We thank Associate Professor A. H. White and Dr B. W. Skelton of the University of Western Australia who collected the data.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: SK1011). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Allen, F. H., Davies, J. E., Galloy, J. J., Johnson, O., Kennard, O., Macrae, C. F., Mitchell, E. M., Mitchell, G. F., Smith, J. M. & Watson, D. G. (1991). *J. Chem. Inf. Comput. Sci.* **31**, 187–204.

Crane, J. D. & Fenton, D. E. (1990). *J. Chem. Soc. Dalton Trans.* pp. 3647–3653.

Cros, G., Laurent, J.-P. & Dahan, F. (1987). *Inorg. Chem.* **26**, 596–599.

Hall, S. R., Flack, H. D. & Stewart, J. M. (1992). Editors. *Xtal3.2 Reference Manual.* Universities of Western Australia, Australia, Geneva, Switzerland, and Maryland, USA.

Nishida, Y., Takahashi, K. & Kida, S. (1981). *Mem. Fac. Sci. Kyushu Univ. Ser. C*, **13**, 27–34.

Yanagi, K. & Minobe, M. (1987). *Acta Cryst.* C**43**, 2060–2063.

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A Biologically Active Gold Complex: Trichloro[(2-pyridyl)methanol-*N*]gold(III)

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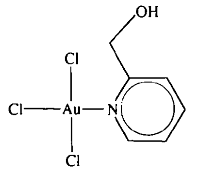
(*Received 29 March 1995; accepted 19 June 1995*)

Abstract

The crystal structure of the title complex, $[AuCl_3(C_6H_7NO)]$, has been determined by X-ray diffraction. The coordination geometry around the Au^{III} atom is square planar. The bond lengths and angles in the complex agree with the literature values.

Comment

Interest in gold compounds has been growing in recent years as some possess anti-arthritic and anti-tumour properties (Ni Dhubhghaill & Sadler, 1993; Sadler & Sue, 1994). Most studies, however, have centered on the activity of gold(I) compounds and very little is known about gold(III) compounds. In the course of our studies of the activity of gold(III) complexes, we have determined the structure of the title complex, $AuCl_3Hpm$, by X-ray diffraction.



$AuCl_3Hpm$

The Au atom in $AuCl_3Hpm$ shows the usual square-planar coordination geometry, and is coordinated by three Cl atoms and the N atom of the pyridine ring. The Au atom is also essentially coplanar with the pyridine ring, the angle between the coordination plane and the pyridine ring being 73.0 (3)°. The O atom deviates from the pyridine ring plane by 0.76 (2) Å. Bond lengths and angles around the Au atom and in the rest of the molecule are in agreement with values from the literature (Holowczak, Stanel & Wong, 1985; Hollis & Lippard, 1983; Timkovich & Tulinsky, 1977).

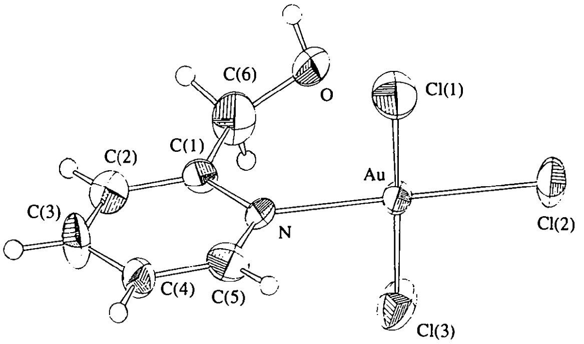


Fig. 1. *ORTEP*II (Johnson, 1976) drawing of $AuCl_3Hpm$. Displacement ellipsoids are shown at the 50% probability level for non-H atoms and H atoms are represented by small spheres of arbitrary radii.

Experimental

The compound was prepared as described in the literature (Dar *et al.*, 1992) and was recrystallized from ethyl ether.

Crystal data

$[AuCl_3(C_6H_7NO)]$
$M_r = 412.43$
Monoclinic
$P2_1/n$
$a = 7.826\ (2)$ Å
$b = 14.606\ (4)$ Å
$c = 8.830\ (3)$ Å
$\beta = 96.58\ (2)°$
$V = 1002.7\ (5)$ Å^3
$Z = 4$
$D_x = 2.727$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 17$–$23°$
$\mu = 15.4$ mm^{-1}
$T = 298$ K
Prism
0.5 × 0.4 × 0.4 mm
Yellow

Data collection

Nonius CAD-4 diffractometer

$R_{int} = 0.0405$
$\theta_{max} = 26.9°$

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$\omega/2\theta$ scans
Absorption correction:
ψ scans
$T_{\min} = 0.59$, $T_{\max} = 0.99$
2406 measured reflections
2180 independent reflections
1796 observed reflections
$[F > 4\sigma(F)]$

$h = -9 \rightarrow 9$
$k = 0 \rightarrow 18$
$l = 0 \rightarrow 11$
2 standard reflections
monitored every 400
reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.0515$
$wR(F^2) = 0.1410$
$S = 1.265$
2180 reflections
113 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2 + 1.51P]$
where $P = [\max(F_o^2,0) + 2F_c^2]/3$

