



Synthesis, crystal structure and Hirshfeld surface analysis of di- μ_2 -iodido-bis[(2,2'-biquinoline- κ^2N,N')copper(I)]

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Keywords: crystal structure; Hirshfeld surface analysis; π - π stacking; biquinoline; copper complex.

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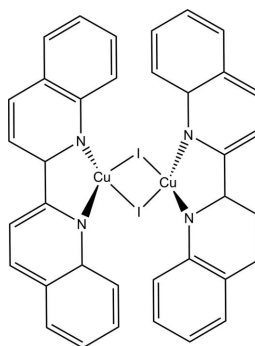
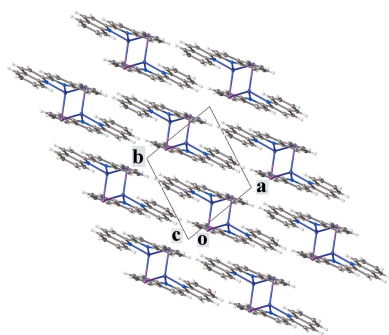
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The molecular and crystal structures of the title compound, [Cu₂I₂(C₁₈H₁₂N₂)₂], were examined by single-crystal X-ray diffraction and Hirshfeld surface analysis. The Cu atom is coordinated in a distorted tetrahedral geometry by two N atoms from the 2,2'-biquinoline ligands and the two μ_2 -bridging iodide ligands. The molecules are in contact *via* π - π -stacking interactions. Hirshfeld surface analysis showed that the most important contributions to the intermolecular interactions are H···H (39.7%), H···I/I···H (17.8%), C···H/H···C (17.5%), C···C (16.5%), N···C/C···N (3.9%) and N···H/H···N (3.5%).

1. Chemical context

Metal complexes with N-heterocyclic ligands find wide applications in various fields such as catalysis and medicine, among others (Delgado-Rebollo *et al.*, 2019; Novikov *et al.*, 2021; Fong, 2016; Artemjev *et al.*, 2022). Copper(I) bipyridine complexes are of interest because of their structural peculiarities, cuprophilic interactions, and important photochemical properties. Therefore, bipyridine-type systems are often the ligands of choice to explore new metal complexes with potentially useful properties (Ferraro *et al.*, 2022; Starosta *et al.*, 2012; Vatsadze *et al.*, 2010). 2,2'-Biquinoline is an important and widely employed diimine ligand. The geometry of the resulting metal derivatives depends on the ligand and counterion, the metal:ligand ratio and the solvent and synthetic conditions. Here we report the preparation and structural characterization of a copper iodide complex with 2,2'-biquinoline. We used Hirshfeld surface analysis to estimate the contribution of non-covalent interactions to the crystal structure.



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Table 1
 Selected geometric parameters (Å, °).

I1—Cu1	2.5734 (2)	Cu1—N2	2.0900 (14)
I1—Cu1 ⁱ	2.6487 (2)	Cu1—N1	2.0930 (13)
Cu1—I1—Cu1 ⁱ	68.829 (8)	N2—Cu1—I1 ⁱ	110.91 (4)
N2—Cu1—N1	79.28 (5)	N1—Cu1—I1 ⁱ	106.99 (4)
N2—Cu1—I1	122.14 (4)	I1—Cu1—I1 ⁱ	111.171 (8)
N1—Cu1—I1	122.34 (4)		

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

2. Structural commentary

The title compound crystallizes in the centrosymmetric space group $P\bar{1}$ with one crystallographically independent molecule in the unit cell. The molecular structure is illustrated in Fig. 1. The Cu atom is coordinated in a distorted tetrahedral geometry (Table 1) by two nitrogen atoms from the 2,2'-biquinoline ligands and the two μ_2 -bridged iodide ligands. The Cu1—I1 and Cu1ⁱ—I1 distances [symmetry code: (i) $-x + 1, -y, -z + 1$] are 2.5734 (2) and 2.6487 (2) Å, which are close to the distances in similar compounds (Sun *et al.*, 2013; Starosta *et al.*, 2012) with a substituted quinoline ligand. The Cu—N distances of 2.0930 (13) and 2.0900 (14) Å are almost equal within standard uncertainty.

