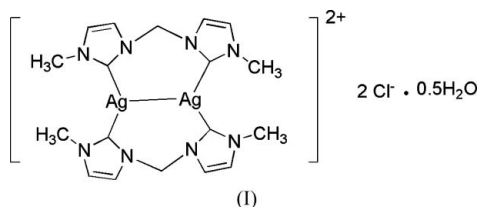


Bis[μ -3,3'-dimethyl-3,3'-methylenebis(2,3-dihydro-1H-imidazole)]disilver(I)(Ag—Ag) dichloride hemihydrate**Da-Qi Wang**Department of Chemistry, Liaocheng University,
Liaocheng, Shandong 252059, People's
Republic of ChinaCorrespondence e-mail:
wangdqchem@yahoo.com.cn**Key indicators**Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
Disorder in solvent or counterion
 R factor = 0.044
 wR factor = 0.122
Data-to-parameter ratio = 14.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title compound, $[\text{Ag}_2(\text{C}_9\text{H}_{12}\text{N}_4)_2]\text{Cl}_2 \cdot 0.5\text{H}_2\text{O}$, each Ag^{I} atom is coordinated by two C atoms of two heterocyclic carbene ligands, displaying a nearly linear geometry. The Ag—Ag separation is quite long, indicating a very weak metal–metal interaction.

Received 23 May 2006
Accepted 9 June 2006**Comment**

Since the discovery of stable imidazolin-2-ylidenes, which were isolated and structurally characterized by Arduengo *et al.* (1991), much interest has been generated in the chemistry of both free heteroatom carbenes and metal complexes of these ligands. Heterocyclic carbenes derived from imidazolium ions form complexes with many transition metals and a large number of heterocyclic carbene complexes of transition metals have been reported (Arnold, 2002; Garrison & Youngs, 2005; Xu *et al.*, 2000). The silver carbene complexes are important, since they have been used as carbene-transfer reagents to prepare carbene complexes of other metals (Wang & Lin, 1998).



The asymmetric unit of the title compound, (I), consists of two Ag^{I} atoms and two imidazolin-2-ylidene ligands, two discrete chloride ions and one half-molecule of water (Fig. 1). The two Ag^{I} atoms are linked by two imidazolylidene ligands into a metallacycle. Each Ag^{I} atom is bicoordinated and displays a linear geometry, or a T-shaped form if the Ag—Ag interaction is taken into account. The Ag—C bond lengths (Table 1) are comparable to the values reported for other $[\text{Ag}(\text{carbene})_2]^+$ complexes (Chen & Liu, 2003; Chen *et al.*, 2002). On the other hand, the Ag—Ag bond is quite long compared with those found in other disilver complexes (Catalano & Malwitz, 2003; Garrison & Youngs, 2005), implying that the Ag—Ag interaction is weak.

Experimental

1,1'-Dimethyl-3,3'-methyleneimidazolium dichloride was prepared according to the procedure of Vogt *et al.* (2005). Silver oxide (0.23 g, 1.0 mmol) was added to a solution of 1,1'-dimethyl-3,3'-methyleneimidazolium dichloride (0.25 g, 1.0 mmol) in dichloromethane (20 ml) and the suspension was stirred overnight. The resultant white

solid was filtered off and washed with diethyl ether. Recrystallization from a hot dimethyl sulfoxide solution gave colourless crystals. Analysis found: C 33.25, H 3.94, N, 17.25%; calculated for $C_{18}H_{25}Ag_2Cl_2N_8O_{0.5}$: C 33.36, H 3.89, N 17.29%.

