Lists of structure factors and anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: DU1061). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(Benzenethiolato-κS)triphenyltin(IV), $[Sn(C_6H_5S)(C_6H_5)_3]$ (I), and Bis(benzenethiolato-κS)diphenyltin(IV), $[Sn(C_6H_5S)_2(C_6H_5)_2]$ (II)

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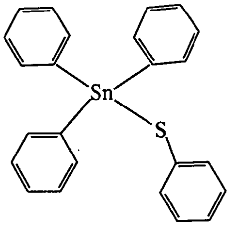
Abstract

The structures of the title compounds, $[(Ph)_3Sn(SPh)]$ (I) and $[(Ph)_2Sn(SPh)_2]$ (II), where Ph = C_6H_5, have been determined by single-crystal X-ray diffraction experiments. In both, the Sn atom has a coordination number of four. The first compound presents a quite regular tetrahedral geometry about the Sn atom, while in the second a greater distortion from the ideal angle of 109.5° is observed. The atomic distances and angles in the phenyl rings are in good agreement with those of a regular hexagon, larger distortions being observed in the second compound.

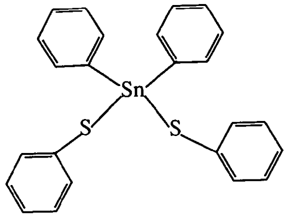
Comment

Crystallographic studies of compounds of the $R_xSn(SPh)_y$ family form part of our research. These compounds are fragments of heterobimetallic complexes, since their reactions with Nb compounds result in Nb—Sn bonds. Heterobimetallic complexes, especially those containing sulfur, are of considerable interest because of their applications in several catalytic processes (Müller, Watkins & Dahl, 1976; Kwart, Schuit & Gates, 1980). Understanding the structural differences between the Sn ligands can be useful in the study of the properties of these complexes.

The two related structures $[(Ph)_3Sn(SPh)]$ (I) and $[(Ph)_2Sn(SPh)_2]$ (II) have been determined by single-crystal X-ray diffraction. Similar structures containing Sn—C and Sn—S bonds have been reported elsewhere (Chieh & Trotter, 1970; Clarke, Cradwick & Wardell, 1973).



(I)



(II)

The Sn—C bond lengths obtained in the present work are all in good agreement with one another. The mean values, 2.138 (3) in (I) and 2.127 (2) Å in (II), are comparable to 2.144 (14) Å in $[(Ph)_4Sn]$ (Chieh & Trotter, 1970) and 2.126 Å in $[(Ph)_3Sn(SC_6H_4\text{-}p\text{-}{}^tBu)]$ (Clarke *et al.*, 1973). The Sn—S and S—C bond lengths in compounds (I) and (II) also agree with those obtained by Clarke *et al.* (1973) [2.413(3) and 1.784 (9) Å, respectively].

All phenyl rings were refined without any constraints. Values of distances and angles in the rings show no significant differences from those of a perfect hexagon.

Substitution of Ph groups by SPh groups in the structure causes a greater distortion from regular tetrahedral geometry about the Sn atom. This can be seen by comparing the values of angles around Sn in compound (II) [from 102.4 (2) to 119.3 (2)°], in compound (I) [from 106.4 (1) to 112.4 (1)°] and in $[(Ph)_4Sn]$ [from 108.8 (4) to 110.8 (9)° (Chieh & Trotter, 1970)]. We also observe that the introduction of SPh groups leads to structures of lower symmetry, since the crystal systems are tetragonal for $[(Ph)_4Sn]$ (Chieh & Trotter, 1970), monoclinic for $[(Ph)_3Sn(SPh)]$ and triclinic for $[(Ph)_2Sn(SPh)_2]$.

