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## **[*N,N'*-Bis(4-bromobenzylidene)-2,2-dimethylpropane- $\kappa^2N,N'$ ]iodidocopper(I). Corrigendum**

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The chemical name of the title compound in the paper by Kia, Fun & Kargar [*Acta Cryst.* (2009), **E65**, m289] is corrected.

In the paper by Kia, Fun & Kargar [*Acta Cryst.* (2009), **E65**, m289], the chemical name given in the *Title* should be '*[N,N'*-Bis(4-bromobenzylidene)-2,2-dimethylpropane-1,3-diamine- $\kappa^2N,N'$ ]iodidocopper(I)'

# [*N,N'*-Bis(4-bromobenzylidene)-2,2-dimethylpropane- $\kappa^2$ *N,N'*]iodidocopper(I)

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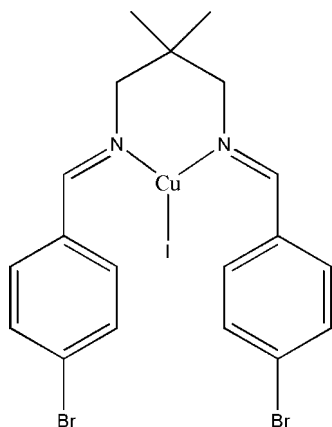
Received 21 January 2009; accepted 12 February 2009

Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.012$  Å;  $R$  factor = 0.050;  $wR$  factor = 0.112; data-to-parameter ratio = 16.0.

The title compound,  $[\text{CuI}(\text{C}_{19}\text{H}_{20}\text{Br}_2\text{N}_2)]$ , lies across a crystallographic mirror plane. The coordination around the copper centre is distorted trigonal planar, with a bite angle of  $94.7(3)^\circ$ . A six-membered chelate ring in a chair conformation is formed by the coordination of the imine N atoms of the bidentate ligand to the  $\text{Cu}^{\text{I}}$  atom. This conformation is required by the crystallographic mirror symmetry. The interplanar angle between the benzene rings is  $74.85(19)^\circ$ . The crystal structure exhibits weak intermolecular  $\text{C}-\text{H}\cdots\pi$  interactions, which link the molecules into chains along the  $b$  axis.

## Related literature

For the puckering parameters, see: Cremer & Pople (1975). For related literature and the catalytic applications see, for example: Killian *et al.* (1996); Jung *et al.* (1996); Small *et al.* (1998). For a related structure, see: Kia *et al.* (2009). For the stability of the temperature controller, see Cosier & Glazer (1986).



## Experimental

### Crystal data

|   |   |
|---|---|
| $[\text{CuI}(\text{C}_{19}\text{H}_{20}\text{Br}_2\text{N}_2)]$ | $V = 2116.8(4) \text{ \AA}^3$             |
| $M_r = 626.63$  | $Z = 4$                                   |
| Monoclinic, $C2/m$  | Mo $K\alpha$ radiation                    |
| $a = 16.2224(15) \text{ \AA}$                                   | $\mu = 6.27 \text{ mm}^{-1}$              |
| $b = 12.2807(12) \text{ \AA}$                                   | $T = 100 \text{ K}$                       |
| $c = 10.6292(12) \text{ \AA}$                                   | $0.58 \times 0.09 \times 0.05 \text{ mm}$ |
| $\beta = 91.599(6)^\circ$                                       |   |

### Data collection

|  |  |
|--|--|
| Bruker SMART APEXII CCD area-detector diffractometer     | 10374 measured reflections             |
| Absorption correction: multi-scan (SADABS; Bruker, 2005) | 1936 independent reflections           |
| $T_{\text{min}} = 0.119$ , $T_{\text{max}} = 0.714$      | 1474 reflections with $I > 2\sigma(I)$ |
|  | $R_{\text{int}} = 0.099$               |

### Refinement

|                                 |  |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.050$ | 121 parameters                                       |
| $wR(F^2) = 0.112$               | H-atom parameters constrained                        |
| $S = 1.16$                      | $\Delta\rho_{\text{max}} = 2.64 \text{ e \AA}^{-3}$  |
| 1936 reflections                | $\Delta\rho_{\text{min}} = -0.99 \text{ e \AA}^{-3}$ |

**Table 1**

Hydrogen-bond geometry (Å, °).

