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[μ-1,1′-Bis(2,4,6-trimethylbenzyl)-3,3′-(2,3,5,6-tetramethyl-*p*-phenylenedibenzimidazole)-2,2′-diylidene]-di-μ-bromo-disilver(I)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.037
wR factor = 0.089
Data-to-parameter ratio = 16.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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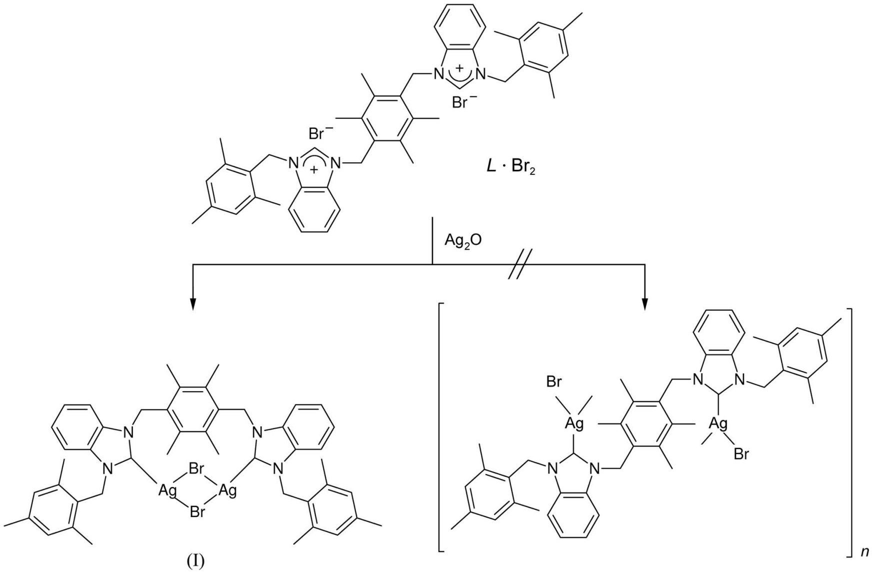
The title compound, $[Ag_2Br_2(C_{46}H_{50}N_4)]$, contains a bulky bis(*N*-heterocyclic carbene) ligand, comprising two benzimidazolium groups linked through a 2,3,5,6-tetramethyl-1,4-xylylene bridge. The compound was formed by reaction of the bromide salt of the ligand with Ag_2O in dichloromethane. The discrete compound is formed in preference to a postulated coordination polymer. Each Ag^I atom is coordinated by the carbene C atom and two Br atoms in a trigonal–planar geometry.

Comment

There has been growing interest in the coordination chemistry of silver(I) derivatives containing *N*-heterocyclic carbene (NHC) ligands, due to potential applications in NHC transfer for the synthesis of transition metal–carbene complexes (Garrison *et al.*, 2005; Wang & Lin, 1998; Baker *et al.*, 2005; Fremont *et al.*, 2005; Lee *et al.*, 2004). Some of them also display antimicrobial activity (Melaiye *et al.*, 2005; Garrison *et al.*, 2005), and catalytic activity for the ring-opening polymerization of lactides and transesterification of esters (Sentman *et al.*, 2005). Some have also been shown to have potential applications in materials science (Lee *et al.*, 2002; Liu *et al.*, 2003).



(I)

The title compound, (I) (Fig. 1), was formed by reaction of the NHC ligand salt LBr_2 with Ag_2O (see reaction scheme). The discrete compound (I) is formed in preference to a postulated coordination polymer. Each Ag^I atom is coordinated by the carbene C atom and two Br atoms in a trigonal–planar geometry (Table 1).

Experimental

A suspension of the ligand salt $L\text{Br}_2$ (1.0 g, 1.22 mmol) and Ag_2O (0.28 g, 1.22 mmol) in dichloromethane (50 ml) was stirred at room temparature for 24 h with exclusion of light. The colour of the mixture gradually changed from black to white. The suspension was then filtered and washed with dichloromethane (2 × 10 ml). The volume of the combined filtrate was reduced to *ca* 10 ml and *n*-hexane (15 ml) was added to afford a white solid. After recrystallization from dichloromethane–*n*-hexane (10:15 ml), the title complex was obtained as a colourless solid (yield 0.88 g, 85%).

Crystal data

$[\text{Ag}_2\text{Br}_2(\text{C}_{46}\text{H}_{50}\text{N}_4)]$
$M_r = 1034.46$
Triclinic, $P\bar{1}$
$a = 9.0005$ (5) Å
$b = 15.8848$ (8) Å
$c = 16.7023$ (10) Å
$\alpha = 61.286$ (4)°
$\beta = 78.137$ (5)°
$\gamma = 83.419$ (5)°
$V = 2049.2$ (2) Å^3
$Z = 2$
$D_x = 1.677$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.94$ mm^{-1}
$T = 293$ (2) K
Plate, colourless
0.60 × 0.44 × 0.08 mm

Data collection

Stoe IPDS 2 diffractometer
ω scans
Absorption correction: integration *X-RED* (Stoe & Cie, 2002)
$T_{\min} = 0.083$, $T_{\max} = 0.815$
29913 measured reflections
8059 independent reflections
6003 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.060$
$\theta_{\max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.089$
$S = 1.01$
8059 reflections
496 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.4769P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.77$ e Å^{-3}
$\Delta\rho_{\min} = -0.62$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—Br1	2.4577 (5)	Ag2—Br2	2.5076 (5)
Ag1—Br2	3.4639 (7)	Ag1—C7	2.104 (3)
Ag2—Br1	2.9483 (6)	Ag2—C36	2.128 (3)
Br1—Ag1—Br2	99.54 (2)	C36—Ag2—Br1	98.21 (9)
C7—Ag1—Br1	165.54 (11)	C36—Ag2—Br2	147.61 (9)
C7—Ag1—Br2	94.49 (11)	Ag1—Br1—Ag2	70.769 (15)
Br1—Ag2—Br2	113.43 (2)	Ag1—Br2—Ag2	61.358 (14)

H atoms were placed in idealized positions and refined using a riding model, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ (aromatic H) or C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ (methyl H). The methyl groups were allowed to rotate about their local threefold axes. Rigid-bond restraints (Rollet, 1970) were applied to Ag2/Br1 and Ag2/Br2 so that the anisotropic displacement components of each pair of atoms were restrained to be equal along the line joining them.

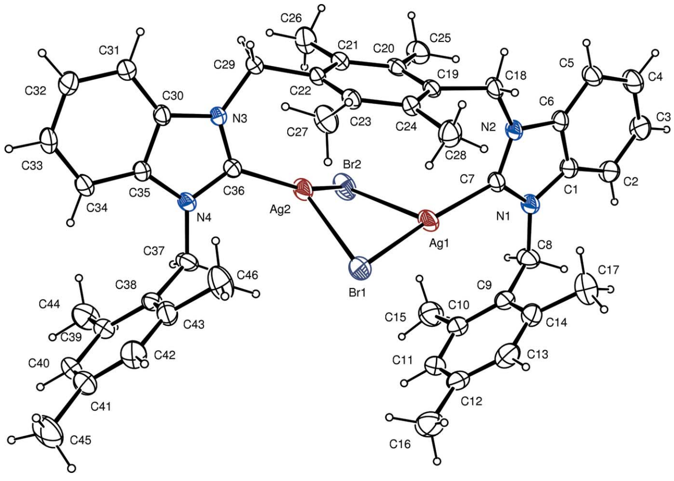


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Version 1.64.02; Farrugia, 1999).

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