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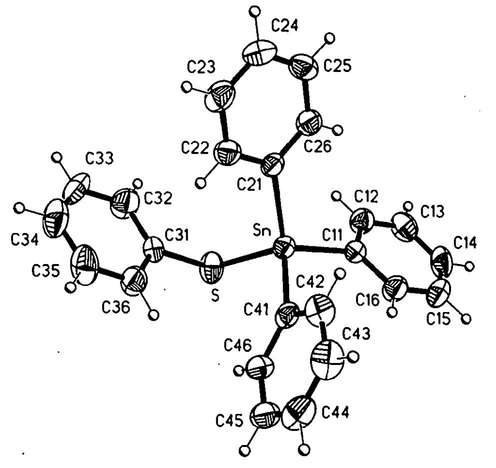

Fig. 1. A view of the molecule [(Ph)$_3$Sn(SPh)], showing 40% probability ellipsoids.

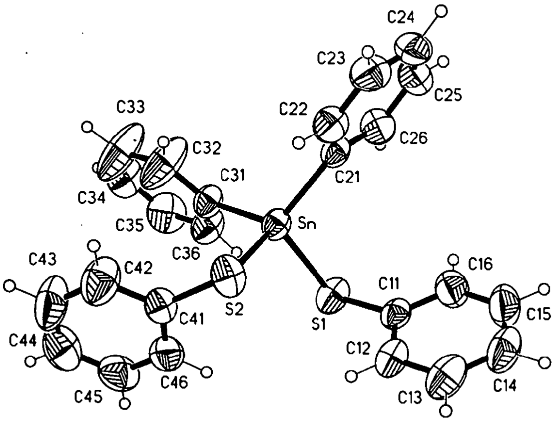

Fig. 2. A view of the molecule [(Ph)$_2$Sn(SPh)$_2$], showing 40% probability ellipsoids.

Experimental

Compound (I)

Crystal data

[Sn(C$_6$H$_5$S)(C$_6$H$_5$)$_3$]
M_r = 459.1
Monoclinic
$P2_1/c$
a = 7.745 (2) Å
b = 16.411 (3) Å
c = 16.120 (3) Å
β = 93.56 (3)°
V = 2044.9 (10) Å^3
Z = 4
D_x = 1.491 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 52 reflections
θ = 4-20°
μ = 1.356 mm^{-1}
T = 293 K
Irregular shape
Diameter ranging from 0.2 to 0.3 mm
Colourless

Data collection

Siemens $P4$ diffractometer
$\theta/2\theta$ scans
Absorption correction: none
4508 measured reflections
2195 independent reflections
2080 observed reflections [$F > 4.0\sigma(F)$]
$R_{\rm int}$ = 0.06

$\theta_{\rm max}$ = 22.5°
$h = -7 \rightarrow 7$
$k = 0 \rightarrow 16$
$l = 0 \rightarrow 16$
3 standard reflections monitored every 247 reflections
intensity variation: none

Refinement

Refinement on F
R = 0.031
wR = 0.050
S = 0.94
2080 reflections
235 parameters
H-atom parameters not refined
Calculated weights $w = 1/[\sigma^2(F) + 0.0025F^2]$

$(\Delta/\sigma)_{\rm max}$ = 0.005
$\Delta\rho_{\rm max}$ = 0.85 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.67 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

