

# Chlorido[1-phenyl-3-(2,3,5,6-tetra-methylbenzyl)benzimidazol-2-ylidene]-silver(I)

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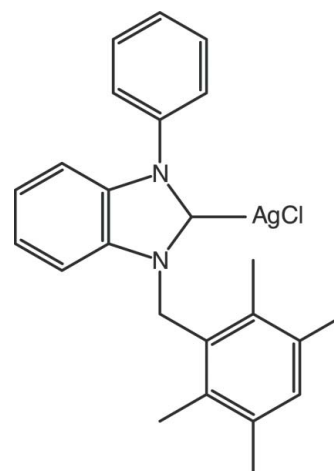
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.080; data-to-parameter ratio = 20.6.

In the title compound,  $[\text{AgCl}(\text{C}_{24}\text{H}_{24}\text{N}_2)]$ , the terminal phenyl and tetramethylbenzene rings [which form a dihedral angle of  $87.92$  ( $14$ ) $^\circ$ ] make dihedral angles of  $59.59$  ( $11$ ) and  $83.19$  ( $12$ ) $^\circ$  with respect to the central benzimidazole ring system. The Ag—C and Ag—Cl single-bond lengths are  $2.087$  ( $3$ ) and  $2.3267$  ( $9$ ) Å. The C—Ag—Cl bond angle is  $172.84$  ( $7$ ) $^\circ$ . C—H $\cdots\pi$  interactions contribute to the stabilization of the crystal structure. A very weak  $\pi$ — $\pi$  stacking interaction between adjacent tetramethylbenzene rings [centroid—centroid distance =  $4.0610$  ( $18$ ) Å] is also observed.

## Related literature

For the synthesis, see: Yigit *et al.* (2012); Özdemir *et al.* (2010c). For applications of silver *N*-heterocyclic carbene complexes in synthesis, catalysis, nanomaterials, and biology, see: Arduengo *et al.* (1993); Guerret *et al.* (1997); Patil *et al.* (2011); Özdemir *et al.* (2010b); Liao *et al.* (2008). For related compounds, see: Patil *et al.* (2010); Zhou *et al.* (2008); Berding *et al.* (2009). For bond-length data, see: Özdemir *et al.* (2010a); Allen *et al.* (1987).



## Experimental

### Crystal data

$[\text{AgCl}(\text{C}_{24}\text{H}_{24}\text{N}_2)]$   
 $M_r = 483.77$   
 Monoclinic,  $P2_1/n$   
 $a = 9.1439$  (2) Å  
 $b = 18.7633$  (4) Å  
 $c = 13.2710$  (3) Å  
 $\beta = 109.899$  (1) $^\circ$

$V = 2140.96$  (8) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.08$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.35 \times 0.22 \times 0.20$  mm

### Data collection

Bruker Kappa APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{\min} = 0.752$ ,  $T_{\max} = 0.806$

19846 measured reflections  
 5288 independent reflections  
 3354 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.040$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.080$   
 $S = 1.01$   
 5288 reflections

257 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.38$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.38$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å,  $^\circ$ ).

Cg2 and Cg3 are the centroids of the C1—C6 benzene and C8—C13 phenyl rings, respectively.

| <i>D</i> —H $\cdots$ <i>A</i> | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
|-------------------------------|-------------|---------------------|-----------------------|-------------------------|
| C9—H9···Cg2 <sup>i</sup>      | 0.93        | 2.69                | 3.507 (4)             | 147                     |
| C22—H22A···Cg3 <sup>ii</sup>  | 0.96        | 2.80                | 3.525 (4)             | 133                     |

Symmetry codes: (i)  $-x, -y + 2, -z$ ; (ii)  $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$ .

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5223).

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## supplementary materials

*Acta Cryst.* (2012). E68, m590–m591 [doi:10.1107/S1600536812012998]

## Chlorido[1-phenyl-3-(2,3,5,6-tetramethylbenzyl)benzimidazol-2-ylidene]silver(I)

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### Comment

*N*-Heterocyclic carbene complexes (NHCs) have developed significantly in organometallic chemistry and homogenous catalysis since discovered, and have become extremely popular. Silver NHC complexes have particular interest because of their wide use as ligand transfer agents for the synthesis other metal-NHC complexes, catalysis, nanomaterials, and also biological activity as antimicrobial agents (Arduengo *et al.*, 1993; Guerret *et al.*, 1997; Patil *et al.*, 2011; Özdemir *et al.*, 2010b; Liao *et al.*, 2008; Patil *et al.*, 2010; Zhou *et al.*, 2008; Berding *et al.*, 2009).

In connection with our papers on the synthesis of the new complexes with *N*-heterocyclic carbene ligands, (Yigit *et al.*, 2012; Özdemir *et al.*, 2010c), we report here the crystal structure of the title compound, chlorido-[1-phenyl-3-(2,3,5,6-tetramethylbenzyl)benzimidazol-2-ylidene]silver (I).