The quinoline fragments in the biquinoline ligand adopt, as expected, a planar geometry. The maximum and minimum deviations of the atoms from these planes are between -0.018 (2) and 0.026 (2) Å. The angle between the quinolines described by rings 1/2 (as defined in Fig. 1) is 5.08 (9)° and between 3/4 is 0.59 (8)°. Then, the quinoline formed by rings 1 and 2 (ring 5) makes an angle of 7.56 (5)° with the quinoline described by rings 3/4 (ring 6).

3. Supramolecular features

The crystal packing is shown in Fig. 2, viewed down the *c* axis. Molecules both within the layers and between them are

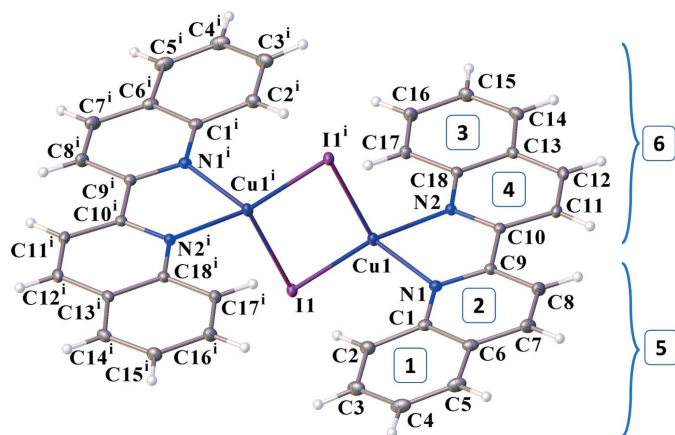


Figure 1
 Molecular structure of the title compound, including atom and ring labelling. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $-x + 1, -y, -z + 1$.]

connected by π - π -stacking interactions between six-membered rings of the quinoline rings. The π - π -stacking interaction parameters are presented in Table 2. Ring 4, defined by N2/C18/C10—C13 in Fig. 1, participates in the shortest interactions. The contact with another ring 4, related by the symmetry operation $-x, -y + 1, -z + 1$, is perhaps the most efficient, based on the distance, the angle between the planes, and the shift between ring centroids.

4. Database survey

A search in the Cambridge Structural Database (CSD, Version 5.43, update of 2022; Groom *et al.*, 2016) showed only a few hits for bis[(μ_2 -halogen)-2,2'-biquinoline-di-copper(I)]. We only found data for compounds with substituted quinoline rings in position-4 with carboxylate fragments. All compounds crystallize in the triclinic space group $P\bar{1}$. In IRIVIP (Vatsadze *et al.*, 2010), *n*-hexyl carboxylate groups are attached to the quinoline rings at position 4. In YIJFAA, YIJFEE, and YIJFII (Sun *et al.*, 2013), ethyl carboxylate fragments are attached, and in PAYKIL (Starosta *et al.*, 2012), there are methyl carboxylate fragments. In IRIVIP and YIJFAA, instead of the iodine atom, as in the title structure, there are chlorine atoms; in YIJFEE, there are bromine atoms. In other structures, the copper atoms are bonded through iodine atoms.

5. Hirshfeld surface analysis

Crystal Explorer21 was used to calculate the Hirshfeld surfaces and two-dimensional fingerprint plots (Spackman *et al.*, 2021). The donor-acceptor groups are visualized using a standard (high) surface resolution and d_{norm} surfaces are mapped over a fixed colour scale from -0.0579 (red) to 1.3919 (blue) a.u., as illustrated in Fig. 3(a). Red spots on the surface