$\text{Cg1}$  is the centroid of the  $\text{C1}-\text{C6}$  benzene ring.

| $D-\text{H}\cdots A$                              | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{C8}-\text{H8A}\cdots\text{Cg1}^{\text{i}}$ | 0.99         | 2.83               | 3.631 (9)   | 138                  |

Symmetry code: (i)  $-x + \frac{1}{2}, -y + \frac{1}{2}, -z$ .

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZZ2161).

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## supporting information

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**[*N,N'*-Bis(4-bromobenzylidene)-2,2-dimethylpropane- $\kappa^2$ *N,N'*]iodidocopper(I)**

Reza Kia, Hoong-Kun Fun and Hadi Kargar

**S1. Comment**

In recent years, an increasing amount of research has been focused on the design and preparation of mono- or dinuclear mixed ligand transition metal complexes with neutral, chelating nitrogen-containing ligands. Early and late transition metal complexes of this type have been extensively used as catalysts for a wide categories of reactions, including olefin polymerization (Killian *et al.*, 1996) and oxygen activation (Jung *et al.*, 1996). In this context, diverse chelating Schiff base type ligands, amines and pyridine derivatives (Small *et al.*, 1998) have successfully been applied in the preparation of these homogeneous catalysts. Here we report the crystal structure of an aldimine Schiff base ligand with copper(I) iodide. To the best of our knowledge, only one such related compound has been published (Kia *et al.*, 2009). The title compound is the second tricoordinate complex of an aldimine bis-Schiff base ligand with copper(I) iodide adopting trigonal planar geometry.

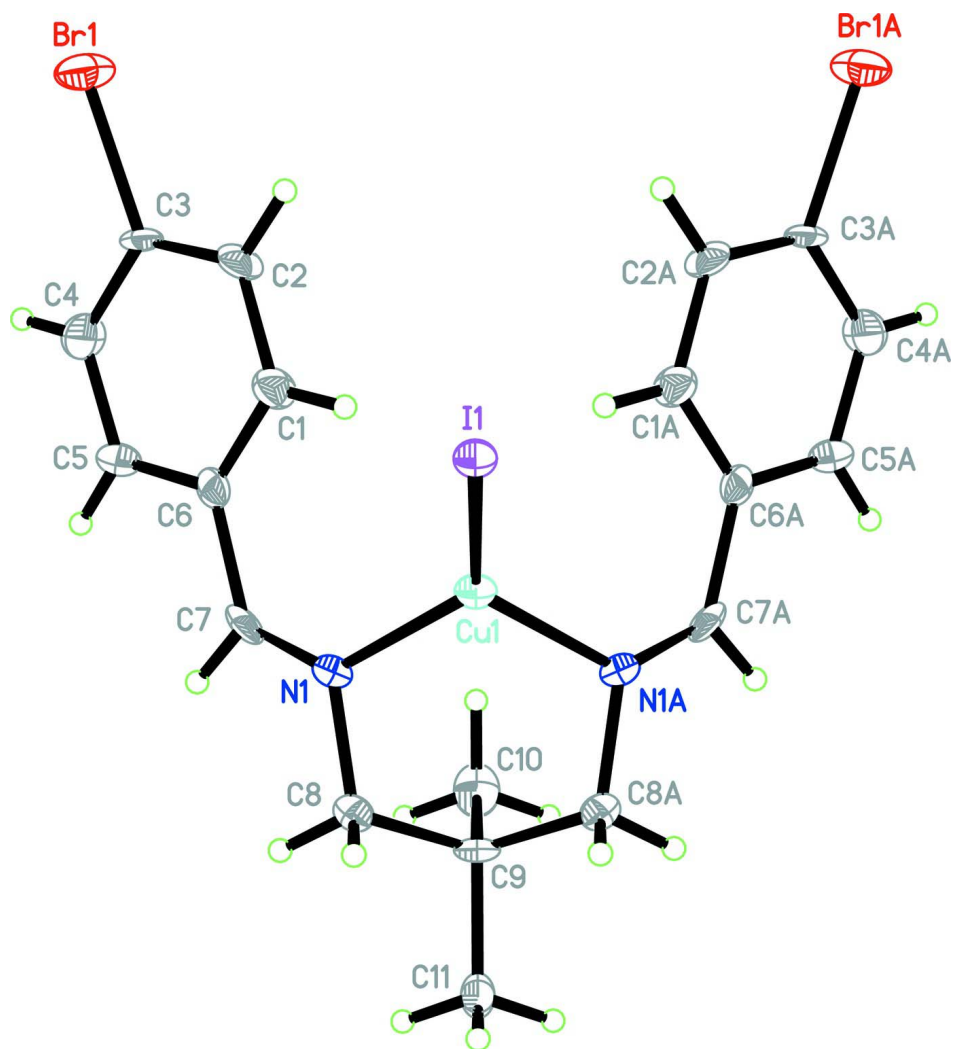
The title compound, I, Fig. 1, lies across a crystallographic mirror plane. Atoms I1, Cu1, C9, C10 and C11 lies on this mirror plane. The asymmetric unit of (I) is composed of one-half of the molecule. The coordination around the copper centre is distorted trigonal planar, with a bite angle of 94.7 (3)°. The deviation of the Cu atom from the N1/N1A/I1 plane is -0.105 (4) Å. A six-membered chelate ring with a chair conformation is formed by the coordination of iminic N atoms of the bidentate ligand to the Cu(I) atom, with ring puckering parameters (Cremer & Pople, 1975) of  $Q = 0.696$  (7) Å,  $\Theta = 172.2$  (6)°,  $\Phi = 180$  (5)°. This conformation is required if the local symmetry of the metal coordination site is in accordance with the mirror plane that passes through the metal atom normal to the line connecting the nitrogen atoms. The dihedral angle between the phenyl rings is 74.85 (19)°. The crystal structure is stabilized by weak intermolecular C—H $\cdots$  $\pi$  interactions ( $Cg1$  is the centroid of the C1–C6 benzene ring) which link the molecules into chains along the *b*-axis (Fig. 2 and Table 1).