In the title compound (I), (Fig. 1), the five- and six-membered rings (N1/N2/C1/C6/C7) and (C1–C6) of the benzimidazole groups are almost co-planar with maximum deviations of -0.012 (2) Å for N1 and 0.012 (3) Å for C6, respectively. The dihedral angle between them is 4.53 (16)°. The C8–C13 phenyl and C15–C20 benzene rings make dihedral angles of 59.59 (11)° and 83.19 (12)°, respectively, with respect to the mean plane of the central N1/N2/C1–C7 benzimidazole ring system, while they make a dihedral angle of 87.92 (14)° with each other. The Ag–C and Ag–Cl single bond lengths are 2.087 (3) Å and 2.3267 (9) Å. The C–Ag–Cl bond angle is 172.84 (7)°. The values of the geometrical parameters of (I) are in agreement with those reported for similar compounds (Allen *et al.*, 1987; Özdemir *et al.*, 2010a).

The crystal structure is stabilized by C–H... $\pi$  interactions (Table 1) and weak  $\pi$ - $\pi$  stacking interactions between adjacent (C15–C20: *Cg*4) benzene rings [*Cg*4...*Cg*4(1 - *x*, 2 - *y*, 1 - *z*) = 4.0610 (18) Å]. Fig. 2 shows the packing of (I) in the unit cell, viewed along the *a* axis.

### Experimental

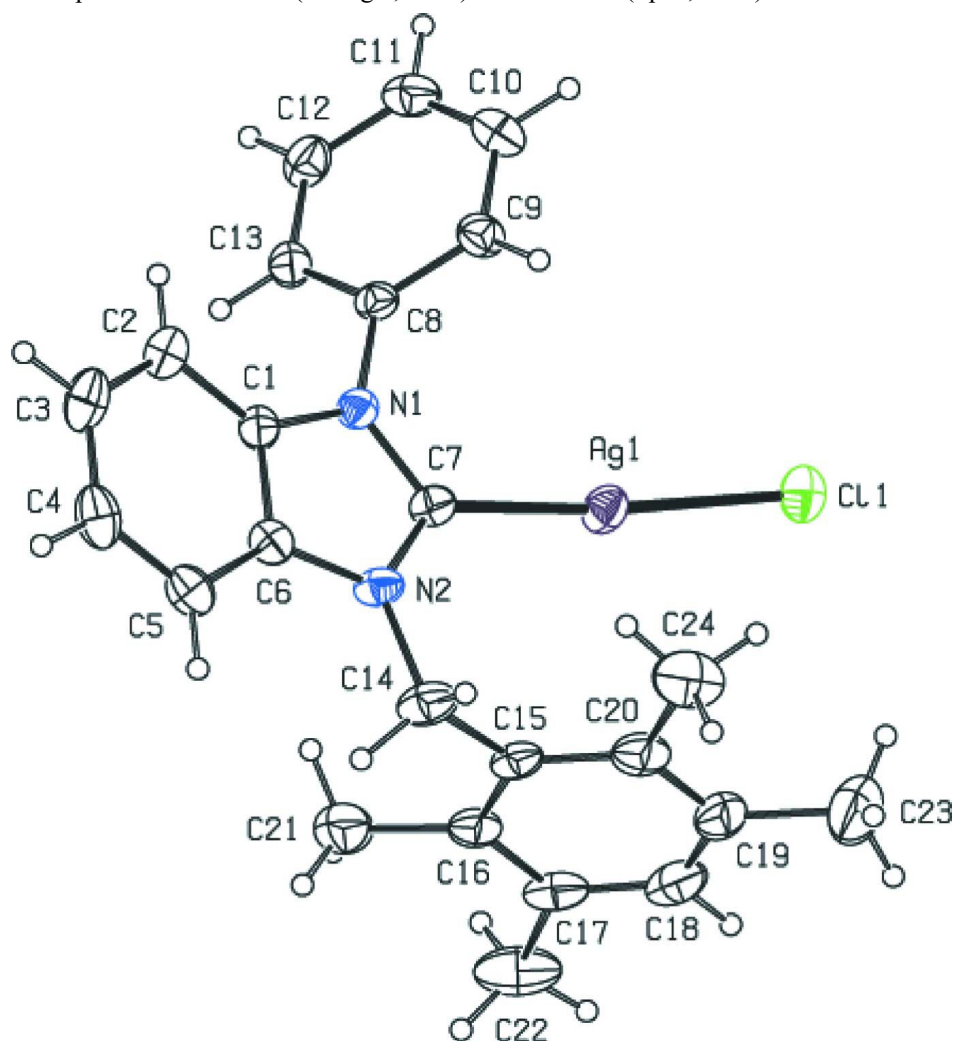
For the originally reported synthesis, see: Yigit *et al.* (2012); Özdemir *et al.* (2010c). Single crystals of the title compound were obtained by recrystallization from dichloromethane/hexane at room temperature. (Yields: 0.281 g; 84%. M.p.: 524–525 K).