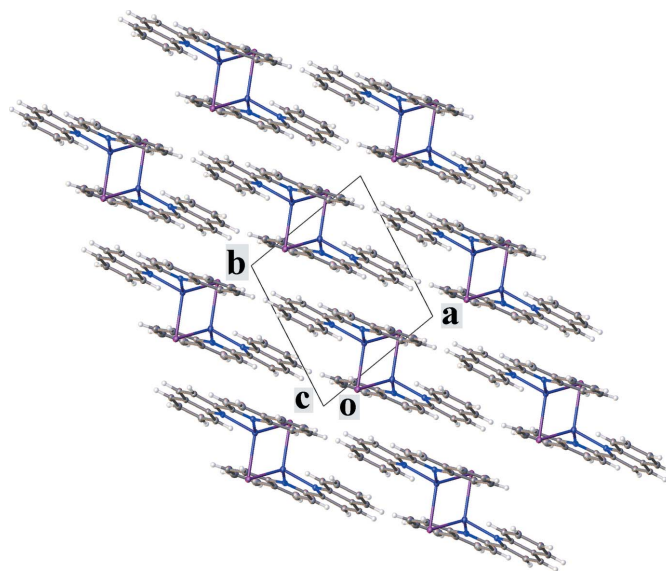


Figure 2
 View along the *c* axis of the crystal packing of the title compound, showing the stacking of layers formed by the Cu complex.

Table 2

π - π -stacking interaction parameters (\AA , $^\circ$).

Ring 1	Ring No.	Ring 2	Ring No.	Angle	Centroid-centroid distance	Shift distance between ring centroids
C1-C6	1	C1-C6($-x + 1, -y, -z + 2$)	1	0.000	3.874	1.459
C13-C18	3	N1/C1/C6-C9($-x + 1, -y + 1, -z + 1$)	2	4.772	3.711	1.480
		N2/C18/C10-C13($-x, -y + 1, -z + 1$)	4	0.590	3.665	1.602
N1/C1/C6-C9	2	N2/C18/C10-C13($-x + 1, -y + 1, -z + 1$)	4	5.301	3.564	1.139
		C13-C18($-x + 1, -y + 1, -z + 1$)	3	4.772	3.711	1.283
N2/C18/C10-C13	4	N2/C18/C10-C13($-x, -y + 1, -z + 1$)	4	0.000	3.652	1.555
		C13-C18($-x, -y + 1, -z + 1$)	3	0.590	3.665	1.579
		N1/C1/C6-C9($-x + 1, -y + 1, -z + 1$)	2	5.301	3.564	1.068

correspond to $C \cdots C$ and $I \cdots H$ interactions. The presence of π -stacking interactions is confirmed by the characteristic red and blue triangles on the shape-index surface [Fig. 3(b)]. Fingerprint plots of the most important non-covalent interactions for the title compound are shown in Fig. 4. The largest contribution to the crystal packing is made by contacts of the $H \cdots H$ type (39.7%). Then contacts of the $H \cdots I/I \cdots H$ and $C \cdots H/H \cdots C$ types make approximately equal contributions (17.8 and 17.5%, respectively). $C \cdots C$ interactions responsible for π -stacking contribute 16.5%. Contacts that contribute less than 1% are not shown in Fig. 4.

6. Synthesis and crystallization

The title compound was prepared by refluxing CuI with one equivalent of 2,2'-biquinoline in ethanol for 24 h. The compound precipitates as a purple solid in 87% yield. Found (%): C, 48.39; H, 2.71; N, 6.27. for $C_{36}H_{24}Cu_2I_2N_4$. Calculated (%): C, 48.61; H, 2.64; N, 6.19.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. C-bound H atoms were placed at calculated positions ($C-H = 0.95 \text{ \AA}$) and refined using a riding model with [$U_{iso}(H) = 1.2U_{eq}(C)$].

Acknowledgements

Authors contributions are as follows: Conceptualization, AWT, AGT and TAL; methodology, APN, AGT; validation: AWT, AGT; formal analysis: APN, AGT, TAL; investigation: AWT, AGT and TAL; resources, AGT, TAL; data curation, APN, EKK; writing (original draft), AWT; writing (review and

editing), APN, AGT, TAL; visualization, AWT, TAL; supervision, AWT, AGT; project administration, AGT; funding acquisition, AGT, TAL.

