

# Crystal structure of (acetonitrile- $\kappa N$ )iodido(2-(naphthalen-1-yl)-6-{1-[(2,4,6-trimethylphenyl)-imino]ethyl}pyridine- $\kappa^2 N, N'$ )copper(I)

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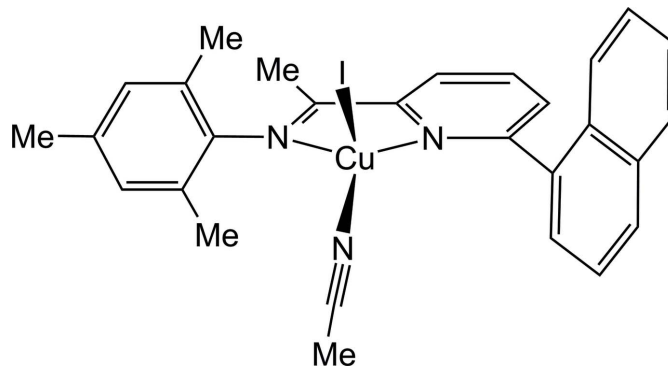
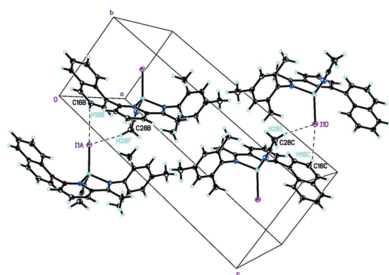
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UK.**Keywords:** crystal structure; copper(I) complex;  
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In the mononuclear title complex, [CuI(C<sub>2</sub>H<sub>3</sub>N)(C<sub>26</sub>H<sub>24</sub>N<sub>2</sub>)], the Cu<sup>I</sup> ion has a distorted tetrahedral coordination environment, defined by two N atoms of the chelating 2-(naphthalen-1-yl)-6-[(2,4,6-trimethylphenyl)imino]pyridine ligand, one N atom of an acetonitrile ligand and one iodide ligand. Within the complex, there are weak intramolecular C—H···N hydrogen bonds, while weak intermolecular C—H···I interactions between complex molecules, help to facilitate a three-dimensional network.

## 1. Chemical context

Coordination complexes of copper(I) halides bearing a variety of co-ligands have been of interest in coordination chemistry (Karahana *et al.*, 2015; Dennehy *et al.*, 2011; Oshio *et al.*, 1996; Seward *et al.*, 2003) due, in some measure, to their preparative accessibility, structural variability, magnetic properties (Oshio *et al.*, 1996) and their relevance to biological or medicinal applications (Corey *et al.*, 1987; Dias *et al.*, 2006). The role of copper(I) is evident in several biologically important reactions, such as a dioxygen carrier and models for several enzymes (Krupanidhi *et al.*, 2008). Elsewhere, these compounds have been reported to be luminescent (Aslanidis *et al.*, 2010; Gallego *et al.*, 2012) and exhibit corrosion inhibiting properties (Tian *et al.*, 2004). The structures of metal complexes bearing naphthyl-substituted *N,N*-pyridine-alkylamides were reported by Armitage *et al.* (2015) and related structures were presented by Wattanakanjana *et al.* (2014). Cotton *et al.* (1999) highlighted details of the affinity of nitrile ligands for Cu<sup>I</sup> ions. Within this context, we report herein the crystal structure of the title complex, [CuI(C<sub>2</sub>H<sub>3</sub>N)(C<sub>26</sub>H<sub>24</sub>N<sub>2</sub>)].