**S2. Experimental**

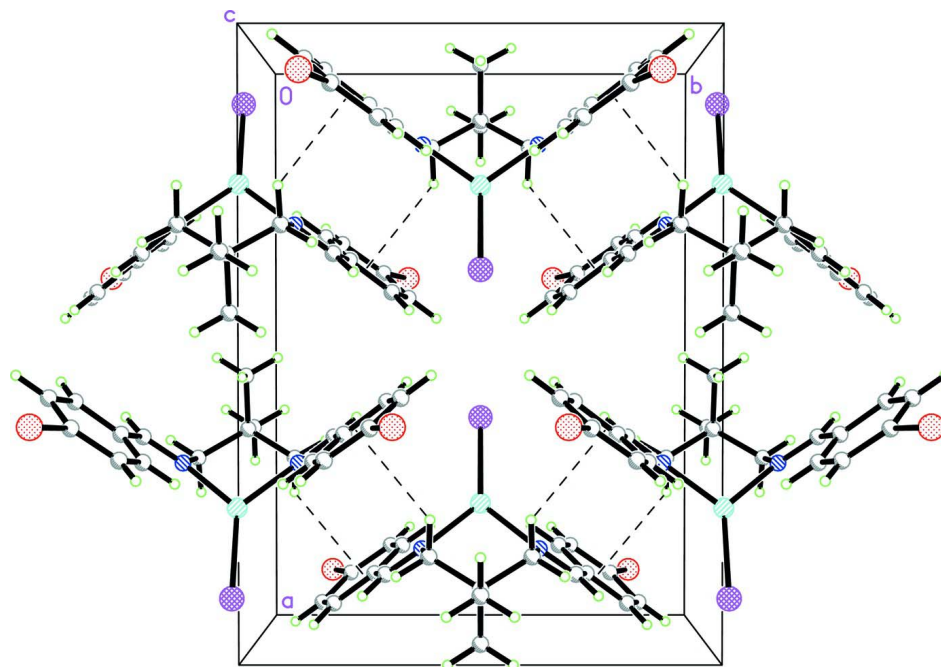
*N,N'*-Bis(4-bromobenzylidene)-2,2-dimethylpropane (783 mg, 2 mmol) was added dropwise to a suspension of CuI (380 mg, 2.0 mmol) in 50 ml of THF. After 15 min a clear yellowish solution was obtained. The volume of the reaction mixture was reduced until the formation of a yellow precipitate occurred. Single crystals suitable for X-ray diffraction were grown from the acetonitrile solution.

**S3. Refinement**

All H atoms were positioned geometrically with C—H = 0.95–0.99 Å and refined in a riding model approximation with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The highest peak (2.64 e. Å<sup>-3</sup>) is located 1.02 Å from I1 and the deepest hole (-0.99 e. Å<sup>-3</sup>) is located 0.58 Å from H10A.

**Figure 1**

The molecular structure of (I), showing 40% probability displacement ellipsoids and the atomic numbering. Symmetry code for A atoms;  $x, -y + 1, z$ .