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

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Sn	0.3896 (1)	0.6831 (1)	0.4597 (1)	0.045 (1)
S	0.7005 (2)	0.6956 (1)	0.4819 (1)	0.060 (1)
C(11)	0.3343 (4)	0.6238 (2)	0.3426 (2)	0.046 (1)
C(12)	0.3957 (5)	0.5472 (2)	0.3244 (2)	0.053 (1)
C(13)	0.3580 (5)	0.5141 (3)	0.2471 (3)	0.067 (2)
C(14)	0.2629 (5)	0.5548 (3)	0.1874 (3)	0.068 (2)
C(15)	0.1986 (6)	0.6299 (3)	0.2042 (3)	0.068 (2)
C(16)	0.2334 (6)	0.6643 (3)	0.2811 (3)	0.060 (1)
C(21)	0.2878 (4)	0.6174 (2)	0.5604 (2)	0.046 (1)
C(22)	0.2973 (5)	0.6488 (2)	0.6397 (2)	0.054 (1)
C(23)	0.2299 (5)	0.6066 (3)	0.7040 (2)	0.066 (2)
C(24)	0.1519 (5)	0.5315 (3)	0.6895 (3)	0.064 (2)
C(25)	0.1431 (5)	0.5005 (2)	0.6109 (3)	0.060 (1)
C(26)	0.2113 (5)	0.5422 (2)	0.5470 (2)	0.056 (1)
C(31)	0.7209 (4)	0.7266 (2)	0.5883 (2)	0.046 (1)
C(32)	0.7921 (7)	0.6732 (3)	0.6457 (3)	0.069 (2)
C(33)	0.8127 (9)	0.6979 (3)	0.7286 (3)	0.093 (2)
C(34)	0.7639 (6)	0.7740 (4)	0.7519 (3)	0.084 (2)
C(35)	0.6914 (8)	0.8253 (3)	0.6951 (4)	0.082 (2)
C(36)	0.6733 (6)	0.8033 (2)	0.6135 (3)	0.062 (2)
C(41)	0.2905 (5)	0.8044 (2)	0.4494 (2)	0.047 (1)
C(42)	0.1151 (7)	0.8188 (2)	0.4544 (3)	0.065 (2)
C(43)	0.0472 (6)	0.8954 (3)	0.4424 (3)	0.079 (2)
C(44)	0.1527 (7)	0.9597 (3)	0.4252 (3)	0.072 (2)
C(45)	0.3260 (7)	0.9470 (2)	0.4214 (3)	0.067 (2)
C(46)	0.3954 (5)	0.8705 (2)	0.4318 (2)	0.054 (1)

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

Sn—S	2.421 (1)	C(25)—C(26)	1.369 (6)
Sn—C(11)	2.142 (3)	C(26)—C(21)	1.378 (5)
Sn—C(21)	2.139 (3)	C(31)—C(32)	1.365 (6)
Sn—C(41)	2.134 (4)	C(32)—C(33)	1.397 (8)
S—C(31)	1.787 (4)	C(33)—C(34)	1.363 (8)
C(11)—C(12)	1.383 (5)	C(34)—C(35)	1.342 (7)
C(12)—C(13)	1.375 (6)	C(35)—C(36)	1.363 (7)
C(13)—C(14)	1.351 (6)	C(36)—C(31)	1.379 (5)
C(14)—C(15)	1.362 (7)	C(41)—C(42)	1.386 (7)
C(15)—C(16)	1.373 (6)	C(42)—C(43)	1.371 (6)
C(16)—C(11)	1.392 (5)	C(43)—C(44)	1.374 (7)
C(21)—C(22)	1.377 (5)	C(44)—C(45)	1.363 (8)
C(22)—C(23)	1.375 (6)	C(45)—C(46)	1.370 (6)
C(23)—C(24)	1.385 (6)	C(46)—C(41)	1.395 (5)
C(24)—C(25)	1.362 (6)		
S—Sn—C(11)	108.2 (1)	C(23)—C(24)—C(25)	119.0 (4)
S—Sn—C(21)	109.9 (1)	C(24)—C(25)—C(26)	120.9 (4)
C(11)—Sn—C(21)	112.1 (1)	C(21)—C(26)—C(25)	120.8 (3)
S—Sn—C(41)	106.4 (1)	S—C(31)—C(32)	118.4 (3)
C(11)—Sn—C(41)	107.7 (1)	S—C(31)—C(36)	122.2 (3)

C(21)—Sn—C(41)	112.4 (1)	C(32)—C(31)—C(36)	119.4 (4)
Sn—S—C(31)	101.2 (1)	C(31)—C(32)—C(33)	118.7 (4)
Sn—C(11)—C(12)	123.2 (3)	C(32)—C(33)—C(34)	120.8 (5)
Sn—C(11)—C(16)	119.0 (3)	C(33)—C(34)—C(35)	119.9 (5)
C(12)—C(11)—C(16)	117.9 (3)	C(34)—C(35)—C(36)	120.4 (5)
C(11)—C(12)—C(13)	119.6 (3)	C(31)—C(36)—C(35)	120.8 (4)
C(12)—C(13)—C(14)	121.8 (4)	Sn—C(41)—C(42)	120.2 (3)
C(13)—C(14)—C(15)	119.7 (4)	Sn—C(41)—C(46)	121.9 (3)
C(14)—C(15)—C(16)	119.8 (4)	C(42)—C(41)—C(46)	117.7 (3)
C(11)—C(16)—C(15)	121.2 (4)	C(41)—C(42)—C(43)	121.1 (4)
Sn—C(21)—C(22)	121.0 (3)	C(42)—C(43)—C(44)	120.3 (5)
Sn—C(21)—C(26)	120.5 (2)	C(43)—C(44)—C(45)	119.4 (4)
C(22)—C(21)—C(26)	118.5 (3)	C(44)—C(45)—C(46)	121.0 (4)
C(21)—C(22)—C(23)	120.7 (4)	C(41)—C(46)—C(45)	120.5 (4)
C(22)—C(23)—C(24)	120.2 (4)		