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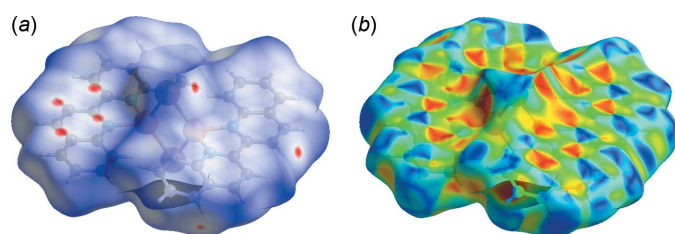


Figure 3

Hirshfeld surface mapped over (a) d_{norm} and (b) shape-index to visualize the interactions in the title compound.

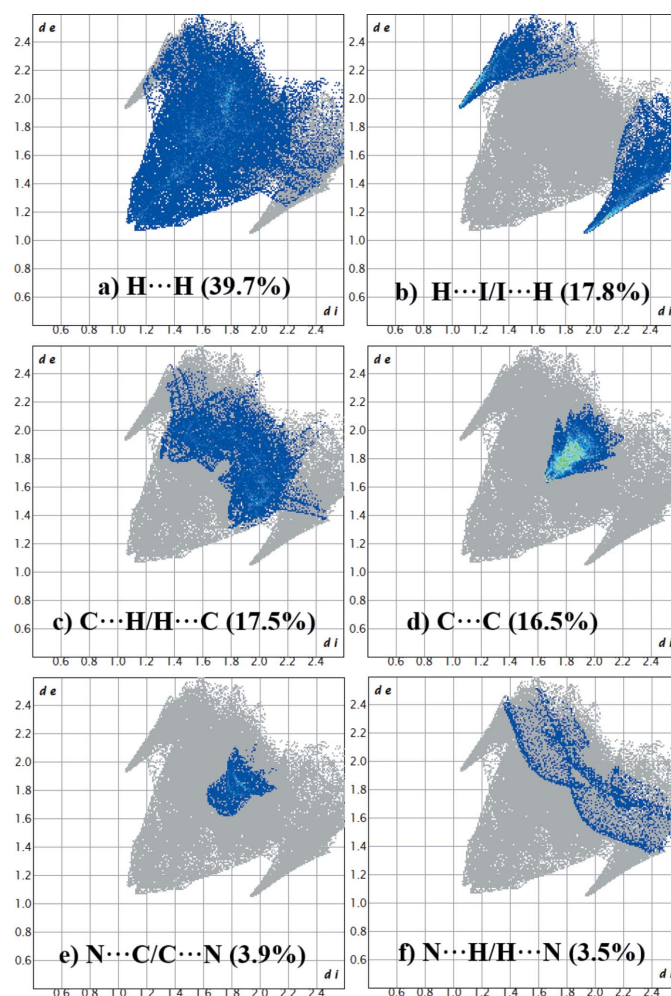


Figure 4

Two-dimensional fingerprint plots for the title compound divided into $H \cdots H$ (39.7%), $H \cdots I/I \cdots H$ (17.8%), $C \cdots H/H \cdots C$ (17.5%), $C \cdots C$ (16.5%), $N \cdots C/C \cdots N$ (3.9%) and $N \cdots H/H \cdots N$ (3.5%) interactions.

Table 3

Experimental details.

