

lengths and angles in Table 2.* The atom-numbering is shown in Fig. 1.

Related literature. The fortuitous preparation of the title compound is described by Thöne (1991). Narrow *ipso* angles in C₆F₅ groups are discussed by Jones (1988). Some Au—C₆F₅ bond lengths are presented by Jones (1992). The tendency of Au atoms in Au^I derivatives to aggregate has been termed 'aurophilicity' by Schmidbaur (1990). A non-parallel arrangement of Au—Cl groups, leading to intermolecular Au...Au contacts, is observed in

* Lists of structure factors, anisotropic thermal parameters, complete bond distances and angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54937 (31 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HA0092]

(dppm)(AuCl)₂ (Schmidbaur, Wohlleben, Wagner, Orama & Huttner, 1977), whereas a *cis* arrangement similar to that of the title compound is seen in (dppm)(AuSiMe₃)₂ (Piana, Wagner & Schubert, 1991).

We thank the Fonds der Chemischen Industrie for financial support.

References

- JONES, P. G. (1988). *J. Organomet. Chem.* **345**, 405–411.
 JONES, P. G. (1992). *Acta Cryst.* **C48**, 1209–1211.
 PIANA, H., WAGNER, H. & SCHUBERT, U. (1991). *Chem. Ber.* **124**, 63–67.
 SCHMIDBAUR, H. (1990). *Gold Bull.* **23**, 11–21.
 SCHMIDBAUR, H., WOHLLEBEN, A., WAGNER, F., ORAMA, O. & HUTTNER, G. (1977). *Chem. Ber.* **110**, 1748–1754.
 SHELDRIK, G. M. (1989). *SHELXTL-Plus*. Version 4.1. Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.
 THÖNE, C. (1991). PhD Thesis. Univ. of Braunschweig, Germany.

Acta Cryst. (1992). **C48**, 1314–1315

Bis[1,1-di(2-pyridyl)ethyl methyl ether-*N,N',O*]copper(II) Di- μ -iodo-bis[iodoargentate(I)]

BY PETER G. JONES

*Institut für Anorganische und Analytische Chemie der Technischen Universität, Hagenring 30,
W-3300 Braunschweig, Germany*

(Received 14 October 1991; accepted 4 December 1991)

Abstract. [Cu(C₁₃H₁₄N₂O)₂][Ag₂I₄], *M_r* = 1215.4, triclinic, *P*1, *a* = 8.5402 (14), *b* = 10.0286 (16), *c* = 10.584 (2) Å, α = 110.221 (10), β = 95.476 (10), γ = 93.420 (12)°, *V* = 842.6 (2) Å³, *Z* = 1, *D_x* = 2.395 Mg m⁻³, λ (Mo *K* α) = 0.71069 Å, μ = 5.424 mm⁻¹, *F*(000) = 563, *T* = 293 K, *R* = 0.034 for 3381 reflections. The Cu atom of the cation lies on a centre of symmetry and is octahedrally coordinated by ligand donor atoms N (at 2.020, 2.000 Å) and O (at 2.393 Å). The centrosymmetric anion displays Ag—I (bridging) 2.780, 2.800, (terminal) 2.679 Å.

Experimental. A pale brown tablet 0.6 × 0.35 × 0.12 mm was mounted in a glass capillary. Using a Stoe four-circle diffractometer, 4493 intensities were registered to $2\theta_{\max} = 55^\circ$ with graphite-monochromated Mo *K* α radiation; 2θ – θ scan mode. Of 3839 unique reflections (*R*_{int} = 0.021, index ranges *h* –11 to 11, *k* –13 to 12, *l* 0 to 13) 3381 with *F* > 4 σ (*F*) were considered observed. The cell constants

were refined from $\pm \omega$ angles of 46 reflections in the 2θ range 20–23°. Three check reflections measured every 100 reflections showed no significant intensity variation. An absorption correction based on ψ scans was applied, with transmission factors 0.53–0.91.