### Refinement

The H atoms were positioned geometrically with C–H = 0.93, C–H = 0.97 and C–H = 0.96 Å, for the aromatic, methylene and methyl H atoms, respectively and refined using a riding model with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$ , where  $x = 1.5$  for the methyl H atoms and  $x = 1.2$  for all other H atoms.

**Computing details**

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

**Figure 1**

The title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

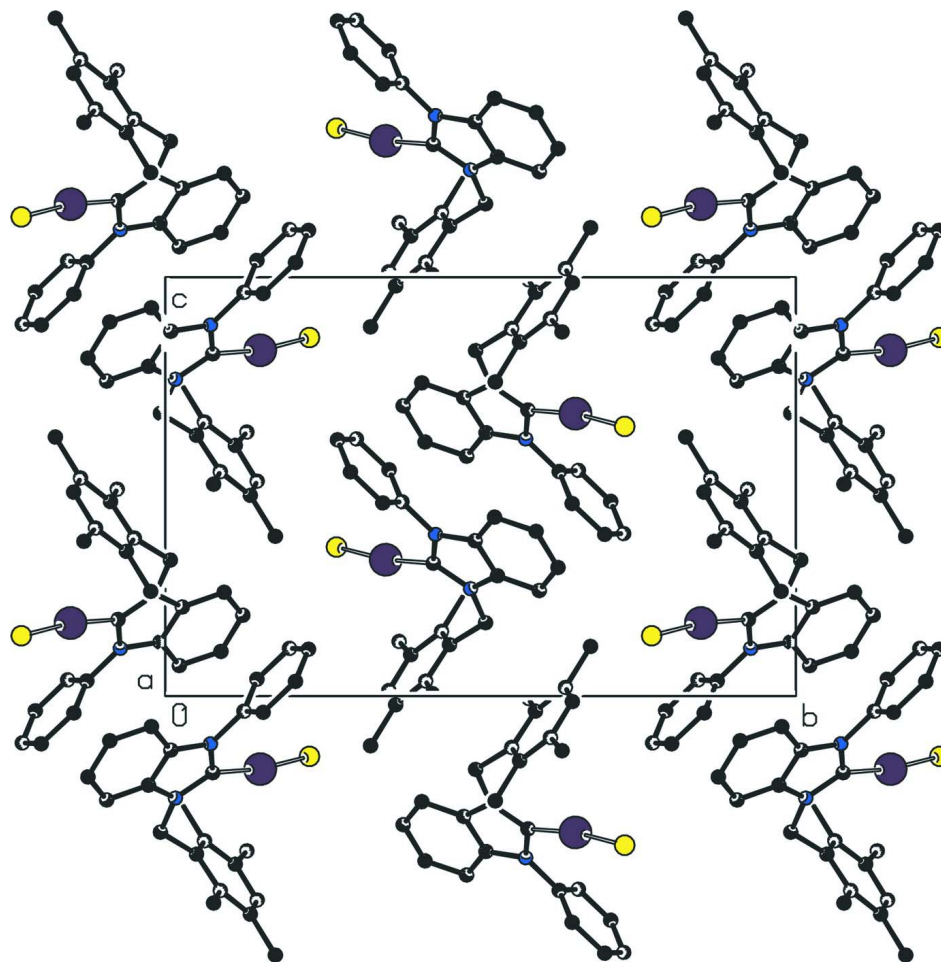


Figure 2

The packing of the title molecule in the unit cell, viewed along the *a* axis. H atoms are omitted for clarity.

### Chlorido[1-phenyl-3-(2,3,5,6-tetramethylbenzyl)benzimidazol-2-ylidene]silver(I)

#### Crystal data

[AgCl(C<sub>24</sub>H<sub>24</sub>N<sub>2</sub>)]

*M<sub>r</sub>* = 483.77

Monoclinic, *P*2<sub>1</sub>/*n*

Hall symbol: -*P* 2<sub>1</sub> *yn*

*a* = 9.1439 (2) Å

*b* = 18.7633 (4) Å

*c* = 13.2710 (3) Å

β = 109.899 (1)°

*V* = 2140.96 (8) Å<sup>3</sup>

*Z* = 4

*F*(000) = 984

*D<sub>x</sub>* = 1.501 Mg m<sup>-3</sup>

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 3354 reflections

θ = 2.4–28.3°

μ = 1.08 mm<sup>-1</sup>

*T* = 296 K

Prism, white

0.35 × 0.22 × 0.20 mm

#### Data collection

Bruker Kappa APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.00 pixels mm<sup>-1</sup>

#### ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

*T<sub>min</sub>* = 0.752, *T<sub>max</sub>* = 0.806

19846 measured reflections

5288 independent reflections  
 3354 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.040$   
 $\theta_{\text{max}} = 28.3^\circ$ ,  $\theta_{\text{min}} = 2.4^\circ$

$h = -10 \rightarrow 12$   
 $k = -25 \rightarrow 16$   
 $l = -17 \rightarrow 17$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.080$   
 $S = 1.01$   
 5288 reflections  
 257 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 0.160P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.38 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.38 \text{ e } \text{\AA}^{-3}$

*Special details*

**Experimental.** *M.p.*: 524–525 K.  $n_{\text{(CN)}} = 1593.31 \text{ cm}^{-1}$ .  $^1\text{H}$  NMR (DMSO)  $\delta$ : 2.11, 2.18 (s, 12H,  $\text{NCH}_2\text{C}_6\text{H}(\text{CH}_3)_4\text{-2,3,5,6}$ ); 5.61 (s, 2H,  $\text{NCH}_2\text{C}_6\text{H}(\text{CH}_3)_4\text{-2,3,5,6}$ ); 6.66–7.87 (m, 10H, Ar-*H*).  $^{13}\text{C}$  NMR (DMSO)  $\delta$ : 16.4, 20.8 ( $\text{NCH}_2\text{C}_6\text{H}(\text{CH}_3)_4\text{-2,3,5,6}$ ); 55.2 ( $\text{NCH}_2\text{C}_6\text{H}(\text{CH}_3)_4\text{-2,3,5,6}$ ); 112.5, 112.8, 124.9, 125.4, 126.8, 129.8, 130.4, 131.3, 132.7, 133.9, 134.6, 138.9 (Ar-*C*); the carbene carbon was not detected. Analysis calculated for  $\text{C}_{24}\text{H}_{24}\text{N}_2\text{AgCl}$ : C 59.58, H 5.00, N 5.79%. Found: C 59.56, H 5.01, N 5.78%.

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement.** Refinement on  $F^2$  for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors  $wR$  and all goodnesses of fit *S* are based on  $F^2$ , conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative  $F^2$ . The observed criterion of  $F^2 > \sigma(F^2)$  is used only for calculating *-R-factor-obs etc.* and is not relevant to the choice of reflections for refinement. *R*-factors based on  $F^2$  are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

|     | <i>x</i>    | <i>y</i>     | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|--------------|----------------------------------|
| Ag1 | 0.25184 (3) | 0.84953 (1)  | 0.17444 (2)  | 0.0476 (1)                       |
| Cl1 | 0.43000 (9) | 0.77142 (4)  | 0.14398 (7)  | 0.0572 (3)                       |
| N1  | -0.0611 (3) | 0.92849 (11) | 0.11403 (17) | 0.0370 (7)                       |
| N2  | 0.1099 (3)  | 0.98412 (11) | 0.24355 (18) | 0.0419 (8)                       |
| C1  | -0.1317 (3) | 0.99141 (14) | 0.1290 (2)   | 0.0383 (9)                       |
| C2  | -0.2743 (3) | 1.02215 (16) | 0.0728 (3)   | 0.0516 (11)                      |
| C3  | -0.3022 (4) | 1.08812 (18) | 0.1066 (3)   | 0.0633 (14)                      |
| C4  | -0.1939 (4) | 1.12282 (17) | 0.1930 (3)   | 0.0600 (13)                      |
| C5  | -0.0523 (4) | 1.09315 (15) | 0.2480 (2)   | 0.0490 (11)                      |
| C6  | -0.0233 (3) | 1.02675 (14) | 0.2127 (2)   | 0.0400 (9)                       |
| C7  | 0.0885 (3)  | 0.92485 (14) | 0.1829 (2)   | 0.0407 (9)                       |
| C8  | -0.1372 (3) | 0.87529 (14) | 0.0361 (2)   | 0.0365 (8)                       |
| C9  | -0.0741 (4) | 0.85480 (15) | -0.0403 (2)  | 0.0458 (10)                      |
| C10 | -0.1480 (4) | 0.80302 (16) | -0.1139 (2)  | 0.0552 (11)                      |
| C11 | -0.2846 (4) | 0.77302 (16) | -0.1119 (2)  | 0.0552 (11)                      |
| C12 | -0.3471 (4) | 0.79363 (16) | -0.0351 (3)  | 0.0536 (11)                      |
| C13 | -0.2733 (3) | 0.84494 (14) | 0.0388 (2)   | 0.0443 (10)                      |

