# [N-(3-Methoxy-2-oxidobenzylidene-κO²)leucinato-κ²N,O](1,10-phenanthroline-κ²N,N′)copper(II) monohydrate

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The asymmetric unit of the title complex, $[Cu(C_{14}H_{17}NO_4)(C_{12}H_8N_2)]\cdot H_2O$, contains two independent $Cu^{II}$ complex molecules and two uncoordinated water molecules. In each complex molecule, the Cu atom is $O,N,O'$-chelated by the tridentate Schiff base ligand and $N,N'$-chelated by the 1,10-phenanthroline ligand in a distorted square-pyramidal geometry. The Cu—N bond distances in the apical directions are 2.298 (4) and 2.268 (4) Å. In the crystal, intermolecular O—H⋯O and C—H⋯O hydrogen bonds together with C—H⋯π interactions result in a three-dimensional supramolecular structure.

## Related literature

For related structures, see: Elena *et al.* (1995); Qiu *et al.* (2008).
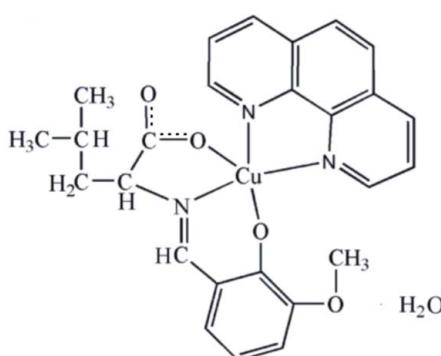


## Experimental

### Crystal data

$[Cu(C_{14}H_{17}NO_4)(C_{12}H_8N_2)]\cdot H_2O$
$M_r = 525.05$
Monoclinic, $P2_1$
$a = 11.1981$ (12) Å
$b = 10.4190$ (11) Å
$c = 21.298$ (2) Å
$\beta = 98.5520$ (10)°
$V = 2457.3$ (5) Å³
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.93$ mm⁻¹
$T = 293$ K
$0.45 \times 0.43 \times 0.41$ mm

### Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.680$, $T_{max} = 0.702$
12981 measured reflections
7382 independent reflections
5544 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.101$
$S = 1.01$
7382 reflections
637 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max} = 0.42$ e Å⁻³
$\Delta\rho_{min} = -0.30$ e Å⁻³
Absolute structure: Flack (1983), 2779 Friedel pairs
Flack parameter: −0.010 (12)

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.919 (4) | Cu2—N4 | 1.934 (4) |
| Cu1—N2 | 2.010 (4) | Cu2—N5 | 2.268 (4) |
| Cu1—N3 | 2.298 (4) | Cu2—N6 | 2.039 (4) |
| Cu1—O1 | 1.960 (3) | Cu2—O5 | 1.953 (4) |
| Cu1—O3 | 1.929 (3) | Cu2—O7 | 1.945 (3) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| O9—H9$A$⋯O2 | 0.85 | 2.22 | 2.715 (7) | 117 |
| O9—H9$B$⋯O2 | 0.85 | 2.20 | 2.715 (7) | 119 |
| O10—H10$A$⋯O6 | 0.85 | 2.27 | 2.805 (8) | 121 |
| O10—H10$B$⋯O6 | 0.85 | 2.27 | 2.805 (8) | 121 |
| C24—H24⋯O10ⁱ | 0.93 | 2.58 | 3.476 (8) | 162 |
| C40—H40$A$⋯O2ⁱⁱ | 0.96 | 2.53 | 3.486 (7) | 176 |
| C43—H43⋯O8ⁱⁱⁱ | 0.93 | 2.48 | 3.172 (6) | 131 |
| C50—H50⋯O9ⁱᵛ | 0.93 | 2.35 | 3.268 (7) | 168 |
| C25—H25⋯Cg1ᵛ | 0.93 | 2.51 | 3.426 (6) | 168 |

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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*.