**Table 1**  
Hydrogen-bond geometry (Å, °).

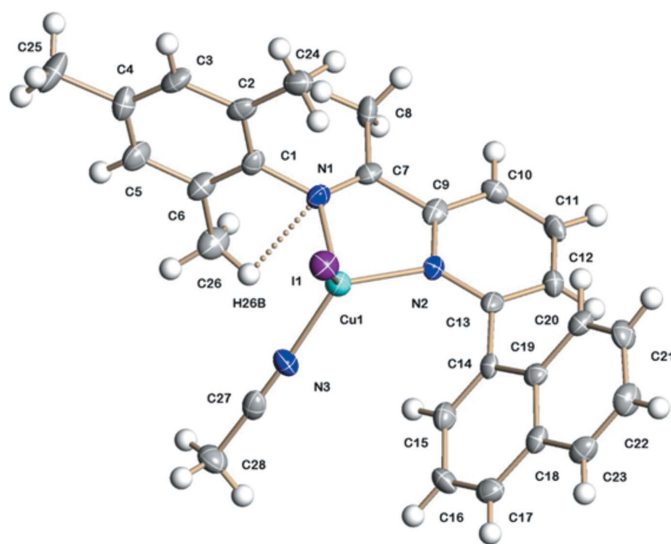
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C26-H26B\cdots N1$	0.98	2.52	2.891 (8)	102

## 2. Structural commentary

The molecular structure of the title complex is shown in Fig. 1. The  $Cu^I$  ion is coordinated by atoms N1 and N2 of the 2-(naphthalen-1-yl)-6-[(2,4,6-trimethylphenyl)imino]pyridine ligand, by atom N3 of an acetonitrile ligand and by an iodide anion (I1), leading to a distorted tetrahedral coordination environment. The two N atoms of the bidentate ligand chelate to  $Cu^I$  with similar  $Cu-N$  bond lengths [ $Cu1-N1 = 2.091$  (4),  $Cu1-N2 = 2.085$  (4) Å]. A comparable  $N,N'$ -binding has been observed in related structures with bis[2-(2-pyridyl)ethyl]amine ligands (Osako *et al.*, 2001). At 1.960 (5) Å, the  $Cu1-N3$  distance is significantly shorter than the  $Cu-N_{pyridine}$  and  $Cu-N_{imine}$  distances. The  $Cu1-I$  distance amounts to 2.5479 (9) Å. The  $N2-Cu1-N1$  bite angle of the chelating ligand is  $78.86$  ( $18$ )°, while the  $N3-Cu-I$  angle between the monodentate acetonitrile and iodide ligands is closer to tetrahedral,  $112.74$  ( $15$ )°. The naphthyl ring system is inclined by  $58.20$  ( $17$ )° to the central  $N=C(CH_3)$ -pyridine moiety, whereas the trimethylphenyl ring is almost perpendicular to the latter, at  $84.8$  ( $3$ )°. Within the complex, an intramolecular  $C-H\cdots N$  hydrogen-bonding interaction is present, stabilizing the molecular conformation (Table 1, Fig. 1).

## 3. Supramolecular features

In the crystal, weak  $C-H\cdots I$  contacts involving a phenyl H atom [ $C16-H16B\cdots I^i$ , 3.958 (6) Å,  $152$ °; symmetry code: (i)



**Figure 1**  
The molecular structure of the title complex, with displacement ellipsoids drawn at the 50% probability level. The  $C-H\cdots N$  hydrogen bond is shown as a dashed line.

$x, y - 1, z$ ] and a H atom of the acetonitrile methyl group [ $[C28-H28B\cdots I^i$ , 4.010 (6) Å,  $109$ °] link the complex molecules, forming a three-dimensional network (Fig. 2).

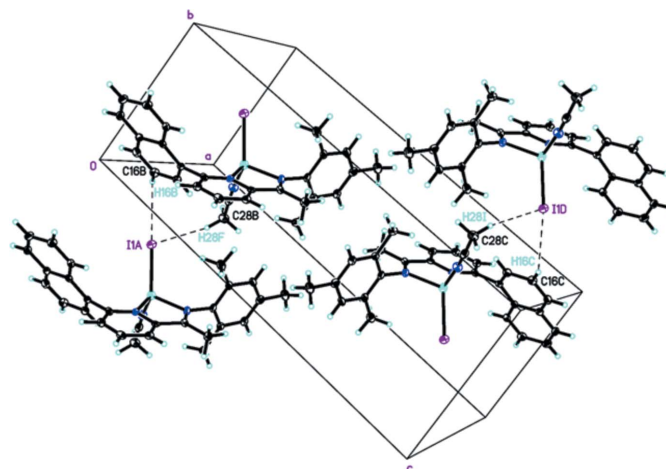
## 4. Synthesis and crystallization

All synthetic manipulations were performed under a nitrogen atmosphere, using standard Schlenk techniques. Solvents were distilled under nitrogen from appropriate drying agents and degassed prior to use (Armarego *et al.*, 1996). The 2-(naphthalen-1-yl)-6-[(2,4,6-trimethylphenyl)imino]pyridine ligand ( $L_{mes}$ ) was synthesized according to a modified literature procedure (Armitage *et al.*, 2015).