|      |            |              |            |             |
|------|------------|--------------|------------|-------------|
| C14  | 0.2555 (4) | 1.00783 (17) | 0.3248 (2) | 0.0575 (11) |
| C15  | 0.3702 (3) | 0.95064 (15) | 0.3774 (2) | 0.0452 (10) |
| C16  | 0.3525 (4) | 0.91300 (16) | 0.4642 (2) | 0.0480 (10) |
| C17  | 0.4668 (4) | 0.86531 (16) | 0.5207 (2) | 0.0579 (11) |
| C18  | 0.5916 (4) | 0.85445 (17) | 0.4869 (3) | 0.0675 (12) |
| C19  | 0.6107 (4) | 0.8891 (2)   | 0.4013 (3) | 0.0639 (11) |
| C20  | 0.4998 (4) | 0.93808 (17) | 0.3455 (2) | 0.0556 (11) |
| C21  | 0.2094 (4) | 0.9235 (2)   | 0.4940 (3) | 0.0758 (14) |
| C22  | 0.4607 (5) | 0.8255 (2)   | 0.6185 (3) | 0.0917 (18) |
| C23  | 0.7508 (5) | 0.8708 (3)   | 0.3695 (4) | 0.115 (2)   |
| C24  | 0.5189 (5) | 0.9767 (2)   | 0.2499 (3) | 0.0853 (17) |
| H2   | -0.34700   | 0.99920      | 0.01520    | 0.0620*     |
| H3   | -0.39630   | 1.11050      | 0.07090    | 0.0760*     |
| H4   | -0.21850   | 1.16730      | 0.21380    | 0.0720*     |
| H5   | 0.02020    | 1.11610      | 0.30560    | 0.0590*     |
| H9   | 0.01720    | 0.87570      | -0.04210   | 0.0550*     |
| H10  | -0.10550   | 0.78830      | -0.16490   | 0.0660*     |
| H11  | -0.33500   | 0.73880      | -0.16250   | 0.0660*     |
| H12  | -0.43850   | 0.77290      | -0.03330   | 0.0640*     |
| H13  | -0.31510   | 0.85920      | 0.09040    | 0.0530*     |
| H14A | 0.22980    | 1.03330      | 0.38010    | 0.0690*     |
| H14B | 0.30560    | 1.04140      | 0.29150    | 0.0690*     |
| H18  | 0.66720    | 0.82180      | 0.52420    | 0.0810*     |
| H21A | 0.22080    | 0.96590      | 0.53640    | 0.1140*     |
| H21B | 0.19590    | 0.88320      | 0.53450    | 0.1140*     |
| H21C | 0.12030    | 0.92820      | 0.43010    | 0.1140*     |
| H22A | 0.37210    | 0.79440      | 0.59830    | 0.1370*     |
| H22B | 0.45230    | 0.85900      | 0.67090    | 0.1370*     |
| H22C | 0.55390    | 0.79790      | 0.64840    | 0.1370*     |
| H23A | 0.71950    | 0.83940      | 0.30890    | 0.1730*     |
| H23B | 0.82820    | 0.84780      | 0.42840    | 0.1730*     |
| H23C | 0.79320    | 0.91370      | 0.35120    | 0.1730*     |
| H24A | 0.59720    | 1.01290      | 0.27490    | 0.1280*     |
| H24B | 0.42190    | 0.99840      | 0.20850    | 0.1280*     |
| H24C | 0.54970    | 0.94330      | 0.20620    | 0.1280*     |

Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$    | $U^{23}$     |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| Ag1 | 0.0405 (1)  | 0.0420 (2)  | 0.0554 (2)  | 0.0047 (1)   | 0.0098 (1)  | -0.0002 (1)  |
| Cl1 | 0.0532 (5)  | 0.0540 (5)  | 0.0682 (5)  | 0.0093 (4)   | 0.0255 (4)  | 0.0036 (4)   |
| N1  | 0.0355 (12) | 0.0364 (13) | 0.0371 (12) | 0.0020 (11)  | 0.0096 (11) | -0.0018 (10) |
| N2  | 0.0431 (14) | 0.0362 (14) | 0.0375 (13) | -0.0034 (11) | 0.0021 (11) | -0.0040 (11) |
| C1  | 0.0378 (15) | 0.0395 (17) | 0.0397 (16) | 0.0031 (14)  | 0.0158 (14) | 0.0020 (13)  |
| C2  | 0.0395 (17) | 0.055 (2)   | 0.060 (2)   | 0.0036 (15)  | 0.0164 (16) | 0.0027 (16)  |
| C3  | 0.048 (2)   | 0.053 (2)   | 0.090 (3)   | 0.0156 (17)  | 0.025 (2)   | 0.0087 (19)  |
| C4  | 0.071 (2)   | 0.0398 (18) | 0.083 (3)   | 0.0081 (19)  | 0.044 (2)   | -0.0009 (18) |
| C5  | 0.062 (2)   | 0.0382 (18) | 0.0521 (19) | -0.0015 (16) | 0.0265 (18) | -0.0025 (14) |
| C6  | 0.0484 (17) | 0.0342 (16) | 0.0389 (16) | 0.0035 (14)  | 0.0169 (14) | 0.0053 (12)  |
| C7  | 0.0400 (16) | 0.0394 (17) | 0.0381 (15) | -0.0002 (14) | 0.0074 (14) | 0.0011 (13)  |