Compound (II)

Crystal data

$[Sn(C_6H_5S)_2(C_6H_5)_2]$
M_r = 491.2
Triclinic
$P\bar{1}$
a = 9.449 (2) Å
b = 10.310 (2) Å
c = 12.430 (2) Å
α = 95.390 (1)°
β = 103.190 (1)°
γ = 107.440 (1)°
V = 1107.5 (5) Å^3
Z = 2
D_x = 1.473 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 33 reflections
θ = 4.5 - 13°
μ = 1.348 mm^{-1}
T = 293 K
Irregular shape
Diameter ranging from 0.2 to 0.3 mm
Colourless

Data collection

Siemens *P*4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
2542 measured reflections
2117 independent reflections
1852 observed reflections $[F > 4.0\sigma(F)]$
R_{int} = 0.02

θ_{max} = 22.5°
$h = -7 \rightarrow 7$
$k = -7 \rightarrow 7$
$l = 0 \rightarrow 9$
3 standard reflections monitored every 247 reflections intensity variation: none

Refinement

Refinement on F
R = 0.030
wR = 0.043
S = 0.82
1852 reflections
244 parameters
H-atom parameters not refined
Calculated weights $w = 1/[\sigma^2(F) + 0.0020F^2]$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (II)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Sn	0.2886 (1)	0.1064 (1)	0.2257 (1)	0.056 (1)
S(2)	0.4491 (2)	0.2024 (2)	0.4140 (1)	0.072 (1)
S(1)	0.0778 (2)	0.1959 (2)	0.1840 (1)	0.073 (1)
C(11)	−0.0328 (6)	0.1212 (5)	0.2734 (5)	0.059 (3)
C(12)	0.0105 (7)	0.1766 (7)	0.3864 (6)	0.077 (3)
C(13)	−0.0815 (9)	0.1219 (9)	0.4529 (6)	0.097 (4)
C(14)	−0.2141 (9)	0.0140 (9)	0.4110 (9)	0.098 (5)
C(15)	−0.2579 (8)	−0.0408 (8)	0.2999 (9)	0.101 (4)
C(16)	−0.1687 (7)	0.0109 (6)	0.2322 (6)	0.082 (3)
C(21)	0.2035 (5)	−0.1108 (5)	0.2202 (4)	0.054 (2)
C(22)	0.2752 (7)	−0.1734 (7)	0.3002 (5)	0.069 (3)
C(23)	0.2228 (8)	−0.3118 (8)	0.2937 (6)	0.082 (4)
C(24)	0.1009 (9)	−0.3939 (7)	0.2072 (7)	0.092 (4)
C(25)	0.0295 (8)	−0.3343 (8)	0.1270 (7)	0.093 (4)
C(26)	0.0806 (7)	−0.1933 (7)	0.1343 (5)	0.073 (3)
C(31)	0.4155 (6)	0.1848 (6)	0.1116 (4)	0.062 (3)
C(32)	0.5476 (11)	0.1628 (11)	0.1104 (8)	0.134 (6)
C(33)	0.6363 (12)	0.2186 (13)	0.0421 (9)	0.161 (8)
C(34)	0.5882 (12)	0.2929 (9)	−0.0294 (7)	0.107 (5)
C(35)	0.4542 (11)	0.3184 (8)	−0.0325 (6)	0.103 (5)
C(36)	0.3691 (8)	0.2643 (7)	0.0385 (5)	0.082 (3)
C(41)	0.5657 (7)	0.3572 (6)	0.3836 (4)	0.061 (3)
C(42)	0.7163 (9)	0.3782 (8)	0.3885 (7)	0.106 (4)
C(43)	0.8059 (9)	0.4969 (10)	0.3642 (8)	0.125 (5)
C(44)	0.7469 (11)	0.5960 (9)	0.3361 (6)	0.104 (4)
C(45)	0.5992 (10)	0.5805 (7)	0.3340 (6)	0.094 (4)
C(46)	0.5108 (8)	0.4629 (7)	0.3594 (5)	0.080 (3)