A solution of 0.0262 g of  $CuI$  (0.137 mmol) in 5 ml of acetonitrile was mixed with a solution of 0.05 g of  $L_{mes}$  (0.134 mmol) in 5 ml of acetonitrile. The mixture was stirred at room temperature for 24 h before evaporating the volatiles. The residue was extracted with *n*-hexane ( $5 \times 3$  ml). The extracts were combined and the solvent removed under reduced pressure to give a red solid which was recrystallized from acetonitrile solution. Yield: 54%. M.p.  $>253$  K (decomp).  $^1H$  NMR (400 MHz,  $CD_2Cl_2$ ):  $\delta$  1.88 [*s*, 6H, *ortho*-( $CH_3$ ) $_2$ ], 1.97 (*s*, 3H,  $N\equiv CCH_3$ ), 2.16 (*s*, 3H,  $N=CCH_3$ ), 2.20 [*s*, 3H, *para*-( $CH_3$ ) $_2$ ], 6.84 (*s*, 2H, Mes-H), 7.39 (*s*, 1H, Nap-H), 7.45 (*t*, *J* 7.8, 2H, Nap-H/Py-H), 7.51 (*s*, 1H, Py-H), 7.73 (*s*, 1H, Py-H), 7.81 (*s*, 2H, Nap-H), 7.87 (*d*, *J* 3.7, 2H, Nap-H), 8.04 (*s*, 1H, Nap-H). IR  $\nu_{max}$  (solid)/ $cm^{-1}$  1620 ( $C=N_{imine}$ ), 1555 ( $C=N_{py}$ ). ESI MS:  $m/z$  428 [ $M-I-MeCN$ ] $^+$ .

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were positioned geometrically, with  $C-H = 0.95$  Å and with  $U_{iso}(H) = 1.2U_{eq}(C)$  for H atoms on  $Csp^2$  and 0.98 Å with  $U_{iso}(H) = 1.5U_{eq}(C)$  for H atoms on  $Csp^3$ .



**Figure 2**  
Part of the crystal structure, showing intermolecular  $C-H\cdots I$  interactions (dashed lines).

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	[CuI(C <sub>2</sub> H <sub>3</sub> N)(C <sub>26</sub> H <sub>24</sub> N <sub>2</sub> )]
$M_r$	595.97
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
$a, b, c$ (Å)	14.689 (3), 8.0775 (15), 21.861 (4)
$\beta$ (°)	103.942 (3)
$V$ (Å <sup>3</sup> )	2517.4 (8)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	2.11
Crystal size (mm)	0.25 × 0.07 × 0.03
Data collection	
Diffractometer	Bruker APEX 2000 CCD area detector
Absorption correction	Multi-scan (SADABS; Bruker, 2001)
$T_{\min}, T_{\max}$	0.679, 0.862
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	19143, 4936, 2757
$R_{\text{int}}$	0.125
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.051, 0.085, 0.77
No. of reflections	4936
No. of parameters	303
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	1.13, -0.81

Computer programs: SMART and SAINT (Bruker, 2001), SHELXS97, SHELXL97 and SHELXTL (Sheldrick, 2008).

## Acknowledgements

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## supporting information

*Acta Cryst.* (2016). E72, 1845-1847 [https://doi.org/10.1107/S2056989016018685]

## Crystal structure of (acetonitrile- $\kappa$ N)iodido(2-(naphthalen-1-yl)-6-{1-[(2,4,6-trimethylphenyl)imino]ethyl}pyridine- $\kappa^2$ N,N'})copper(I)

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### Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

(Acetonitrile- $\kappa$ N)iodido(2-(naphthalen-1-yl)-6-{1-[(2,4,6-trimethylphenyl)imino]ethyl}pyridine- $\kappa^2$ N,N')copper(I)

### Crystal data

[CuI(C<sub>2</sub>H<sub>3</sub>N)(C<sub>26</sub>H<sub>24</sub>N<sub>2</sub>)]