**Figure 2**

The crystal packing of (I), viewed down the *c*-axis, showing C—H... $\pi$  interactions linking the molecules into chains along the *b*-axis.

**[*N,N'*-Bis(4-bromobenzylidene)-2,2-dimethylpropane- $\kappa^2N,N'$ ]iodidocopper(I)**

*Crystal data*

[CuI(C<sub>19</sub>H<sub>20</sub>Br<sub>2</sub>N<sub>2</sub>)]

*M<sub>r</sub>* = 626.63

Monoclinic, *C2/m*

Hall symbol: -*C* 2*y*

*a* = 16.2224 (15) Å

*b* = 12.2807 (12) Å

*c* = 10.6292 (12) Å

$\beta$  = 91.599 (6)°

*V* = 2116.8 (4) Å<sup>3</sup>

*Z* = 4

*F*(000) = 1200

*D<sub>x</sub>* = 1.966 Mg m<sup>-3</sup>

Mo *K* $\alpha$  radiation,  $\lambda$  = 0.71073 Å

Cell parameters from 4080 reflections

$\theta$  = 2.5–29.5°

$\mu$  = 6.27 mm<sup>-1</sup>

*T* = 100 K

Needle, yellow

0.58 × 0.09 × 0.05 mm

*Data collection*

Bruker SMART APEXII CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

*T<sub>min</sub>* = 0.119, *T<sub>max</sub>* = 0.714

10374 measured reflections

1936 independent reflections

1474 reflections with *I* > 2 $\sigma$ (*I*)

*R<sub>int</sub>* = 0.099

$\theta_{\max}$  = 25.0°,  $\theta_{\min}$  = 2.1°

*h* = -19→19

*k* = -14→14

*l* = -12→12

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.050$   
 $wR(F^2) = 0.112$   
 $S = 1.16$   
 1936 reflections  
 121 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 16.0151P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 2.64 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.99 \text{ e } \text{\AA}^{-3}$

*Special details*

**Experimental.** The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted R-factor  $wR$  and goodness 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 threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) 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>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|-------------|--------------|----------------------------------|
| I1   | 0.38486 (4) | 0.5000      | 0.14862 (6)  | 0.0166 (2)                       |
| Br1  | 0.11472 (5) | 0.16378 (8) | 0.54336 (7)  | 0.0309 (3)                       |
| Cu1  | 0.25251 (8) | 0.5000      | 0.02730 (11) | 0.0168 (3)                       |
| N1   | 0.1853 (3)  | 0.3798 (6)  | -0.0519 (5)  | 0.0167 (14)                      |
| C1   | 0.1751 (5)  | 0.3315 (7)  | 0.2223 (7)   | 0.0213 (18)                      |
| H1A  | 0.2085      | 0.3923      | 0.2022       | 0.026*                           |
| C2   | 0.1683 (4)  | 0.3023 (7)  | 0.3463 (7)   | 0.0210 (18)                      |
| H2A  | 0.1957      | 0.3426      | 0.4113       | 0.025*                           |
| C3   | 0.1204 (5)  | 0.2130 (7)  | 0.3742 (6)   | 0.0193 (18)                      |
| C4   | 0.0779 (5)  | 0.1560 (7)  | 0.2811 (8)   | 0.026 (2)                        |
| H4A  | 0.0442      | 0.0958      | 0.3021       | 0.031*                           |
| C5   | 0.0852 (4)  | 0.1878 (7)  | 0.1556 (7)   | 0.0188 (18)                      |
| H5A  | 0.0559      | 0.1496      | 0.0907       | 0.023*                           |
| C6   | 0.1354 (4)  | 0.2756 (7)  | 0.1260 (7)   | 0.0172 (18)                      |
| C7   | 0.1428 (4)  | 0.3030 (7)  | -0.0085 (7)  | 0.0184 (17)                      |
| H7A  | 0.1130      | 0.2590      | -0.0675      | 0.022*                           |
| C8   | 0.1816 (5)  | 0.3967 (7)  | -0.1892 (7)  | 0.0213 (18)                      |
| H8A  | 0.1542      | 0.3330      | -0.2292      | 0.026*                           |
| H8B  | 0.2387      | 0.3997      | -0.2198      | 0.026*                           |
| C9   | 0.1360 (7)  | 0.5000      | -0.2327 (9)  | 0.020 (3)                        |
| C10  | 0.0477 (6)  | 0.5000      | -0.1869 (11) | 0.028 (3)                        |
| H10A | 0.0492      | 0.5000      | -0.0947      | 0.041*                           |
| H10B | 0.0187      | 0.4348      | -0.2177      | 0.041*                           |