Crystal data	
Chemical formula	[Cu ₂ I ₂ (C ₁₈ H ₁₂ N ₂) ₂]
<i>M</i> _r	893.49
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.2032 (2), 9.4084 (3), 10.8312 (3)
α , β , γ (°)	70.9328 (8), 76.1237 (9), 74.2486 (9)
<i>V</i> (Å ³)	749.84 (4)
<i>Z</i>	1
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	3.51
Crystal size (mm)	0.12 × 0.10 × 0.06
Data collection	
Diffraction	Bruker D8 QUEST PHOTON-III CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.656, 0.798
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	22231, 5464, 4875
<i>R</i> _{int}	0.030
(sin θ/λ) _{max} (Å ⁻¹)	0.759
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.021, 0.050, 1.07
No. of reflections	5464
No. of parameters	200
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.93, -1.00

Computer programs: *APEX3* (Bruker, 2018), *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *SHELXTL* (Sheldrick, 2008).

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Synthesis, crystal structure and Hirshfeld surface analysis of di- μ_2 -iodido-bis-[(2,2'-biquinoline- κ^2N,N')copper(I)]

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Computing details

Data collection: *APEX3* (Bruker, 2018); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Di- μ_2 -iodido-bis[(2,2'-biquinoline- κ^2N,N')copper(I)]

Crystal data

[Cu₂I₂(C₁₈H₁₂N₂)₂]

$M_r = 893.49$

Triclinic, $P\bar{1}$

$a = 8.2032$ (2) Å

$b = 9.4084$ (3) Å

$c = 10.8312$ (3) Å

$\alpha = 70.9328$ (8)°

$\beta = 76.1237$ (9)°

$\gamma = 74.2486$ (9)°

$V = 749.84$ (4) Å³

$Z = 1$

$F(000) = 432$

$D_x = 1.979$ Mg m⁻³

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

Cell parameters from 9951 reflections

$\theta = 2.3$ – 32.6 °

$\mu = 3.51$ mm⁻¹

$T = 100$ K

Plate, red

$0.12 \times 0.10 \times 0.06$ mm

Data collection

Bruker D8 QUEST PHOTON-III CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.656$, $T_{\max} = 0.798$

22231 measured reflections

5464 independent reflections

4875 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 32.6$ °, $\theta_{\min} = 2.3$ °

$h = -12 \rightarrow 12$

$k = -14 \rightarrow 14$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.021$

$wR(F^2) = 0.050$

$S = 1.07$

5464 reflections

200 parameters

0 restraints

Primary atom site location: difference Fourier
map

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0241P)^2 + 0.2045P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.93 \text{ e } \text{Å}^{-3}$

$$\Delta\rho_{\min} = -1.00 \text{ e } \text{Å}^{-3}$$

Extinction correction: SHELXL,
 $Fc^* = kFc[1 + 0.001x\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00061 (6)