The structure was solved by the heavy-atom method and subjected to anisotropic full-matrix least-squares refinement on *F*; $\sum w(F_o - F_c)^2$ minimized. H atoms were included in the refinement using a riding model and with fixed isotropic *U*. The weighting scheme was $w^{-1} = \sigma^2(F) + 0.0002F^2$; final *R* = 0.034, with *wR* = 0.048 (for all data *R* = 0.039, *wR* = 0.053); 184 parameters (data to parameter ratio 18.4:1); *S* = 2.4; maximum $\Delta/\sigma = 0.01$; maximum, minimum $\Delta\rho = 1.53, -1.43 \text{ e } \text{Å}^{-3}$. Atomic scattering factors and *f'*, *f''* values were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). The program system used was Siemens *SHELXTL-Plus* (Sheldrick, 1989) on a MicroVAX

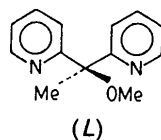
Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

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

	x	y	z	U_{eq}
I(1)	1611.4 (4)	2606.2 (4)	7938.2 (3)	58 (1)
I(2)	-2620.7 (4)	397.7 (4)	9472.3 (4)	66 (1)
Ag	551.8 (6)	943.7 (5)	9251.5 (5)	69 (1)
Cu	5000	5000	5000	33 (1)
C(1)	3295 (5)	5613 (4)	2774 (4)	37 (1)
C(2)	2733 (7)	5864 (6)	1486 (4)	54 (2)
C(3)	5116 (7)	4005 (6)	1574 (5)	58 (2)
O	4853 (3)	5132 (3)	2778 (3)	42 (1)
N(1)	4285 (4)	6926 (4)	5145 (3)	37 (1)
C(12)	3491 (5)	7007 (5)	4019 (4)	45 (2)
C(13)	2865 (6)	8237 (5)	4020 (5)	52 (2)
C(14)	3058 (6)	9413 (5)	5214 (5)	51 (2)
C(15)	3883 (6)	9337 (5)	6365 (5)	46 (2)
C(16)	4495 (6)	8072 (5)	6283 (5)	38 (1)
N(2)	2803 (4)	4176 (4)	4142 (3)	37 (1)
C(22)	2188 (5)	4548 (4)	3105 (4)	52 (2)
C(23)	691 (6)	4038 (6)	2452 (5)	66 (2)
C(24)	-213 (6)	3127 (7)	2903 (6)	66 (2)
C(25)	403 (6)	2755 (7)	3974 (7)	66 (2)
C(26)	1928 (6)	3297 (6)	4578 (5)	51 (2)

II computer. Final atomic coordinates are given in Table 1,* with derived bond lengths and angles in Tables 2. Fig. 1 shows the atom-numbering scheme.

Related literature. The corresponding salt $[\text{CuL}_2]^{2+}[\text{Cu}_2\text{I}_4]^{2-}$ [$L = 1,1$ -di(2-pyridyl)ethyl methyl ether] is isostructural (Bhaduri, Sapre & Jones, 1991). Related Cu compounds have been reported by Basu, Bhaduri, Sapre & Jones (1987). The structure of an $[\text{Ag}_2\text{I}_4]^{2-}$ salt has recently been reported by Helgesson & Jagner (1991), who earlier published structures of $[\text{Ag}_2\text{X}_4]^{2-}$ ($X = \text{Cl}, \text{Br}$) and $[\text{Ag}_4\text{I}_8]^{4-}$ salts (Helgesson & Jagner, 1988, 1990).



We thank the Fonds der Chemischen Industrie for financial support. The crystals were provided by Dr S. Bhaduri and colleagues at the Alchemic Research Centre, Thane, India. Intensity measurements were carried out at the Inorganic Chemistry Institute, University of Göttingen, Germany.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54936 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HA0094]

Table 2. Interatomic distances (\AA) and angles ($^\circ$)

