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# 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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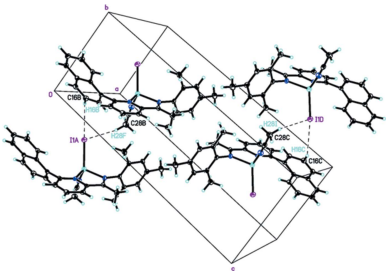
In the mononuclear title complex, $[CuI(C_2H_3N)(C_{26}H_{24}N_2)]$, the $Cu^I$ ion has a distorted tetrahedral coordination environment, defined by two N atoms of the chelating 2-(naphthalen-1-yl)-6-[(2,4,6-trimethylphenyl)imino]pyridine ligand, one N atom of an acetonitrile ligand and one iodide ligand. 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 (Karahan *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-alkyl-amides 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 $Cu^I$ ions. Within this context, we report herein the crystal structure of the title complex, $[CuI(C_2H_3N)(C_{26}H_{24}N_2)]$.



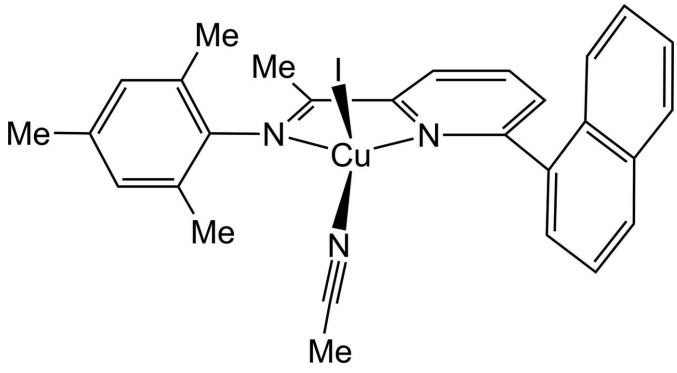


Table 1
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C26—H26$B$···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···N hydrogen-bonding interaction is present, stabilizing the molecular conformation (Table 1, Fig. 1).

## 3. Supramolecular features

In the crystal, weak C—H···I contacts involving a phenyl H atom [C16—H16$B$···I$^{i}$, 3.958 (6) Å, 152°; symmetry code: (i) $x$, $y-1$, $z$] and a H atom of the acetonitrile methyl group [[C28—H28$B$···I$^{i}$, 4.010 (6) Å, 109°] link the complex molecules, forming a three-dimensional network (Fig. 2).

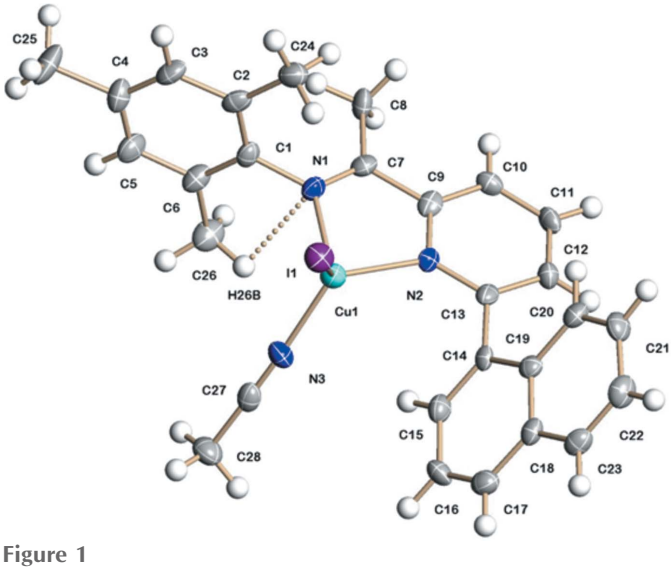



Figure 1
The molecular structure of the title complex, with displacement ellipsoids drawn at the 50% probability level. The C—H···N hydrogen bond is shown as a dashed line.

## 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 × 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). $^{1}$H NMR (400 MHz, $CD_2Cl_2$): $\delta$ 1.88 [*s*, 6H, *ortho*- $(CH_3)_2$], 1.97 (*s*, 3H, N≡C$CH_3$), 2.16 (*s*, 3H, N=C$CH_3$), 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) = 1.2$U_{eq}$(C) for H atoms on C$sp^2$ and 0.98 Å with $U_{iso}$(H) = 1.5$U_{eq}$(C) for H atoms on C$sp^3$.

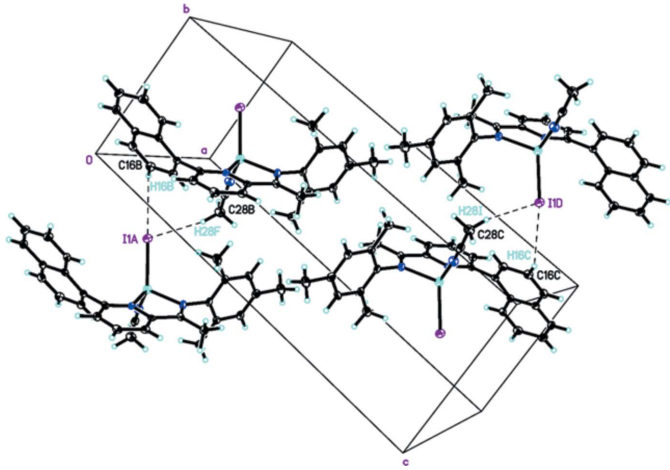



Figure 2
Part of the crystal structure, showing intermolecular C—H···I interactions (dashed lines).

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[CuI(C_2H_3N)(C_{26}H_{24}N_2)]$ |
| $M_r$ | 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$^3$) | 2517.4 (8) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 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 |
| $R_{int}$ | 0.125 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 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 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.13, −0.81 |

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

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# supporting information

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# 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)

**Nada Al-Najjar, Gregory A. Solan and Kuldip Singh**

## Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (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*

$[CuI(C_2H_3N)(C_{26}H_{24}N_2)]$
$M_r = 595.97$
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$^3$
$Z = 4$
$F(000) = 1192$
$D_x = 1.572$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 639 reflections
$\theta = 2.9$–$23.2°$
$\mu = 2.11$ mm$^{-1}$
$T = 150$ K
Needle, orange
0.25 × 0.07 × 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 $I > 2\sigma(I)$
$R_{int} = 0.125$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.4°$
$h = -18 \rightarrow 17$
$k = -9 \rightarrow 9$
$l = -26 \rightarrow 26$

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

$\Delta\rho_{max} = 1.13$ e Å$^{-3}$
$\Delta\rho_{min} = -0.81$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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 |

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|---|---|---|---|
| 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) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C26—H26*B*···N1 | 0.98 | 2.52 | 2.891 (8) | 102 |