Special details

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
II	0.72676 (2)	0.05497 (2)	0.36228 (2)	0.01463 (4)
Cu1	0.47151 (3)	0.14895 (2)	0.52815 (2)	0.01482 (5)
N1	0.50362 (17)	0.22489 (16)	0.68043 (14)	0.0137 (2)
N2	0.32363 (17)	0.37275 (15)	0.48351 (13)	0.0126 (2)
C1	0.5986 (2)	0.14322 (19)	0.77875 (16)	0.0149 (3)
C2	0.7206 (2)	0.0086 (2)	0.76410 (18)	0.0188 (3)
H2	0.7335	-0.0253	0.6881	0.023*
C3	0.8205 (2)	-0.0730 (2)	0.86007 (19)	0.0225 (3)
H3	0.9050	-0.1616	0.8486	0.027*
C4	0.7991 (3)	-0.0268 (2)	0.97589 (19)	0.0235 (4)
H4	0.8658	-0.0869	1.0430	0.028*
C5	0.6831 (2)	0.1034 (2)	0.99178 (18)	0.0221 (3)
H5	0.6688	0.1333	1.0701	0.027*
C6	0.5837 (2)	0.1942 (2)	0.89164 (16)	0.0168 (3)
C7	0.4734 (2)	0.3365 (2)	0.89624 (17)	0.0204 (3)
H7	0.4603	0.3741	0.9702	0.024*
C8	0.3849 (2)	0.4209 (2)	0.79434 (17)	0.0186 (3)
H8	0.3134	0.5187	0.7954	0.022*
C9	0.4017 (2)	0.35984 (18)	0.68682 (16)	0.0134 (3)
C10	0.30656 (19)	0.44564 (18)	0.57445 (16)	0.0130 (3)
C11	0.2064 (2)	0.59515 (18)	0.56565 (17)	0.0151 (3)
H11	0.1989	0.6436	0.6318	0.018*
C12	0.1199 (2)	0.67017 (18)	0.46130 (17)	0.0161 (3)
H12	0.0505	0.7703	0.4552	0.019*
C13	0.1348 (2)	0.59756 (18)	0.36296 (16)	0.0135 (3)
C14	0.0488 (2)	0.6683 (2)	0.25249 (17)	0.0171 (3)
H14	-0.0225	0.7681	0.2431	0.021*
C15	0.0680 (2)	0.5933 (2)	0.15911 (17)	0.0183 (3)
H15	0.0103	0.6413	0.0850	0.022*
C16	0.1738 (2)	0.4440 (2)	0.17292 (17)	0.0181 (3)
H16	0.1868	0.3931	0.1074	0.022*
C17	0.2579 (2)	0.37192 (19)	0.27946 (17)	0.0162 (3)
H17	0.3279	0.2717	0.2876	0.019*
C18	0.23990 (19)	0.44731 (18)	0.37738 (16)	0.0129 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
II	0.01422 (5)	0.01364 (5)	0.01633 (6)	-0.00129 (3)	-0.00081 (3)	-0.00714 (4)
Cu1	0.01437 (9)	0.01477 (9)	0.01559 (10)	0.00062 (7)	-0.00375 (7)	-0.00671 (7)
N1	0.0120 (6)	0.0154 (6)	0.0140 (6)	-0.0033 (5)	-0.0023 (5)	-0.0041 (5)
N2	0.0117 (5)	0.0134 (6)	0.0131 (6)	-0.0013 (5)	-0.0023 (4)	-0.0049 (5)
C1	0.0130 (7)	0.0179 (7)	0.0145 (7)	-0.0057 (6)	-0.0020 (5)	-0.0035 (6)
C2	0.0187 (8)	0.0184 (7)	0.0188 (8)	-0.0028 (6)	-0.0069 (6)	-0.0028 (6)
C3	0.0211 (8)	0.0196 (8)	0.0249 (9)	-0.0041 (7)	-0.0097 (7)	0.0003 (7)
C4	0.0250 (9)	0.0243 (9)	0.0207 (8)	-0.0102 (7)	-0.0117 (7)	0.0042 (7)
C5	0.0252 (9)	0.0282 (9)	0.0150 (7)	-0.0111 (7)	-0.0076 (6)	-0.0013 (7)
C6	0.0149 (7)	0.0234 (8)	0.0133 (7)	-0.0081 (6)	-0.0018 (5)	-0.0036 (6)
C7	0.0183 (8)	0.0309 (9)	0.0160 (8)	-0.0060 (7)	-0.0015 (6)	-0.0121 (7)
C8	0.0170 (7)	0.0244 (8)	0.0175 (8)	-0.0024 (6)	-0.0030 (6)	-0.0113 (7)
C9	0.0113 (6)	0.0162 (7)	0.0138 (7)	-0.0027 (5)	-0.0015 (5)	-0.0059 (6)
C10	0.0103 (6)	0.0148 (6)	0.0145 (7)	-0.0032 (5)	-0.0009 (5)	-0.0053 (5)
C11	0.0147 (7)	0.0140 (6)	0.0186 (7)	-0.0033 (5)	-0.0016 (5)	-0.0077 (6)
C12	0.0152 (7)	0.0118 (6)	0.0206 (8)	-0.0023 (5)	-0.0009 (6)	-0.0055 (6)
C13	0.0116 (6)	0.0118 (6)	0.0159 (7)	-0.0019 (5)	-0.0022 (5)	-0.0026 (5)
C14	0.0137 (7)	0.0162 (7)	0.0181 (8)	-0.0016 (6)	-0.0033 (6)	-0.0012 (6)
C15	0.0175 (7)	0.0188 (7)	0.0166 (7)	-0.0013 (6)	-0.0058 (6)	-0.0023 (6)
C16	0.0175 (7)	0.0212 (8)	0.0164 (7)	-0.0011 (6)	-0.0043 (6)	-0.0077 (6)
C17	0.0152 (7)	0.0162 (7)	0.0180 (7)	-0.0006 (6)	-0.0036 (6)	-0.0072 (6)
C18	0.0104 (6)	0.0135 (6)	0.0145 (7)	-0.0021 (5)	-0.0016 (5)	-0.0041 (5)