|     |             |             |             |              |              |              |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C8  | 0.0363 (15) | 0.0365 (15) | 0.0317 (14) | 0.0037 (13)  | 0.0051 (13)  | 0.0024 (12)  |
| C9  | 0.0493 (17) | 0.0513 (19) | 0.0390 (15) | -0.0054 (15) | 0.0179 (14)  | -0.0013 (14) |
| C10 | 0.074 (2)   | 0.054 (2)   | 0.0415 (18) | -0.0010 (18) | 0.0246 (18)  | -0.0060 (15) |
| C11 | 0.063 (2)   | 0.0477 (19) | 0.0437 (18) | -0.0020 (17) | 0.0036 (17)  | -0.0072 (15) |
| C12 | 0.0391 (17) | 0.053 (2)   | 0.066 (2)   | -0.0026 (15) | 0.0143 (17)  | -0.0038 (17) |
| C13 | 0.0399 (16) | 0.0464 (18) | 0.0474 (17) | 0.0000 (15)  | 0.0161 (14)  | -0.0064 (14) |
| C14 | 0.057 (2)   | 0.0458 (19) | 0.0532 (19) | -0.0074 (17) | -0.0028 (16) | -0.0059 (15) |
| C15 | 0.0407 (17) | 0.0428 (18) | 0.0400 (16) | -0.0072 (14) | -0.0018 (14) | -0.0065 (14) |
| C16 | 0.0478 (18) | 0.0485 (19) | 0.0402 (17) | -0.0133 (15) | 0.0054 (15)  | -0.0108 (14) |
| C17 | 0.066 (2)   | 0.049 (2)   | 0.0400 (17) | -0.0114 (17) | -0.0063 (17) | -0.0023 (15) |
| C18 | 0.057 (2)   | 0.056 (2)   | 0.064 (2)   | 0.0075 (18)  | -0.0126 (19) | -0.0112 (18) |
| C19 | 0.0424 (19) | 0.074 (2)   | 0.066 (2)   | -0.0081 (19) | 0.0065 (18)  | -0.022 (2)   |
| C20 | 0.056 (2)   | 0.056 (2)   | 0.0476 (18) | -0.0213 (17) | 0.0082 (17)  | -0.0109 (16) |
| C21 | 0.064 (2)   | 0.100 (3)   | 0.061 (2)   | -0.014 (2)   | 0.018 (2)    | -0.015 (2)   |
| C22 | 0.123 (4)   | 0.074 (3)   | 0.052 (2)   | -0.023 (3)   | -0.004 (2)   | 0.0150 (19)  |
| C23 | 0.057 (3)   | 0.153 (5)   | 0.131 (4)   | 0.002 (3)    | 0.026 (3)    | -0.044 (4)   |
| C24 | 0.092 (3)   | 0.098 (3)   | 0.068 (3)   | -0.037 (3)   | 0.030 (2)    | -0.003 (2)   |

*Geometric parameters (Å, °)*

|            |            |          |           |
|------------|------------|----------|-----------|
| Ag1—C11    | 2.3267 (9) | C19—C20  | 1.382 (5) |
| Ag1—C7     | 2.087 (3)  | C19—C23  | 1.518 (6) |
| N1—C1      | 1.392 (4)  | C20—C24  | 1.522 (5) |
| N1—C7      | 1.364 (4)  | C2—H2    | 0.9300    |
| N1—C8      | 1.435 (3)  | C3—H3    | 0.9300    |
| N2—C6      | 1.397 (4)  | C4—H4    | 0.9300    |
| N2—C7      | 1.348 (3)  | C5—H5    | 0.9300    |
| N2—C14     | 1.468 (4)  | C9—H9    | 0.9300    |
| C1—C2      | 1.388 (4)  | C10—H10  | 0.9300    |
| C1—C6      | 1.381 (4)  | C11—H11  | 0.9300    |
| C2—C3      | 1.370 (5)  | C12—H12  | 0.9300    |
| C3—C4      | 1.395 (5)  | C13—H13  | 0.9300    |
| C4—C5      | 1.370 (5)  | C14—H14A | 0.9700    |
| C5—C6      | 1.388 (4)  | C14—H14B | 0.9700    |
| C8—C9      | 1.381 (4)  | C18—H18  | 0.9300    |
| C8—C13     | 1.380 (4)  | C21—H21A | 0.9600    |
| C9—C10     | 1.380 (4)  | C21—H21B | 0.9600    |
| C10—C11    | 1.379 (5)  | C21—H21C | 0.9600    |
| C11—C12    | 1.383 (5)  | C22—H22A | 0.9600    |
| C12—C13    | 1.376 (4)  | C22—H22B | 0.9600    |
| C14—C15    | 1.497 (4)  | C22—H22C | 0.9600    |
| C15—C16    | 1.407 (4)  | C23—H23A | 0.9600    |
| C15—C20    | 1.407 (5)  | C23—H23B | 0.9600    |
| C16—C17    | 1.386 (4)  | C23—H23C | 0.9600    |
| C16—C21    | 1.503 (5)  | C24—H24A | 0.9600    |
| C17—C18    | 1.376 (5)  | C24—H24B | 0.9600    |
| C17—C22    | 1.515 (5)  | C24—H24C | 0.9600    |
| C18—C19    | 1.371 (5)  |          |           |
| Cl1—Ag1—C7 | 172.84 (7) | C2—C3—H3 | 119.00    |