I(2)—Ag	2.679 (1)	I(2)—Ag	2.780 (1)
I(2)—Ag ¹	2.800 (1)	Ag...Ag ¹	3.021 (1)
Cu—O	2.393 (3)	Cu—N(1)	2.020 (4)
Cu—N(2)	2.000 (3)	C(1)—C(2)	1.509 (7)
C(1)—O	1.442 (5)	C(1)—C(12)	1.541 (5)
C(1)—C(22)	1.537 (7)	C(3)—O	1.428 (6)
N(1)—C(12)	1.344 (6)	N(1)—C(16)	1.334 (5)
C(12)—C(13)	1.374 (7)	C(13)—C(14)	1.386 (6)
C(14)—C(15)	1.376 (8)	C(15)—C(16)	1.379 (7)
N(2)—C(22)	1.348 (6)	N(2)—C(26)	1.348 (7)
C(22)—C(23)	1.372 (6)	C(23)—C(24)	1.396 (9)
C(24)—C(25)	1.379 (10)	C(25)—C(26)	1.384 (7)
Ag—I(2)—Ag ¹	65.6 (1)	I(1)—Ag—I(2)	124.0 (1)
I(1)—Ag—I(2)	121.5 (1)	I(2)—Ag—I(2)	114.4 (1)
O—Cu—N(1)	72.9 (1)	O—Cu—N(2)	75.4 (1)
N(1)—Cu—N(2)	86.9 (1)	O—Cu—O ⁱⁱ	180.0
N(1)—Cu—O ⁱⁱ	107.1 (1)	N(2)—Cu—O ⁱⁱ	104.6 (1)
N(1)—Cu—N(1 ⁱⁱ)	180.0	N(2)—Cu—N(1 ⁱⁱ)	93.1 (1)
N(2)—Cu—N(2 ⁱⁱ)	180.0	C(2)—C(1)—O	113.1 (4)
C(2)—C(1)—C(12)	111.8 (4)	O—C(1)—C(12)	103.1 (3)
C(2)—C(1)—C(22)	114.1 (4)	O—C(1)—C(22)	107.5 (4)
C(12)—C(1)—C(22)	106.4 (3)	Cu—O—C(1)	95.8 (2)
Cu—O—C(3)	125.5 (3)	C(1)—O—C(3)	115.5 (3)
Cu—N(1)—C(12)	116.2 (2)	Cu—N(1)—C(16)	124.3 (3)
C(12)—N(1)—C(16)	119.4 (4)	C(1)—C(12)—N(1)	114.9 (4)
C(1)—C(12)—C(13)	123.7 (4)	N(1)—C(12)—C(13)	121.4 (3)
C(12)—C(13)—C(14)	118.8 (5)	C(13)—C(14)—C(15)	119.9 (5)
C(14)—C(15)—C(16)	118.0 (4)	N(1)—C(16)—C(15)	122.4 (5)
Cu—N(2)—C(22)	117.7 (3)	Cu—N(2)—C(26)	122.5 (3)
C(22)—N(2)—C(26)	119.8 (4)	C(1)—C(22)—N(2)	113.6 (3)
C(1)—C(22)—C(23)	124.4 (4)	N(2)—C(22)—C(23)	122.0 (5)
C(22)—C(23)—C(24)	118.1 (5)	C(23)—C(24)—C(25)	120.2 (5)
C(24)—C(25)—C(26)	118.6 (6)	N(2)—C(26)—C(25)	121.2 (6)

Symmetry code: (i) $-x, -y, 2-z$; (ii) $1-x, 1-y, 1-z$.

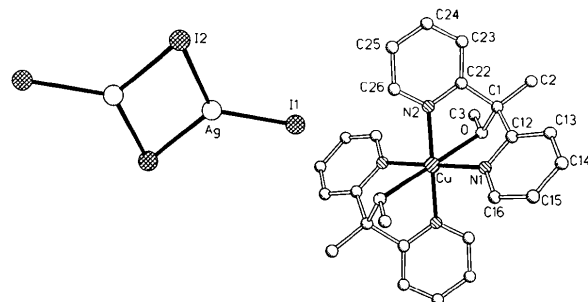


Fig. 1. The title compound in the crystal, showing the atom-numbering scheme of the asymmetric unit. H atoms omitted; radii arbitrary.

References

- BASU, A., BHADURI, S., SAPRE, N. Y. & JONES, P. G. (1987). *J. Chem. Soc. Chem. Commun.* pp. 1724–1725.
- BHADURI, S., SAPRE, N. Y. & JONES, P. G. (1991). *J. Chem. Soc. Dalton Trans.* pp. 2539–2543.
- HELGESSION, G. & JAGNER, S. (1988). *J. Chem. Soc. Dalton Trans.* pp. 2117–2120.
- HELGESSION, G. & JAGNER, S. (1990). *J. Chem. Soc. Dalton Trans.* pp. 2413–2420.
- HELGESSION, G. & JAGNER, S. (1991). *Inorg. Chem.* **30**, 2574–2577.
- SHELDRIK, G. M. (1989). *SHELXTL-Plus*. Version 4.1. Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.