Geometric parameters (Å, °)

II—Cu1	2.5734 (2)	C7—C8	1.369 (3)
II—Cu1 ⁱ	2.6487 (2)	C7—H7	0.9500
Cu1—N2	2.0900 (14)	C8—C9	1.422 (2)
Cu1—N1	2.0930 (13)	C8—H8	0.9500
Cu1—II ⁱ	2.6487 (2)	C9—C10	1.488 (2)
Cu1—Cu1 ⁱ	2.9520 (4)	C10—C11	1.409 (2)
N1—C9	1.330 (2)	C11—C12	1.367 (2)
N1—C1	1.367 (2)	C11—H11	0.9500
N2—C10	1.3354 (19)	C12—C13	1.409 (2)
N2—C18	1.369 (2)	C12—H12	0.9500
C1—C2	1.414 (2)	C13—C14	1.415 (2)
C1—C6	1.421 (2)	C13—C18	1.423 (2)
C2—C3	1.374 (2)	C14—C15	1.369 (2)
C2—H2	0.9500	C14—H14	0.9500
C3—C4	1.415 (3)	C15—C16	1.418 (2)
C3—H3	0.9500	C15—H15	0.9500
C4—C5	1.365 (3)	C16—C17	1.372 (2)
C4—H4	0.9500	C16—H16	0.9500
C5—C6	1.418 (2)	C17—C18	1.418 (2)
C5—H5	0.9500	C17—H17	0.9500