## References

Elena, L., Jose, A. G. V., Jaime, R., Sofia, P. & Antonio, S. (1995). *Polyhedron*, **14**, 663–670.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Qiu, Z., Li, L., Liu, Y., Xu, T. & Wang, D. (2008). *Acta Cryst.* E**64**, m745–m746.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-Ray Instruments Inc., Madison, Wisconsin, USA.

# supporting information

## [*N*-(3-Methoxy-2-oxidobenzylidene-*κO²*)leucinato-*κ²N,O*](1,10-phenanthroline-*κ²N,N′*)copper(II) monohydrate

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### S1. Comment

Schiff bases still play an important role as ligands in metal coordination chemistry even after almost a century since their discovery. Considerable efforts have been devotedd to copper(II) complexes of tridentate Schiff base ligands of *N*-alkylidene or *N*-arylidene alkanato type, due to their structural richness, electrochemical properties as well as a potential model for a number of important biological systems. Herein, we report the synthesis and crystal structure of a new copper(II) complex with a tridentate Schiff base ligand derived from the condensation of *o*-vanillin and *L*-leucine, and with 1,10-phenanthroline.

There are two independent structurses in the crystallographic asymmetric unit except the solvent water moleculars (Fig.1). In either of the two main molecular structures, the central Cu$^{II}$ atom is five-coordinated by one N atom and two O atoms from the tridentate Schiff base ligand and two N atoms from 1,10-phenanthroline ligand, forming a seriously distorted square-pyramidal geometry. The O1, O3, N1, and N2 atoms (or O5, O7, N4, and N6) locate in equatorial plane, and N3 (or N5) in the apital position. The Cu1$^{II}$ atom and Cu2$^{II}$ atom lie 0.1552 (21)Å and 0.0859 (22)Å above theirs equatorial plane, respectively. Similar to that repoted previously (Elena *et al.*, 1995; Qiu *et al.*, 2008), the apital atoms (N3, N5) are much longer from their copper atoms, with the bond distances of Cu1—N3 = 2.298 (4)Å and Cu2—N5 = 2.268 (4)Å (Table 1). The tridentate Schiff base ligands coordinated to copper atoms form two penta-chelated rings(Cu1/O1/C1—C2/N1 and Cu2/O5/C27—C28/N4) and two hexa-chelated rings (Cu1/N1/C7—C9/O3 and Cu2/N4/C33—C35/O7). In each molecular, the penta-chelated ring and hexa-chelated ring have formed their individual dihedral angle 12.64 (22)° and 17.39 (21)°, respectively. The phenanthroline ligands are almost perpendicular to their individual equatorial plane (dihedral angle 89.03 (13)° and 86.24 (14)°).

In the crystal structure, there exist C—H···O and O—H···O hydrogen bonds (Table 2) which link the molecules into a three-dimensional network structure (Fig. 2). Additionally, the intermolecular C—H···*π* interaction [H25···*Cg*$^i$= 2.513 Å, C25···*Cg*$^i$= 3.426 Å, and C25—H25···*Cg*$^i$= 167.55°; symmetry code: (i) -*x*, *y* - 1/2, 1 - *z*; *Cg* is the centroid of the C8—C13 ring] also stablizes the crystal packing, along with the van der Waals forces.

### S2. Experimental

*L*-Leucine (1 mmol, 113.2 mg) and potassium hydroxide (1 mmol, 56.1 mg) were dissolved in hot methanol (10 ml) and added successively to a methanol solution of *o*-vanilline (1 mmol, 152.2 mg). The mixture was then stirred at 323 K for 2 h. Subsequently, an aqueous solution (2 ml) of cupric acetate monohydrate (1 mmol, 199.7 mg) was added dropwise and stirred for 2 h. An methanol solution (5 ml) of 1,10-phenanthroline monohydrate (1 mmol, 198.2 mg) was added dropwise and stirred for 4 h. The resultant solution was held at room temperature for 10 d, single crystals suitable for X-ray diffraction were obtained.