Table 4. *Selected geometric parameters* (Å, °) *for* (II)

Sn—S(1)	2.410 (2)	C(24)—C(25)	1.373 (12)
Sn—S(2)	2.409 (1)	C(25)—C(26)	1.375 (11)
Sn—C(21)	2.129 (5)	C(26)—C(21)	1.373 (6)
Sn—C(31)	2.125 (6)	C(31)—C(32)	1.337 (13)
S(1)—C(11)	1.769 (6)	C(32)—C(33)	1.372 (16)
S(2)—C(41)	1.775 (6)	C(33)—C(34)	1.317 (16)
C(11)—C(12)	1.383 (9)	C(34)—C(35)	1.362 (16)
C(12)—C(13)	1.371 (11)	C(35)—C(36)	1.372 (12)
C(13)—C(14)	1.355 (10)	C(36)—C(31)	1.365 (10)
C(14)—C(15)	1.360 (14)	C(41)—C(42)	1.360 (11)
C(15)—C(16)	1.357 (13)	C(42)—C(43)	1.368 (13)
C(16)—C(11)	1.385 (7)	C(43)—C(44)	1.341 (15)
C(21)—C(22)	1.393 (9)	C(44)—C(45)	1.350 (14)
C(22)—C(23)	1.350 (10)	C(45)—C(46)	1.361 (10)
C(23)—C(24)	1.371 (9)	C(46)—C(41)	1.369 (11)
S(2)—Sn—S(1)	110.8 (1)	C(26)—C(25)—C(24)	119.8 (6)
S(2)—Sn—C(21)	105.7 (1)	C(25)—C(24)—C(23)	119.4 (7)
S(1)—Sn—C(21)	110.2 (1)	C(24)—C(23)—C(22)	121.1 (7)
S(2)—Sn—C(31)	108.4 (1)	C(23)—C(22)—C(21)	120.4 (5)
S(1)—Sn—C(31)	102.4 (2)	Sn—C(31)—C(36)	121.7 (5)
C(21)—Sn—C(31)	119.3 (2)	Sn—C(31)—C(32)	121.7 (6)
Sn—S(2)—C(41)	97.3 (2)	C(36)—C(31)—C(32)	116.6 (7)
Sn—S(1)—C(11)	101.8 (2)	C(31)—C(32)—C(33)	122.9 (10)
S(1)—C(11)—C(12)	120.4 (4)	C(32)—C(33)—C(34)	119.6 (12)
S(1)—C(11)—C(16)	121.5 (5)	C(33)—C(34)—C(35)	120.1 (10)
C(16)—C(11)—C(12)	118.0 (6)	C(34)—C(35)—C(36)	119.3 (8)
C(11)—C(12)—C(13)	119.4 (5)	C(35)—C(36)—C(31)	121.4 (8)
C(12)—C(13)—C(14)	121.7 (8)	S(2)—C(41)—C(46)	121.9 (5)
C(13)—C(14)—C(15)	119.2 (9)	S(2)—C(41)—C(42)	121.0 (6)
C(14)—C(15)—C(16)	120.3 (6)	C(46)—C(41)—C(42)	117.0 (6)
C(15)—C(16)—C(11)	121.3 (6)	C(41)—C(42)—C(43)	121.1 (9)
Sn—C(21)—C(26)	120.4 (5)	C(42)—C(43)—C(44)	120.4 (9)
Sn—C(21)—C(22)	121.1 (3)	C(43)—C(44)—C(45)	120.1 (8)
C(22)—C(21)—C(26)	118.4 (5)	C(44)—C(45)—C(46)	119.4 (8)
C(21)—C(26)—C(25)	120.9 (6)	C(45)—C(46)—C(41)	121.9 (8)