|             |             |               |           |
|-------------|-------------|---------------|-----------|
| C1—N1—C7    | 110.8 (2)   | C4—C3—H3      | 119.00    |
| C1—N1—C8    | 123.9 (2)   | C3—C4—H4      | 119.00    |
| C7—N1—C8    | 125.3 (2)   | C5—C4—H4      | 119.00    |
| C6—N2—C7    | 111.3 (2)   | C4—C5—H5      | 122.00    |
| C6—N2—C14   | 121.6 (2)   | C6—C5—H5      | 122.00    |
| C7—N2—C14   | 126.9 (3)   | C8—C9—H9      | 120.00    |
| N1—C1—C2    | 132.2 (3)   | C10—C9—H9     | 120.00    |
| N1—C1—C6    | 106.3 (2)   | C9—C10—H10    | 120.00    |
| C2—C1—C6    | 121.2 (3)   | C11—C10—H10   | 120.00    |
| C1—C2—C3    | 116.4 (3)   | C10—C11—H11   | 120.00    |
| C2—C3—C4    | 122.1 (3)   | C12—C11—H11   | 120.00    |
| C3—C4—C5    | 121.8 (3)   | C11—C12—H12   | 120.00    |
| C4—C5—C6    | 116.1 (3)   | C13—C12—H12   | 120.00    |
| N2—C6—C1    | 106.0 (2)   | C8—C13—H13    | 120.00    |
| N2—C6—C5    | 131.5 (3)   | C12—C13—H13   | 120.00    |
| C1—C6—C5    | 122.4 (3)   | N2—C14—H14A   | 108.00    |
| Ag1—C7—N1   | 124.81 (18) | N2—C14—H14B   | 108.00    |
| Ag1—C7—N2   | 129.1 (2)   | C15—C14—H14A  | 108.00    |
| N1—C7—N2    | 105.5 (2)   | C15—C14—H14B  | 108.00    |
| N1—C8—C9    | 120.1 (3)   | H14A—C14—H14B | 107.00    |
| N1—C8—C13   | 119.2 (2)   | C17—C18—H18   | 118.00    |
| C9—C8—C13   | 120.7 (3)   | C19—C18—H18   | 118.00    |
| C8—C9—C10   | 119.3 (3)   | C16—C21—H21A  | 109.00    |
| C9—C10—C11  | 120.2 (3)   | C16—C21—H21B  | 109.00    |
| C10—C11—C12 | 120.3 (3)   | C16—C21—H21C  | 109.00    |
| C11—C12—C13 | 119.7 (3)   | H21A—C21—H21B | 110.00    |
| C8—C13—C12  | 119.9 (3)   | H21A—C21—H21C | 109.00    |
| N2—C14—C15  | 116.2 (2)   | H21B—C21—H21C | 110.00    |
| C14—C15—C16 | 119.0 (3)   | C17—C22—H22A  | 110.00    |
| C14—C15—C20 | 120.5 (3)   | C17—C22—H22B  | 109.00    |
| C16—C15—C20 | 120.4 (3)   | C17—C22—H22C  | 109.00    |
| C15—C16—C17 | 119.4 (3)   | H22A—C22—H22B | 109.00    |
| C15—C16—C21 | 120.2 (3)   | H22A—C22—H22C | 109.00    |
| C17—C16—C21 | 120.4 (3)   | H22B—C22—H22C | 109.00    |
| C16—C17—C18 | 118.4 (3)   | C19—C23—H23A  | 109.00    |
| C16—C17—C22 | 122.7 (3)   | C19—C23—H23B  | 109.00    |
| C18—C17—C22 | 118.9 (3)   | C19—C23—H23C  | 109.00    |
| C17—C18—C19 | 123.6 (3)   | H23A—C23—H23B | 109.00    |
| C18—C19—C20 | 118.8 (3)   | H23A—C23—H23C | 110.00    |
| C18—C19—C23 | 118.7 (4)   | H23B—C23—H23C | 109.00    |
| C20—C19—C23 | 122.4 (4)   | C20—C24—H24A  | 109.00    |
| C15—C20—C19 | 119.3 (3)   | C20—C24—H24B  | 109.00    |
| C15—C20—C24 | 121.2 (3)   | C20—C24—H24C  | 109.00    |
| C19—C20—C24 | 119.5 (3)   | H24A—C24—H24B | 109.00    |
| C1—C2—H2    | 122.00      | H24A—C24—H24C | 109.00    |
| C3—C2—H2    | 122.00      | H24B—C24—H24C | 110.00    |
|             |             |               |           |
| C7—N1—C1—C2 | 172.8 (3)   | C4—C5—C6—C1   | -1.7 (4)  |
| C8—N1—C1—C2 | -7.1 (5)    | N1—C8—C9—C10  | 179.3 (2) |