|      |            |        |              |           |
|------|------------|--------|--------------|-----------|
| C11  | 0.1346 (7) | 0.5000 | -0.3771 (10) | 0.024 (3) |
| H11A | 0.1916     | 0.5000 | -0.4055      | 0.036*    |
| H11B | 0.1061     | 0.5652 | -0.4091      | 0.036*    |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$    | $U^{13}$    | $U^{23}$   |
|-----|------------|------------|------------|-------------|-------------|------------|
| I1  | 0.0191 (4) | 0.0171 (4) | 0.0134 (4) | 0.000       | -0.0029 (3) | 0.000      |
| Br1 | 0.0371 (5) | 0.0400 (6) | 0.0154 (4) | -0.0155 (4) | -0.0026 (3) | 0.0048 (4) |
| Cu1 | 0.0195 (7) | 0.0188 (8) | 0.0121 (7) | 0.000       | -0.0020 (5) | 0.000      |
| N1  | 0.020 (3)  | 0.018 (4)  | 0.012 (3)  | 0.001 (3)   | 0.001 (2)   | -0.002 (3) |
| C1  | 0.024 (4)  | 0.021 (5)  | 0.019 (4)  | -0.007 (3)  | 0.002 (3)   | -0.003 (4) |
| C2  | 0.025 (4)  | 0.023 (5)  | 0.015 (4)  | -0.009 (4)  | -0.004 (3)  | -0.007 (4) |
| C3  | 0.031 (4)  | 0.022 (5)  | 0.005 (4)  | -0.003 (4)  | 0.001 (3)   | 0.002 (3)  |
| C4  | 0.031 (5)  | 0.022 (5)  | 0.025 (5)  | -0.010 (4)  | 0.002 (4)   | 0.003 (4)  |
| C5  | 0.018 (4)  | 0.025 (5)  | 0.013 (4)  | -0.001 (3)  | -0.002 (3)  | -0.002 (4) |
| C6  | 0.019 (4)  | 0.014 (5)  | 0.020 (4)  | 0.005 (3)   | 0.004 (3)   | -0.002 (4) |
| C7  | 0.022 (4)  | 0.016 (5)  | 0.017 (4)  | 0.000 (3)   | -0.005 (3)  | -0.010 (4) |
| C8  | 0.031 (4)  | 0.019 (5)  | 0.014 (4)  | -0.003 (4)  | 0.001 (3)   | -0.002 (4) |
| C9  | 0.029 (6)  | 0.024 (7)  | 0.007 (5)  | 0.000       | 0.003 (4)   | 0.000      |
| C10 | 0.022 (6)  | 0.034 (8)  | 0.027 (7)  | 0.000       | -0.009 (5)  | 0.000      |
| C11 | 0.038 (7)  | 0.020 (7)  | 0.015 (6)  | 0.000       | -0.006 (5)  | 0.000      |

*Geometric parameters (Å, °)*

|                         |             |                    |            |
|-------------------------|-------------|--------------------|------------|
| I1—Cu1                  | 2.4735 (14) | C5—C6              | 1.392 (11) |
| Br1—C3                  | 1.902 (7)   | C5—H5A             | 0.9500     |
| Cu1—N1                  | 2.006 (6)   | C6—C7              | 1.477 (11) |
| Cu1—N1 <sup>i</sup>     | 2.006 (6)   | C7—H7A             | 0.9500     |
| N1—C7                   | 1.263 (10)  | C8—C9              | 1.533 (10) |
| N1—C8                   | 1.474 (9)   | C8—H8A             | 0.9900     |
| C1—C2                   | 1.374 (11)  | C8—H8B             | 0.9900     |
| C1—C6                   | 1.378 (10)  | C9—C10             | 1.527 (15) |
| C1—H1A                  | 0.9500      | C9—C8 <sup>i</sup> | 1.533 (10) |
| C2—C3                   | 1.381 (11)  | C9—C11             | 1.535 (14) |
| C2—H2A                  | 0.9500      | C10—H10A           | 0.9800     |
| C3—C4                   | 1.381 (11)  | C10—H10B           | 0.9800     |
| C4—C5                   | 1.398 (11)  | C11—H11A           | 0.9800     |
| C4—H4A                  | 0.9500      | C11—H11B           | 0.9801     |
| N1—Cu1—N1 <sup>i</sup>  | 94.8 (4)    | C5—C6—C7           | 117.3 (7)  |
| N1—Cu1—I1               | 132.24 (18) | N1—C7—C6           | 125.7 (7)  |
| N1 <sup>i</sup> —Cu1—I1 | 132.24 (18) | N1—C7—H7A          | 117.1      |
| C7—N1—C8                | 117.4 (6)   | C6—C7—H7A          | 117.1      |
| C7—N1—Cu1               | 133.8 (5)   | N1—C8—C9           | 114.9 (7)  |
| C8—N1—Cu1               | 108.5 (5)   | N1—C8—H8A          | 108.5      |
| C2—C1—C6                | 122.3 (8)   | C9—C8—H8A          | 108.5      |
| C2—C1—H1A               | 118.9       | N1—C8—H8B          | 108.5      |