For compound (I), θ scans were made from 0.50° on the low-angle side of $K\alpha_1$ to 0.50° on the high-angle side of $K\alpha_2$. For compound (II), θ scans were made from 0.40° on the low-angle side of $K\alpha_1$ to 0.40° on the high-angle side of $K\alpha_2$. For both compounds, backgrounds were measured with stationary crystal and stationary counter at the beginning and end of the scan, each for 0.5% of the total scan time. The relatively low upper limit for data collection, $(\sin\theta)/\lambda$ = 0.55 Å^{-1}, is justified by satisfactory final results obtained by the structure refinements. Data collection: *XSCANS* (Fait, 1991). Cell refinement, data reduction, structure solution and refinement, and preparation of the material for publication were performed using the *SHELXTL-Plus* (Sheldrick, 1990) package.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: SH1090). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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[2,6-Bis(2-pyrimidinylthiomethyl)pyridine]dichlorocopper(II) Methanol Solvate

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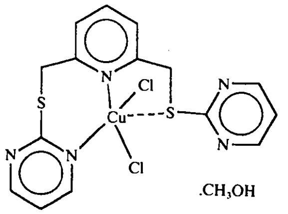
Abstract

In the title compound, [CuCl$_2$(C$_{15}$H$_{13}$N$_5$S$_2$)].CH$_3$OH, the Cu^{2+} ion has square-pyramidal coordination geometry. The basal plane of the pyramid is formed by two Cl$^-$ ions, one pyridine N atom and one pyrimidine N atom. The fifth coordination site is occupied by the S atom of a thiomethyl group. The methanol molecule occupies an otherwise empty space in the structure.

Comment

The coordination chemistry of 2,6-bis(*R*-thiomethyl)pyridine changes considerably with the nature of the *R* group (Teixidor, Sánchez-Castelló, Lucena, Escriche, Kivekäs, Sundberg & Casabó, 1991). The present ligand, 2,6-bis(2-pyrimidinylthiomethyl)pyridine, in the title compound, (I), has seven potential donor atoms, which afford a large number of different possible coordination modes. The title complex is a new example of this series and shows an asymmetric coordination mode of the multidentate ligand.



(I)

The structure consists of molecular complex units and methanol molecules. The complex is depicted in Fig. 1. The ligand is coordinated in a tridentate manner to the Cu^{2+} ion. The two Cl$^-$ ions and two ligand N atoms form the equatorial plane around the Cu^{2+} ion. The fifth coordination site is occupied by the S atom of a thiomethyl group. The Cu—Cl distances are similar whereas Cu—N(1) and

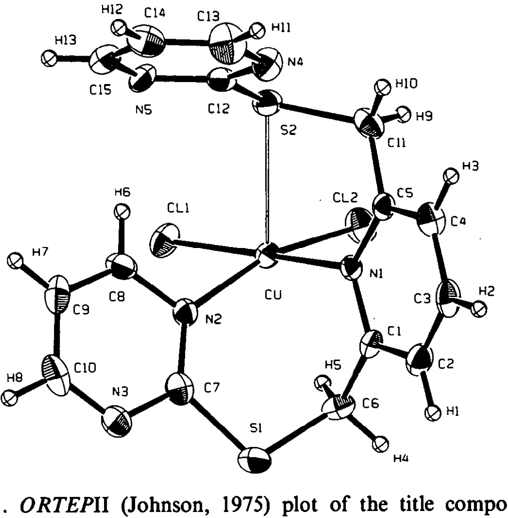


Fig. 1. *ORTEP*II (Johnson, 1975) plot of the title compound. Displacement ellipsoids are shown at 30% probability levels, except for those of the H atoms which are drawn with an isotropic displacement factor of 1.0.

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