|               |              |                 |            |
|---------------|--------------|-----------------|------------|
| C7—N1—C1—C6   | -2.1 (3)     | C9—C8—C13—C12   | 0.1 (4)    |
| C8—N1—C1—C6   | 178.0 (2)    | C13—C8—C9—C10   | -0.5 (4)   |
| C1—N1—C7—Ag1  | -169.48 (19) | N1—C8—C13—C12   | -179.7 (3) |
| C8—N1—C7—Ag1  | 10.4 (4)     | C8—C9—C10—C11   | 1.0 (4)    |
| C1—N1—C7—N2   | 2.2 (3)      | C9—C10—C11—C12  | -1.1 (5)   |
| C8—N1—C7—N2   | -178.0 (2)   | C10—C11—C12—C13 | 0.8 (5)    |
| C7—N1—C8—C13  | 122.9 (3)    | C11—C12—C13—C8  | -0.3 (4)   |
| C1—N1—C8—C9   | 123.0 (3)    | N2—C14—C15—C16  | -83.2 (3)  |
| C7—N1—C8—C9   | -56.9 (4)    | N2—C14—C15—C20  | 101.2 (3)  |
| C1—N1—C8—C13  | -57.2 (4)    | C14—C15—C16—C17 | -173.2 (3) |
| C7—N2—C14—C15 | -26.7 (4)    | C14—C15—C16—C21 | 7.9 (4)    |
| C6—N2—C7—N1   | -1.4 (3)     | C20—C15—C16—C17 | 2.4 (4)    |
| C14—N2—C7—N1  | -175.3 (3)   | C20—C15—C16—C21 | -176.5 (3) |
| C6—N2—C14—C15 | 160.1 (3)    | C14—C15—C20—C19 | 174.6 (3)  |
| C14—N2—C6—C1  | 174.4 (2)    | C14—C15—C20—C24 | -6.2 (4)   |
| C7—N2—C6—C5   | -176.4 (3)   | C16—C15—C20—C19 | -0.9 (4)   |
| C14—N2—C6—C5  | -2.2 (5)     | C16—C15—C20—C24 | 178.3 (3)  |
| C6—N2—C7—Ag1  | 169.7 (2)    | C15—C16—C17—C18 | -2.5 (4)   |
| C14—N2—C7—Ag1 | -4.1 (4)     | C15—C16—C17—C22 | 176.8 (3)  |
| C7—N2—C6—C1   | 0.2 (3)      | C21—C16—C17—C18 | 176.4 (3)  |
| N1—C1—C2—C3   | -175.7 (3)   | C21—C16—C17—C22 | -4.3 (5)   |
| N1—C1—C6—C5   | 178.1 (3)    | C16—C17—C18—C19 | 1.1 (5)    |
| C6—C1—C2—C3   | -1.5 (5)     | C22—C17—C18—C19 | -178.2 (3) |
| C2—C1—C6—C5   | 2.5 (4)      | C17—C18—C19—C20 | 0.4 (5)    |
| C2—C1—C6—N2   | -174.4 (3)   | C17—C18—C19—C23 | -178.0 (4) |
| N1—C1—C6—N2   | 1.1 (3)      | C18—C19—C20—C15 | -0.5 (5)   |
| C1—C2—C3—C4   | -0.2 (5)     | C18—C19—C20—C24 | -179.7 (3) |
| C2—C3—C4—C5   | 1.0 (6)      | C23—C19—C20—C15 | 177.9 (3)  |
| C3—C4—C5—C6   | 0.0 (5)      | C23—C19—C20—C24 | -1.3 (5)   |
| C4—C5—C6—N2   | 174.4 (3)    |                 |            |

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

Cg2 and Cg3 are the centroids of the C1—C6 benzene and C8—C13 phenyl rings, respectively.

| $D-H\cdots A$                       | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------------------|-------|-------------|-------------|---------------|
| C9—H9 $\cdots$ Cg2 <sup>i</sup>     | 0.93  | 2.69        | 3.507 (4)   | 147           |
| C22—H22A $\cdots$ Cg3 <sup>ii</sup> | 0.96  | 2.80        | 3.525 (4)   | 133           |

Symmetry codes: (i)  $-x, -y+2, -z$ ; (ii)  $x+1/2, -y+3/2, z+1/2$ .