$(\Delta/\sigma)_{\max} = 0.074$
$\Delta\rho_{\max} = 3.1$ e Å^{-3}
$\Delta\rho_{\min} = -3.3$ e Å^{-3}
Extinction correction: none
Atomic scattering factors
from *SHELXTL-Plus*
(Sheldrick, 1990)

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

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

	x	y	z	$U_{\rm eq}$
Au	0.1801 (1)	0.1156 (1)	0.0890 (1)	0.024 (1)
Cl(1)	0.4666 (5)	0.1222 (3)	0.0708 (5)	0.047 (1)
Cl(2)	0.1250 (5)	0.1925 (2)	−0.1339 (4)	0.041 (1)
Cl(3)	−0.1068 (4)	0.1033 (3)	0.1086 (4)	0.045 (1)
N	0.2268 (11)	0.0457 (7)	0.2869 (11)	0.025 (2)
C(1)	0.2083 (18)	0.0839 (8)	0.4264 (13)	0.030 (3)
C(2)	0.2413 (19)	0.0301 (10)	0.5509 (16)	0.041 (3)
C(3)	0.2945 (21)	−0.0581 (10)	0.5444 (16)	0.045 (4)
C(4)	0.3135 (19)	−0.0957 (9)	0.4006 (15)	0.039 (3)
C(5)	0.2810 (19)	−0.0430 (9)	0.2788 (17)	0.041 (3)
C(6)	0.1581 (25)	0.1813 (9)	0.4385 (17)	0.052 (4)
O	0.2155 (15)	0.2386 (7)	0.3313 (11)	0.044 (2)

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

Au—N	2.021 (9)	C(1)—C(2)	1.35 (2)
Au—Cl(2)	2.265 (3)	C(1)—C(6)	1.48 (2)
Au—Cl(1)	2.268 (4)	C(2)—C(3)	1.36 (2)
Au—Cl(3)	2.278 (4)	C(3)—C(4)	1.41 (2)
N—C(1)	1.374 (14)	C(4)—C(5)	1.32 (2)
N—C(5)	1.37 (2)	C(6)—O	1.38 (2)
N—Au—Cl(2)	179.2 (3)	N—C(1)—C(2)	117.6 (11)
N—Au—Cl(1)	90.0 (3)	N—C(1)—C(6)	120.6 (11)
Cl(2)—Au—Cl(1)	90.52 (14)	C(2)—C(1)—C(6)	121.8 (12)
N—Au—Cl(3)	88.7 (3)	C(3)—C(2)—C(1)	123.2 (14)
Cl(2)—Au—Cl(3)	90.80 (14)	C(2)—C(3)—C(4)	118.3 (12)
Cl(1)—Au—Cl(3)	177.87 (14)	C(3)—C(4)—C(5)	118.5 (13)
C(1)—N—C(5)	119.8 (11)	N—C(5)—C(4)	122.7 (14)
C(1)—N—Au	122.9 (8)	O—C(6)—C(1)	115.0 (13)
C(5)—N—Au	117.4 (9)		

The H atom bonded to O was located from a difference Fourier map; other H atoms were placed in calculated positions. H atoms were refined with a common isotropic displacement parameter. The highest values of $\Delta\rho$ are near the heavy atoms and are probably the result of uncorrected thermal motion or inadequacies in the scattering factors.

Data collection: Nonius CAD-4 software. Cell refinement: Nonius CAD-4 software. Data reduction: Nonius CAD-4 software. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976).

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: NA1179). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Dar, A., Moss, K., Cottrill, M. S., Parish, R. V., McAuliffe, C. A., Pritchard, R. G., Beagley, B. & Sandbank, J. (1992). *J. Chem. Soc. Dalton Trans.* pp. 1907–1913.

Hollis, L. S. & Lippard, S. J. (1983). *J. Am. Chem. Soc.* **105**, 4293–4299.

Holowczak, M. S., Stanel, M. D. & Wong, G. G. (1985). *J. Am. Chem. Soc.* **107**, 5789–5790.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Ni Dhubhghaill, O. M. & Sadler, P. J. (1993). *Metal Complexes in Cancer Chemotherapy*, edited by B. K. Keppler, pp. 221–248. Weinheim: VCH.

Sadler, P. J. & Sue, R. E. (1994). *Metal Based Drugs*, **1**, 107–144.

Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.

Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Timkovich, R. & Tulinsky, A. (1977). *Inorg. Chem.* **16**, 962–963.

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Diphenyltin Diiodide

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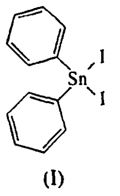
(Received 30 August 1995; accepted 15 December 1995)

Abstract

The title compound, diiododiphenyltin, [SnI$_2$(C$_6$H$_5$)$_2$], has essentially tetrahedral coordination geometry with intermolecular I···I and Sn···I separations close to the sum of the appropriate van der Waals radii.

Comment

The title compound, (I), consists of essentially individual Ph$_2$SnI$_2$ molecules separated by I···I and Sn···I distances close to the sum of the appropriate van der Waals radii; the van der Waals radii for Sn and I were taken to be 2.20 and 1.95–2.12 Å, respectively (Huheey,



(I)

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