$M_r = 595.97$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.689$  (3) Å

$b = 8.0775$  (15) Å

$c = 21.861$  (4) Å

$\beta = 103.942$  (3)°

$V = 2517.4$  (8) Å<sup>3</sup>

$Z = 4$

$F(000) = 1192$

$D_x = 1.572$  Mg m<sup>-3</sup>

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

Cell parameters from 639 reflections

$\theta = 2.9$ – $23.2$ °

$\mu = 2.11$  mm<sup>-1</sup>

$T = 150$  K

Needle, orange

$0.25 \times 0.07 \times 0.03$  mm

### Data collection

Bruker APEX 2000 CCD area detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.679$ ,  $T_{\max} = 0.862$

19143 measured reflections

4936 independent reflections

2757 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.125$

$\theta_{\max} = 26.0$ °,  $\theta_{\min} = 1.4$ °

$h = -18 \rightarrow 17$

$k = -9 \rightarrow 9$

$l = -26 \rightarrow 26$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.085$

$S = 0.77$

4936 reflections

303 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

$$w = 1/[\sigma^2(F_o^2) + (0.0178P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$

$$\Delta\rho_{\max} = 1.13 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.81 \text{ e } \text{\AA}^{-3}$$

### 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.

**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  $F^2 > 2\text{sigma}(F^2)$  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 ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.27041 (5)	0.46133 (9)	0.24724 (3)	0.0280 (2)
I1	0.27321 (3)	0.69329 (5)	0.16873 (2)	0.03325 (13)
N1	0.2948 (3)	0.5389 (6)	0.3410 (2)	0.0241 (12)
N2	0.1440 (3)	0.3972 (5)	0.2685 (2)	0.0196 (11)
N3	0.3532 (3)	0.2768 (6)	0.2390 (2)	0.0307 (13)
C1	0.3799 (4)	0.6189 (7)	0.3735 (3)	0.0241 (14)
C2	0.3847 (4)	0.7897 (8)	0.3723 (3)	0.0277 (15)
C3	0.4709 (4)	0.8651 (7)	0.3999 (3)	0.0309 (16)
H3	0.4755	0.9824	0.3996	0.037*
C4	0.5483 (4)	0.7737 (8)	0.4270 (3)	0.0322 (16)
C5	0.5416 (4)	0.6047 (8)	0.4277 (3)	0.0335 (16)
H5	0.5956	0.5412	0.4463	0.040*
C6	0.4569 (4)	0.5231 (7)	0.4015 (3)	0.0293 (15)
C7	0.2277 (4)	0.5153 (7)	0.3683 (3)	0.0245 (14)
C8	0.2289 (4)	0.5595 (7)	0.4358 (2)	0.0293 (15)
H8A	0.2892	0.6104	0.4560	0.044*
H8B	0.2200	0.4590	0.4588	0.044*
H8C	0.1781	0.6378	0.4363	0.044*
C9	0.1407 (4)	0.4362 (7)	0.3290 (3)	0.0237 (14)
C10	0.0617 (4)	0.4098 (7)	0.3511 (3)	0.0246 (14)
H10	0.0612	0.4389	0.3931	0.030*
C11	-0.0174 (4)	0.3404 (7)	0.3115 (3)	0.0260 (15)
H11	-0.0723	0.3197	0.3260	0.031*
C12	-0.0143 (4)	0.3028 (7)	0.2511 (3)	0.0249 (14)
H12	-0.0679	0.2569	0.2230	0.030*
C13	0.0668 (4)	0.3312 (7)	0.2308 (3)	0.0224 (14)
C14	0.0726 (4)	0.2803 (7)	0.1655 (3)	0.0193 (13)
C15	0.1401 (4)	0.1717 (7)	0.1593 (3)	0.0281 (15)
H15	0.1865	0.1391	0.1956	0.034*
C16	0.1429 (4)	0.1057 (7)	0.0993 (3)	0.0282 (15)
H16	0.1905	0.0295	0.0955	0.034*
C17	0.0766 (4)	0.1533 (7)	0.0478 (3)	0.0303 (16)