|                            |            |                          |            |
|----------------------------|------------|--------------------------|------------|
| C6—C1—H1A                  | 118.9      | C9—C8—H8B                | 108.5      |
| C1—C2—C3                   | 118.3 (7)  | H8A—C8—H8B               | 107.5      |
| C1—C2—H2A                  | 120.9      | C10—C9—C8 <sup>i</sup>   | 110.7 (6)  |
| C3—C2—H2A                  | 120.9      | C10—C9—C8                | 110.7 (6)  |
| C4—C3—C2                   | 121.4 (7)  | C8 <sup>i</sup> —C9—C8   | 111.7 (9)  |
| C4—C3—Br1                  | 118.7 (6)  | C10—C9—C11               | 109.3 (9)  |
| C2—C3—Br1                  | 119.8 (6)  | C8 <sup>i</sup> —C9—C11  | 107.1 (6)  |
| C3—C4—C5                   | 119.2 (8)  | C8—C9—C11                | 107.1 (6)  |
| C3—C4—H4A                  | 120.4      | C9—C10—H10A              | 108.7      |
| C5—C4—H4A                  | 120.4      | C9—C10—H10B              | 109.8      |
| C6—C5—C4                   | 119.8 (7)  | H10A—C10—H10B            | 109.5      |
| C6—C5—H5A                  | 120.1      | C9—C11—H11A              | 108.6      |
| C4—C5—H5A                  | 120.1      | C9—C11—H11B              | 109.9      |
| C1—C6—C5                   | 118.9 (7)  | H11A—C11—H11B            | 109.5      |
| C1—C6—C7                   | 123.8 (7)  |                          |            |
|                            |            |                          |            |
| N1 <sup>i</sup> —Cu1—N1—C7 | -119.0 (7) | C4—C5—C6—C1              | -1.9 (11)  |
| I1—Cu1—N1—C7               | 70.2 (8)   | C4—C5—C6—C7              | 178.0 (7)  |
| N1 <sup>i</sup> —Cu1—N1—C8 | 54.2 (5)   | C8—N1—C7—C6              | -177.4 (7) |
| I1—Cu1—N1—C8               | -116.5 (4) | Cu1—N1—C7—C6             | -4.5 (12)  |
| C6—C1—C2—C3                | 0.8 (12)   | C1—C6—C7—N1              | -0.3 (12)  |
| C1—C2—C3—C4                | -2.2 (12)  | C5—C6—C7—N1              | 179.8 (7)  |
| C1—C2—C3—Br1               | 175.9 (6)  | C7—N1—C8—C9              | 109.6 (8)  |
| C2—C3—C4—C5                | 1.6 (13)   | Cu1—N1—C8—C9             | -64.9 (7)  |
| Br1—C3—C4—C5               | -176.6 (6) | N1—C8—C9—C10             | -57.8 (9)  |
| C3—C4—C5—C6                | 0.5 (12)   | N1—C8—C9—C8 <sup>i</sup> | 66.0 (10)  |
| C2—C1—C6—C5                | 1.3 (12)   | N1—C8—C9—C11             | -176.9 (7) |
| C2—C1—C6—C7                | -178.6 (7) |                          |            |

Symmetry code: (i)  $x, -y+1, z$ .

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

| $D-H\cdots A$                           | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-------|-------------|-------------|---------------|
| C8—H8A <sup>ii</sup> ⋯Cg1 <sup>ii</sup> | 0.99  | 2.83        | 3.631 (9)   | 138           |

Symmetry code: (ii)  $-x+1/2, -y+1/2, -z$ .