## S3. Refinement

All the H atoms were placed in geometrically calculated positions with C—H = 0.93–0.98Å and O—H = 0.85 Å and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for the others.
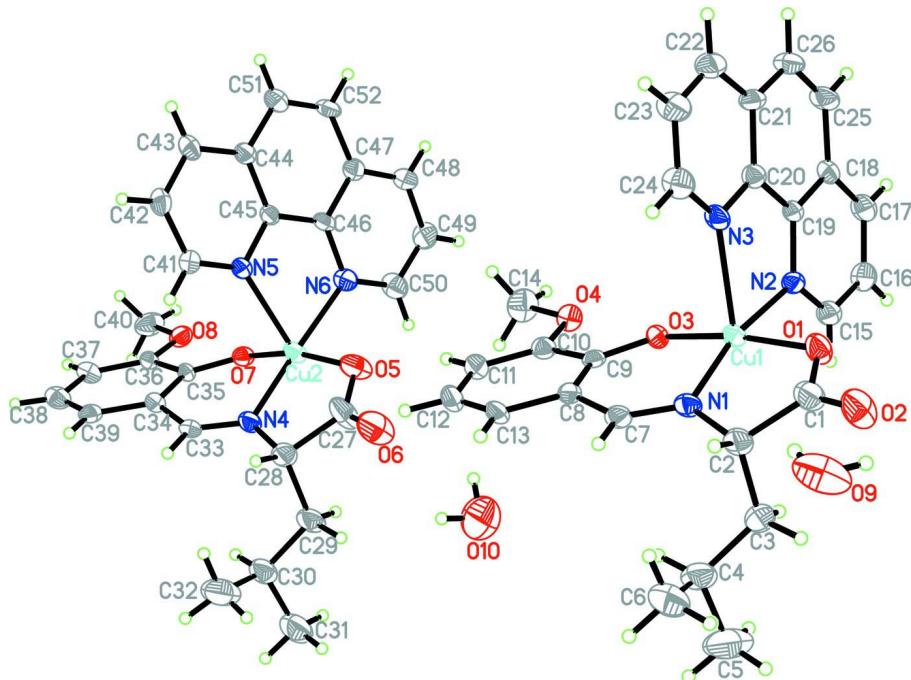


**Figure 1**

The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.
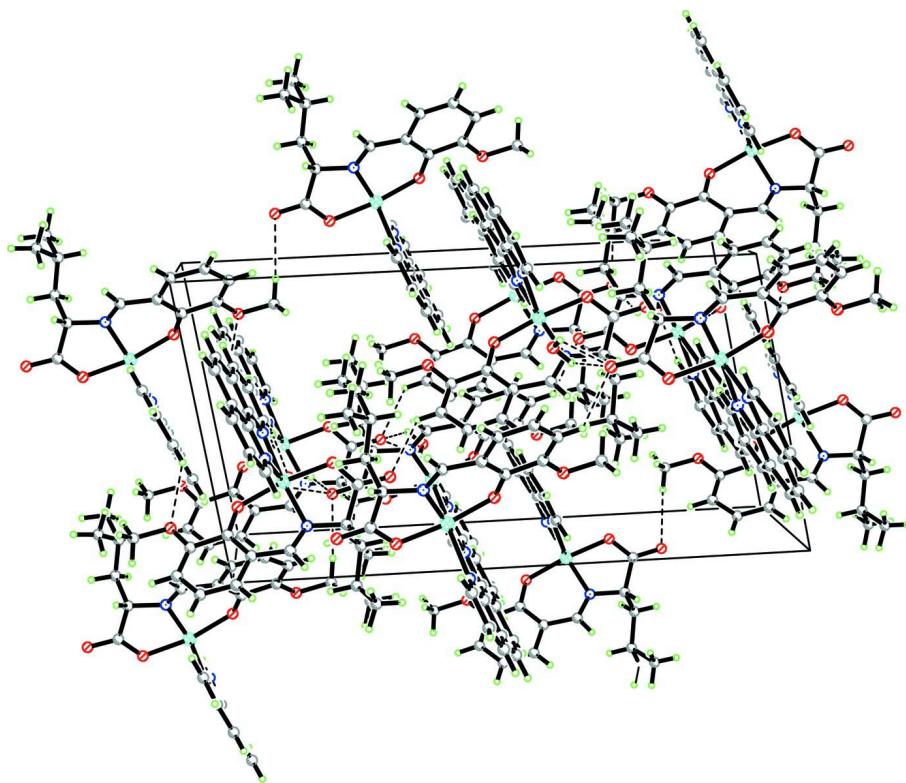
**Figure 2**

Packing diagram of the title compound.