H17	0.0781	0.1087	0.0079	0.036*
C18	0.0056 (4)	0.2669 (7)	0.0517 (3)	0.0244 (15)
C19	0.0043 (4)	0.3361 (7)	0.1116 (3)	0.0224 (14)
C20	-0.0648 (4)	0.4581 (7)	0.1131 (3)	0.0266 (15)
H20	-0.0671	0.5070	0.1522	0.032*
C21	-0.1273 (4)	0.5060 (7)	0.0600 (3)	0.0305 (16)
H21	-0.1712	0.5906	0.0626	0.037*
C22	-0.1293 (4)	0.4334 (8)	0.0006 (3)	0.0337 (16)
H22	-0.1754	0.4644	-0.0361	0.040*
C23	-0.0625 (4)	0.3175 (7)	-0.0021 (3)	0.0294 (15)
H23	-0.0620	0.2693	-0.0417	0.035*
C24	0.3003 (4)	0.8937 (7)	0.3427 (3)	0.0347 (17)
H24A	0.2747	0.8572	0.2992	0.052*
H24B	0.3189	1.0102	0.3428	0.052*
H24C	0.2524	0.8811	0.3668	0.052*
C25	0.6418 (4)	0.8592 (8)	0.4547 (3)	0.051 (2)
H25A	0.6356	0.9314	0.4895	0.076*
H25B	0.6598	0.9255	0.4220	0.076*
H25C	0.6901	0.7755	0.4704	0.076*
C26	0.4524 (4)	0.3376 (7)	0.4039 (3)	0.0379 (17)
H26A	0.5139	0.2910	0.4037	0.057*
H26B	0.4055	0.2970	0.3672	0.057*
H26C	0.4347	0.3036	0.4426	0.057*
C27	0.4029 (4)	0.1710 (8)	0.2387 (3)	0.0284 (15)
C28	0.4682 (4)	0.0349 (7)	0.2396 (3)	0.0367 (17)
H28A	0.5068	0.0200	0.2825	0.055*
H28B	0.5088	0.0601	0.2112	0.055*
H28C	0.4330	-0.0670	0.2257	0.055*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0280 (4)	0.0304 (5)	0.0269 (4)	-0.0010 (4)	0.0089 (4)	-0.0029 (4)
I1	0.0350 (2)	0.0339 (3)	0.0303 (2)	0.0026 (2)	0.00674 (18)	0.0044 (2)
N1	0.024 (3)	0.027 (3)	0.021 (3)	-0.003 (2)	0.002 (2)	-0.003 (2)
N2	0.018 (3)	0.021 (3)	0.018 (3)	0.001 (2)	0.000 (2)	0.003 (2)
N3	0.025 (3)	0.033 (3)	0.037 (3)	0.004 (3)	0.012 (3)	-0.002 (3)
C1	0.022 (4)	0.032 (4)	0.017 (3)	-0.005 (3)	0.002 (3)	-0.002 (3)
C2	0.038 (4)	0.029 (4)	0.017 (3)	-0.007 (3)	0.009 (3)	-0.006 (3)
C3	0.040 (4)	0.025 (4)	0.028 (4)	-0.013 (3)	0.008 (3)	-0.006 (3)
C4	0.024 (4)	0.042 (5)	0.028 (4)	-0.008 (3)	0.001 (3)	0.007 (3)
C5	0.033 (4)	0.033 (4)	0.028 (4)	-0.004 (3)	-0.004 (3)	-0.001 (3)
C6	0.036 (4)	0.028 (4)	0.022 (4)	-0.009 (3)	0.003 (3)	0.002 (3)
C7	0.029 (4)	0.018 (3)	0.025 (4)	-0.003 (3)	0.005 (3)	-0.003 (3)
C8	0.018 (3)	0.039 (4)	0.030 (4)	-0.008 (3)	0.005 (3)	0.002 (3)
C9	0.027 (4)	0.015 (3)	0.027 (4)	-0.001 (3)	0.003 (3)	0.007 (3)
C10	0.029 (4)	0.024 (4)	0.024 (4)	0.004 (3)	0.012 (3)	0.002 (3)
C11	0.021 (3)	0.024 (4)	0.037 (4)	-0.001 (3)	0.016 (3)	0.002 (3)

