

Xian-Wu Dong, Wei Li, Hai-Yan Liu and Jian-Fang Ma*

Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

Correspondence e-mail:
jianfangma@yahoo.com.cn

Key indicators

Single-crystal X-ray study
 $T = 291$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.031
 wR factor = 0.096
Data-to-parameter ratio = 19.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Di- μ -chloro-bis[bis(3-methylisoquinoline- κ N)silver(I)]

The title dinuclear compound, $[\text{Ag}_2\text{Cl}_2(\text{C}_{10}\text{H}_9\text{N})_4]$, has C_2 symmetry. The Ag^{I} ion is coordinated by two methylisoquinoline molecules and two Cl^- anions with a distorted tetrahedral geometry. The distance of 3.0630 (9) Å between the two Ag atoms suggests the existence of an Ag–Ag bonding interaction within the dinuclear complex molecule.

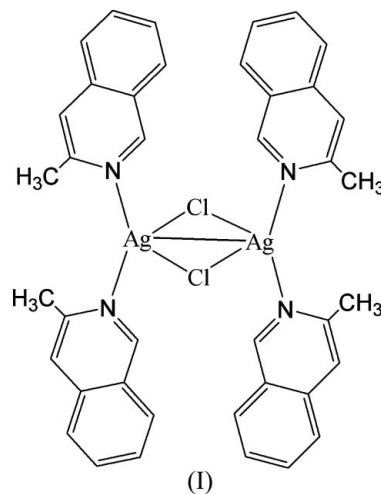
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Comment

The Ag^{I} ion exhibits flexible coordination geometry (Sharma & Rogers, 1998). For silver halides, 1:1 crystalline adducts are usually obtained (Mills & White, 1985). In our previous work, a 1:2 adduct of $[\text{Ag}L_2]\text{NO}_3$ ($L = 3$ -methylisoquinoline) was reported (Dong *et al.*, 2005). We present here the structure of another 1:2 adduct $[\text{AgClL}_2]_2$, (I).



The molecular structure of (I) is shown in Fig. 1. Compound (I) shows a dinuclear structure, with the mid-point of the Ag–Ag bond located on a twofold axis. The structure is similar to that found in $[\text{AgBr}(2\text{Me-py})_2]_2$ (Mills & White, 1985). Each Ag^{I} ion is coordinated by two methylisoquinoline molecules with normal Ag–N bond distances (Table 1). Two Ag^{I} ions are further bridged by two Cl^- anions to form the dinuclear structure. Thus, the Ag^{I} ion has a distorted tetrahedral coordination geometry. The Ag–Ag distance of 3.0630 (9) Å is identical to the sum of the covalent radii for the silver atoms and suggests the existence of metal–metal bonding within the dinuclear molecule.

Experimental

AgCl (0.072 g, 0.5 mmol) was dissolved in an aqueous solution of NH_3 (14 M, 5 ml), then a solution of 3-methylisoquinoline (0.143 g,

1.0 mmol) in methanol (2 ml) was added, and a white precipitate formed immediately. The precipitate was collected by filtration, washed with water and dissolved in acetonitrile. Crystals of (I) were obtained by evaporating the solution for several days at room temperature.

Crystal data

[Ag₂Cl₂(C₁₀H₉N)₄]
M_r = 859.37
 Monoclinic, C2/c
a = 24.760 (5) Å
b = 10.963 (5) Å
c = 16.881 (5) Å
 β = 126.328 (5) $^\circ$
V = 3692 (2) Å³
Z = 4

D_x = 1.546 Mg m⁻³
 Mo K α radiation
 Cell parameters from 11437 reflections
 θ = 2.1–27.5 $^\circ$
 μ = 1.24 mm⁻¹
T = 291 (2) K
 Block, colorless
 0.27 × 0.22 × 0.21 mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.711, *T_{max}* = 0.776
 17327 measured reflections

4228 independent reflections
 2635 reflections with *I* > 2 σ (*I*)
R_{int} = 0.037
 θ_{\max} = 27.5 $^\circ$
h = -32 → 25
k = -14 → 14
l = -21 → 21

Refinement

Refinement on *F*²
R [*F*² > 2 σ (*F*²)] = 0.031
wR (*F*²) = 0.096
S = 0.88
 4228 reflections
 219 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0537P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.52 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.81 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, $^\circ$).

Ag1–N1	2.299 (2)	Ag1–Cl ⁱ	2.6671 (10)
Ag1–N2	2.306 (3)	Ag1–Ag1 ⁱ	3.0630 (9)
Ag1–Cl	2.6612 (11)		
N1–Ag1–N2	130.96 (8)	N2–Ag1–Cl ⁱ	95.56 (6)
N1–Ag1–Cl	96.53 (7)	Cl–Ag1–Cl ⁱ	106.02 (3)
N2–Ag1–Cl	112.58 (7)	Ag1–Cl–Ag1 ⁱ	70.18 (3)
N1–Ag1–Cl ⁱ	113.83 (6)		

Symmetry code: (i) $-x + 2, y, -z + \frac{3}{2}$.

Methyl H atoms were placed at calculated positions with C–H = 0.96 Å and the torsion angles refined to fit the electron density. Aromatic H atoms were positioned geometrically with C–H = 0.93 Å and refined as riding atoms. *U*_{iso}(H) was set as 1.2 or 1.5 times *U*_{eq}(C).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*;

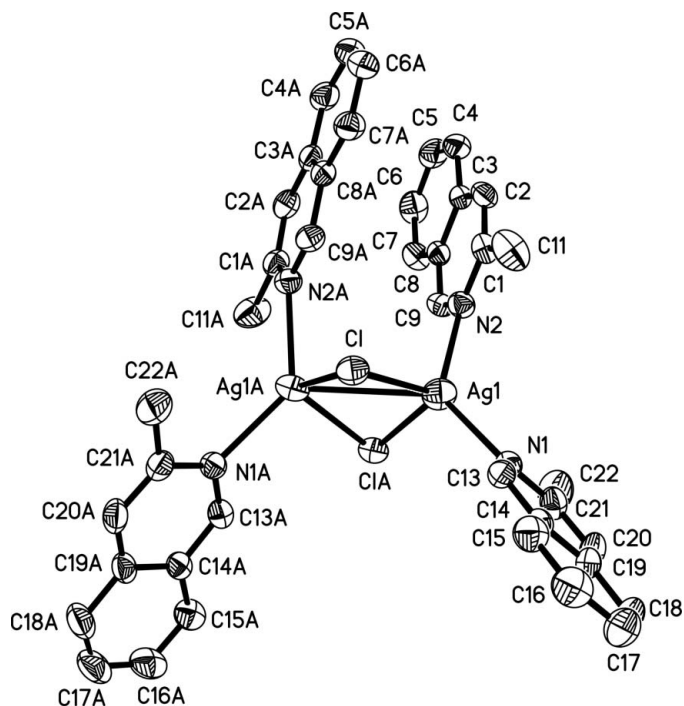


Figure 1

The molecular structure of (I), with 30% probability displacement ellipsoids [symmetry code: (A) $2 - x, y, \frac{3}{2} - z$]. H atoms have been omitted for clarity.

program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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