C6—C7	1.406 (3)		
Cu1—I1—Cu1 ⁱ	68.829 (8)	C8—C7—H7	119.9
N2—Cu1—N1	79.28 (5)	C6—C7—H7	119.9
N2—Cu1—I1	122.14 (4)	C7—C8—C9	118.99 (16)
N1—Cu1—I1	122.34 (4)	C7—C8—H8	120.5
N2—Cu1—I1 ⁱ	110.91 (4)	C9—C8—H8	120.5
N1—Cu1—I1 ⁱ	106.99 (4)	N1—C9—C8	122.17 (15)
I1—Cu1—I1 ⁱ	111.171 (8)	N1—C9—C10	116.58 (13)
N2—Cu1—Cu1 ⁱ	141.62 (4)	C8—C9—C10	121.24 (15)
N1—Cu1—Cu1 ⁱ	136.76 (4)	N2—C10—C11	122.82 (15)
I1—Cu1—Cu1 ⁱ	56.791 (7)	N2—C10—C9	115.92 (14)
I1 ⁱ —Cu1—Cu1 ⁱ	54.380 (7)	C11—C10—C9	121.26 (14)
C9—N1—C1	119.18 (14)	C12—C11—C10	119.63 (14)
C9—N1—Cu1	113.35 (11)	C12—C11—H11	120.2
C1—N1—Cu1	126.92 (11)	C10—C11—H11	120.2
C10—N2—C18	118.23 (14)	C11—C12—C13	119.38 (15)
C10—N2—Cu1	113.89 (11)	C11—C12—H12	120.3
C18—N2—Cu1	127.82 (10)	C13—C12—H12	120.3
N1—C1—C2	118.85 (15)	C12—C13—C14	122.40 (15)
N1—C1—C6	121.75 (15)	C12—C13—C18	117.93 (15)
C2—C1—C6	119.33 (16)	C14—C13—C18	119.67 (14)
C3—C2—C1	119.82 (17)	C15—C14—C13	120.22 (16)
C3—C2—H2	120.1	C15—C14—H14	119.9
C1—C2—H2	120.1	C13—C14—H14	119.9
C2—C3—C4	120.78 (18)	C14—C15—C16	120.11 (16)
C2—C3—H3	119.6	C14—C15—H15	119.9
C4—C3—H3	119.6	C16—C15—H15	119.9
C5—C4—C3	120.43 (17)	C17—C16—C15	121.04 (15)
C5—C4—H4	119.8	C17—C16—H16	119.5
C3—C4—H4	119.8	C15—C16—H16	119.5
C4—C5—C6	120.13 (17)	C16—C17—C18	119.85 (15)
C4—C5—H5	119.9	C16—C17—H17	120.1
C6—C5—H5	119.9	C18—C17—H17	120.1
C7—C6—C5	122.99 (16)	N2—C18—C17	118.90 (14)
C7—C6—C1	117.63 (16)	N2—C18—C13	122.00 (14)
C5—C6—C1	119.34 (17)	C17—C18—C13	119.10 (15)
C8—C7—C6	120.15 (15)		
C9—N1—C1—C2	-173.05 (15)	C18—N2—C10—C9	-179.42 (13)
Cu1—N1—C1—C2	16.1 (2)	Cu1—N2—C10—C9	3.07 (17)
C9—N1—C1—C6	3.8 (2)	N1—C9—C10—N2	4.8 (2)
Cu1—N1—C1—C6	-166.98 (11)	C8—C9—C10—N2	-175.83 (14)
N1—C1—C2—C3	178.35 (16)	N1—C9—C10—C11	-174.64 (14)
C6—C1—C2—C3	1.4 (3)	C8—C9—C10—C11	4.7 (2)
C1—C2—C3—C4	2.0 (3)	N2—C10—C11—C12	0.9 (2)
C2—C3—C4—C5	-2.6 (3)	C9—C10—C11—C12	-179.63 (15)
C3—C4—C5—C6	-0.4 (3)	C10—C11—C12—C13	-1.0 (2)

C4—C5—C6—C7	-174.13 (17)	C11—C12—C13—C14	179.90 (16)
C4—C5—C6—C1	3.8 (3)	C11—C12—C13—C18	0.2 (2)
N1—C1—C6—C7	-3.1 (2)	C12—C13—C14—C15	179.67 (15)
C2—C1—C6—C7	173.76 (16)	C18—C13—C14—C15	-0.7 (2)
N1—C1—C6—C5	178.82 (15)	C13—C14—C15—C16	0.2 (3)
C2—C1—C6—C5	-4.3 (2)	C14—C15—C16—C17	0.3 (3)
C5—C6—C7—C8	177.99 (17)	C15—C16—C17—C18	-0.3 (3)
C1—C6—C7—C8	0.0 (2)	C10—N2—C18—C17	179.51 (14)
C6—C7—C8—C9	2.2 (3)	Cu1—N2—C18—C17	-3.4 (2)
C1—N1—C9—C8	-1.5 (2)	C10—N2—C18—C13	-0.9 (2)
Cu1—N1—C9—C8	170.55 (12)	Cu1—N2—C18—C13	176.23 (11)
C1—N1—C9—C10	177.85 (13)	C16—C17—C18—N2	179.42 (15)
Cu1—N1—C9—C10	-10.14 (17)	C16—C17—C18—C13	-0.2 (2)
C7—C8—C9—N1	-1.6 (3)	C12—C13—C18—N2	0.7 (2)
C7—C8—C9—C10	179.14 (15)	C14—C13—C18—N2	-178.92 (15)
C18—N2—C10—C11	0.1 (2)	C12—C13—C18—C17	-179.65 (15)
Cu1—N2—C10—C11	-177.45 (12)	C14—C13—C18—C17	0.7 (2)

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