C12	0.018 (3)	0.028 (4)	0.029 (4)	-0.001 (3)	0.006 (3)	0.001 (3)
C13	0.021 (3)	0.014 (3)	0.030 (4)	0.002 (3)	0.002 (3)	-0.002 (3)
C14	0.014 (3)	0.021 (3)	0.023 (3)	-0.005 (3)	0.004 (3)	0.003 (3)
C15	0.022 (3)	0.027 (4)	0.033 (4)	0.000 (3)	0.001 (3)	0.003 (3)
C16	0.026 (4)	0.029 (4)	0.034 (4)	0.005 (3)	0.014 (3)	0.000 (3)
C17	0.034 (4)	0.028 (4)	0.031 (4)	-0.006 (3)	0.011 (3)	-0.005 (3)
C18	0.021 (3)	0.025 (4)	0.026 (4)	-0.006 (3)	0.002 (3)	0.003 (3)
C19	0.024 (3)	0.018 (4)	0.025 (3)	-0.004 (3)	0.006 (3)	-0.001 (3)
C20	0.027 (4)	0.024 (4)	0.026 (4)	-0.007 (3)	0.003 (3)	-0.002 (3)
C21	0.023 (4)	0.029 (4)	0.038 (4)	0.007 (3)	0.004 (3)	0.004 (3)
C22	0.031 (4)	0.036 (4)	0.029 (4)	-0.001 (3)	-0.001 (3)	0.008 (3)
C23	0.034 (4)	0.034 (4)	0.020 (3)	-0.008 (3)	0.007 (3)	-0.001 (3)
C24	0.038 (4)	0.032 (4)	0.037 (4)	-0.004 (3)	0.014 (3)	-0.008 (3)
C25	0.041 (4)	0.047 (5)	0.054 (5)	-0.024 (4)	-0.008 (4)	0.001 (4)
C26	0.042 (4)	0.032 (4)	0.034 (4)	0.001 (3)	-0.002 (3)	0.007 (3)
C27	0.024 (4)	0.040 (4)	0.022 (3)	-0.006 (3)	0.006 (3)	0.000 (3)
C28	0.035 (4)	0.031 (4)	0.046 (4)	0.006 (3)	0.014 (3)	0.000 (3)

*Geometric parameters (Å, °)*

Cu1—N3	1.960 (5)	C13—C14	1.507 (7)
Cu1—N2	2.085 (4)	C14—C15	1.355 (7)
Cu1—N1	2.091 (4)	C14—C19	1.426 (7)
Cu1—I1	2.5479 (9)	C15—C16	1.427 (7)
N1—C7	1.282 (7)	C15—H15	0.9500
N1—C1	1.434 (6)	C16—C17	1.354 (7)
N2—C13	1.342 (6)	C16—H16	0.9500
N2—C9	1.372 (6)	C17—C18	1.408 (7)
N3—C27	1.125 (7)	C17—H17	0.9500
C1—C2	1.382 (7)	C18—C23	1.409 (7)
C1—C6	1.386 (7)	C18—C19	1.427 (7)
C2—C3	1.403 (7)	C19—C20	1.420 (7)
C2—C24	1.508 (7)	C20—C21	1.351 (7)
C3—C4	1.366 (8)	C20—H20	0.9500
C3—H3	0.9500	C21—C22	1.420 (8)
C4—C5	1.369 (8)	C21—H21	0.9500
C4—C25	1.527 (7)	C22—C23	1.368 (7)
C5—C6	1.402 (7)	C22—H22	0.9500
C5—H5	0.9500	C23—H23	0.9500
C6—C26	1.501 (7)	C24—H24A	0.9800
C7—C9	1.500 (7)	C24—H24B	0.9800
C7—C8	1.515 (7)	C24—H24C	0.9800
C8—H8A	0.9800	C25—H25A	0.9800
C8—H8B	0.9800	C25—H25B	0.9800
C8—H8C	0.9800	C25—H25C	0.9800
C9—C10	1.377 (7)	C26—H26A	0.9800
C10—C11	1.389 (7)	C26—H26B	0.9800
C10—H10	0.9500	C26—H26C	0.9800