Crystal data

$[Ag_2(C_9H_{12}N_4)_2]Cl_2 \cdot 0.5H_2O$
 $M_r = 648.10$
 Monoclinic, $P2_1/c$
 $a = 7.436 (3) \text{ \AA}$
 $b = 12.498 (4) \text{ \AA}$
 $c = 25.382 (8) \text{ \AA}$
 $\beta = 95.702 (6)^\circ$
 $V = 2347.3 (14) \text{ \AA}^3$

$Z = 4$
 $D_x = 1.834 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 1.92 \text{ mm}^{-1}$
 $T = 298 (2) \text{ K}$
 Plate, colourless
 $0.36 \times 0.14 \times 0.07 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.545, T_{\max} = 0.877$

11631 measured reflections
 4076 independent reflections
 2895 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.056$
 $\theta_{\max} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.122$
 $S = 1.04$
 4076 reflections
 280 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2 + 0.2797P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.59 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.67 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

Ag1—C1	2.095 (5)	Ag2—C4	2.098 (5)
Ag1—C10	2.113 (5)	Ag2—C13	2.105 (5)
Ag1—Ag2	3.3179 (11)		
C1—Ag1—C10	164.79 (19)	C4—Ag2—C13	168.65 (18)
C1—Ag1—Ag2	94.51 (13)	C4—Ag2—Ag1	96.39 (12)
C10—Ag1—Ag2	96.81 (14)	C13—Ag2—Ag1	94.95 (13)

Water H atoms were located in a difference Fourier map and were refined as riding in their as-found positions, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. H atoms bound to C atoms were placed in calculated positions ($C-H = 0.93-0.97 \text{ \AA}$) and allowed to ride during subsequent refinement, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The highest peak in the difference Fourier map is located 0.87 \AA from atom C11.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve

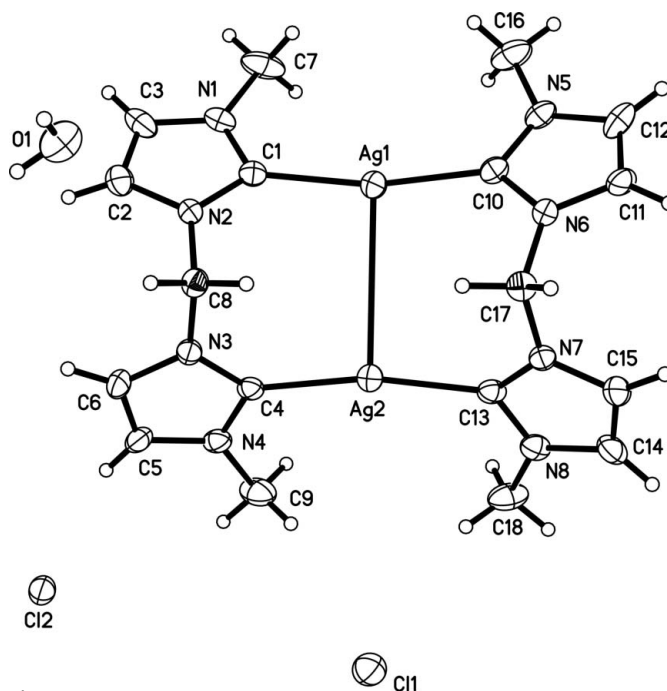


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

References

Arduengo, A. J., Harlow, R. L. & Kline, M. (1991). *J. Am. Chem. Soc.* **113**, 361–363.
 Arnold, P. L. (2002). *Heteroat. Chem.* **13**, 534–539.
 Bruker (1998). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
 Catalano, V. J. & Malwitz, M. A. (2003). *Inorg. Chem.* **42**, 5483–5485.
 Chen, W. & Liu, F. (2003). *J. Organomet. Chem.* **673**, 5–12.
 Chen, W., Wu, B. & Matsumoto, K. (2002). *J. Organomet. Chem.* **654**, 233–236.
 Garrison, J. C. & Youngs, W. J. (2005). *Chem. Rev.* **105**, 3978–4008.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.
 Sheldrick, G. M. (1997b). SHELXTL. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
 Vogt, M., Pons, V. & Heinekey, D. M. (2005). *Organometallics*, **24**, 1832–1836.
 Wang, H. M. J. & Lin, I. J. B. (1998). *Organometallics*, **17**, 972–975.
 Xu, L., Chen, W. & Xiao, J. (2000). *Organometallics*, **19**, 1123–1127.