C11—C12	1.364 (7)	C27—C28	1.456 (8)
C11—H11	0.9500	C28—H28A	0.9800
C12—C13	1.387 (7)	C28—H28B	0.9800
C12—H12	0.9500	C28—H28C	0.9800
N3—Cu1—N2	115.94 (19)	C15—C14—C19	120.5 (5)
N3—Cu1—N1	110.75 (19)	C15—C14—C13	118.8 (5)
N2—Cu1—N1	78.86 (18)	C19—C14—C13	120.5 (5)
N3—Cu1—I1	112.74 (15)	C14—C15—C16	121.2 (5)
N2—Cu1—I1	119.51 (12)	C14—C15—H15	119.4
N1—Cu1—I1	114.43 (13)	C16—C15—H15	119.4
C7—N1—C1	120.8 (5)	C17—C16—C15	118.9 (6)
C7—N1—Cu1	116.2 (4)	C17—C16—H16	120.5
C1—N1—Cu1	122.9 (4)	C15—C16—H16	120.5
C13—N2—C9	117.5 (5)	C16—C17—C18	122.0 (6)
C13—N2—Cu1	128.9 (4)	C16—C17—H17	119.0
C9—N2—Cu1	113.5 (4)	C18—C17—H17	119.0
C27—N3—Cu1	175.3 (5)	C17—C18—C23	121.7 (6)
C2—C1—C6	121.7 (6)	C17—C18—C19	119.0 (5)
C2—C1—N1	118.9 (5)	C23—C18—C19	119.2 (5)
C6—C1—N1	119.2 (5)	C20—C19—C14	124.3 (5)
C1—C2—C3	118.0 (6)	C20—C19—C18	117.5 (5)
C1—C2—C24	121.6 (5)	C14—C19—C18	118.2 (5)
C3—C2—C24	120.4 (6)	C21—C20—C19	121.4 (6)
C4—C3—C2	121.5 (6)	C21—C20—H20	119.3
C4—C3—H3	119.2	C19—C20—H20	119.3
C2—C3—H3	119.2	C20—C21—C22	121.8 (6)
C3—C4—C5	119.3 (6)	C20—C21—H21	119.1
C3—C4—C25	120.2 (6)	C22—C21—H21	119.1
C5—C4—C25	120.5 (6)	C23—C22—C21	117.8 (6)
C4—C5—C6	121.6 (6)	C23—C22—H22	121.1
C4—C5—H5	119.2	C21—C22—H22	121.1
C6—C5—H5	119.2	C22—C23—C18	122.3 (6)
C1—C6—C5	117.9 (6)	C22—C23—H23	118.8
C1—C6—C26	122.3 (6)	C18—C23—H23	118.8
C5—C6—C26	119.8 (6)	C2—C24—H24A	109.5
N1—C7—C9	116.2 (5)	C2—C24—H24B	109.5
N1—C7—C8	126.0 (5)	H24A—C24—H24B	109.5
C9—C7—C8	117.8 (5)	C2—C24—H24C	109.5
C7—C8—H8A	109.5	H24A—C24—H24C	109.5
C7—C8—H8B	109.5	H24B—C24—H24C	109.5
H8A—C8—H8B	109.5	C4—C25—H25A	109.5
C7—C8—H8C	109.5	C4—C25—H25B	109.5
H8A—C8—H8C	109.5	H25A—C25—H25B	109.5
H8B—C8—H8C	109.5	C4—C25—H25C	109.5
N2—C9—C10	122.0 (5)	H25A—C25—H25C	109.5
N2—C9—C7	115.2 (5)	H25B—C25—H25C	109.5
C10—C9—C7	122.7 (5)	C6—C26—H26A	109.5



C9—C10—C11	119.6 (5)	C6—C26—H26B	109.5
C9—C10—H10	120.2	H26A—C26—H26B	109.5
C11—C10—H10	120.2	C6—C26—H26C	109.5
C12—C11—C10	118.3 (5)	H26A—C26—H26C	109.5
C12—C11—H11	120.8	H26B—C26—H26C	109.5
C10—C11—H11	120.8	N3—C27—C28	178.7 (7)
C11—C12—C13	120.2 (5)	C27—C28—H28A	109.5
C11—C12—H12	119.9	C27—C28—H28B	109.5
C13—C12—H12	119.9	H28A—C28—H28B	109.5
N2—C13—C12	122.2 (5)	C27—C28—H28C	109.5
N2—C13—C14	117.2 (5)	H28A—C28—H28C	109.5
C12—C13—C14	120.5 (5)	H28B—C28—H28C	109.5
N3—Cu1—N1—C7	-113.7 (4)	N1—C7—C9—N2	0.5 (7)
N2—Cu1—N1—C7	0.1 (4)	C8—C7—C9—N2	-179.3 (5)
I1—Cu1—N1—C7	117.6 (4)	N1—C7—C9—C10	-177.1 (5)
N3—Cu1—N1—C1	68.3 (5)	C8—C7—C9—C10	3.0 (8)
N2—Cu1—N1—C1	-178.0 (5)	N2—C9—C10—C11	0.6 (8)
I1—Cu1—N1—C1	-60.5 (4)	C7—C9—C10—C11	178.1 (5)
N3—Cu1—N2—C13	-74.9 (5)	C9—C10—C11—C12	-1.0 (8)
N1—Cu1—N2—C13	177.3 (5)	C10—C11—C12—C13	1.0 (9)
I1—Cu1—N2—C13	65.3 (5)	C9—N2—C13—C12	0.2 (8)
N3—Cu1—N2—C9	108.0 (4)	Cu1—N2—C13—C12	-176.7 (4)
N1—Cu1—N2—C9	0.2 (4)	C9—N2—C13—C14	-176.8 (5)
I1—Cu1—N2—C9	-111.7 (3)	Cu1—N2—C13—C14	6.3 (7)
C7—N1—C1—C2	-86.8 (7)	C11—C12—C13—N2	-0.7 (9)
Cu1—N1—C1—C2	91.2 (6)	C11—C12—C13—C14	176.2 (5)
C7—N1—C1—C6	97.6 (7)	N2—C13—C14—C15	56.3 (7)
Cu1—N1—C1—C6	-84.4 (6)	C12—C13—C14—C15	-120.8 (6)
C6—C1—C2—C3	0.7 (9)	N2—C13—C14—C19	-128.1 (5)
N1—C1—C2—C3	-174.8 (5)	C12—C13—C14—C19	54.8 (8)
C6—C1—C2—C24	-179.1 (5)	C19—C14—C15—C16	-2.4 (8)
N1—C1—C2—C24	5.4 (8)	C13—C14—C15—C16	173.3 (5)
C1—C2—C3—C4	0.2 (9)	C14—C15—C16—C17	0.1 (9)
C24—C2—C3—C4	180.0 (5)	C15—C16—C17—C18	0.5 (9)
C2—C3—C4—C5	-0.3 (9)	C16—C17—C18—C23	179.2 (6)
C2—C3—C4—C25	178.0 (5)	C16—C17—C18—C19	1.1 (8)
C3—C4—C5—C6	-0.5 (10)	C15—C14—C19—C20	-175.4 (5)
C25—C4—C5—C6	-178.8 (5)	C13—C14—C19—C20	9.0 (8)
C2—C1—C6—C5	-1.4 (9)	C15—C14—C19—C18	3.9 (8)
N1—C1—C6—C5	174.1 (5)	C13—C14—C19—C18	-171.7 (5)
C2—C1—C6—C26	179.1 (5)	C17—C18—C19—C20	176.1 (5)
N1—C1—C6—C26	-5.4 (9)	C23—C18—C19—C20	-2.1 (8)
C4—C5—C6—C1	1.3 (9)	C17—C18—C19—C14	-3.2 (8)
C4—C5—C6—C26	-179.2 (6)	C23—C18—C19—C14	178.6 (5)
C1—N1—C7—C9	177.8 (5)	C14—C19—C20—C21	179.7 (5)
Cu1—N1—C7—C9	-0.3 (7)	C18—C19—C20—C21	0.5 (8)
C1—N1—C7—C8	-2.4 (9)	C19—C20—C21—C22	2.1 (9)

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Cu1—N1—C7—C8	179.5 (4)	C20—C21—C22—C23	-3.0 (9)
C13—N2—C9—C10	-0.2 (8)	C21—C22—C23—C18	1.3 (9)
Cu1—N2—C9—C10	177.2 (4)	C17—C18—C23—C22	-176.9 (5)
C13—N2—C9—C7	-177.8 (5)	C19—C18—C23—C22	1.2 (9)
Cu1—N2—C9—C7	-0.5 (6)		

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*Hydrogen-bond geometry (Å, °)*

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<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C26—H26B...N1	0.98	2.52	2.891 (8)	102

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