**[*N*-(3-Methoxy-2-oxidobenzylidene-$\kappa O^2$)leucinato- $\kappa^2 N,O$](1,10-phenanthroline- $\kappa^2 N,N'$)copper(II) monohydrate**

*Crystal data*

| | |
|---|---|
| [Cu(C$_{14}$H$_{17}$NO$_4$)(C$_{12}$H$_8$N$_2$)]·H$_2$O | $F(000) = 1092$ |
| $M_r = 525.05$ | $D_x = 1.419$ Mg m$^{-3}$ |
| Monoclinic, $P2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2yb | Cell parameters from 4089 reflections |
| $a = 11.1981$ (12) Å | $\theta = 2.2$–$26.8°$ |
| $b = 10.4190$ (11) Å | $\mu = 0.93$ mm$^{-1}$ |
| $c = 21.298$ (2) Å | $T = 293$ K |
| $\beta = 98.552$ (1)° | Block, blue |
| $V = 2457.3$ (5) Å$^3$ | $0.45 \times 0.43 \times 0.41$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART 1000 CCD area-detector diffractometer | 12981 measured reflections |
| | 7382 independent reflections |
| Radiation source: fine-focus sealed tube | 5544 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.027$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -13 \rightarrow 11$ |
| | $k = -11 \rightarrow 12$ |
| $T_{min} = 0.680$, $T_{max} = 0.702$ | $l = -25 \rightarrow 25$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | H-atom parameters constrained |
| $wR(F^2) = 0.101$ | $w = 1/[\sigma^2(F_o^2) + (0.0508P)^2]$ |
| $S = 1.01$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 7382 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 637 parameters | $\Delta\rho_{max} = 0.42$ e Å$^{-3}$ |
| 1 restraint | $\Delta\rho_{min} = -0.30$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 2779 Friedel pairs |
| Secondary atom site location: difference Fourier map | Absolute structure parameter: −0.010 (12) |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.19614 (5) | 0.73977 (4) | 0.38068 (3) | 0.03585 (18) |
| Cu2 | 0.69306 (5) | 0.85315 (5) | 0.88162 (3) | 0.0400 (2) |
| N1 | 0.3237 (3) | 0.8364 (4) | 0.35210 (16) | 0.0402 (9) |
| N2 | 0.0776 (3) | 0.6083 (4) | 0.40247 (18) | 0.0336 (10) |
| N3 | 0.0348 (3) | 0.8640 (4) | 0.3981 (2) | 0.0388 (10) |
| N4 | 0.8351 (3) | 0.9294 (4) | 0.85529 (17) | 0.0426 (10) |
| N5 | 0.5893 (3) | 1.0317 (4) | 0.90173 (19) | 0.0359 (10) |
| N6 | 0.5344 (4) | 0.7771 (4) | 0.9006 (2) | 0.0427 (12) |
| O1 | 0.1368 (3) | 0.7246 (4) | 0.28967 (15) | 0.0522 (10) |
| O2 | 0.1742 (4) | 0.7864 (4) | 0.19411 (19) | 0.0757 (15) |
| O3 | 0.2733 (3) | 0.7420 (4) | 0.46790 (14) | 0.0348 (7) |
| O4 | 0.3396 (3) | 0.7325 (4) | 0.59119 (15) | 0.0429 (8) |
| O5 | 0.6398 (3) | 0.8405 (5) | 0.79026 (17) | 0.0636 (12) |
| O6 | 0.6919 (4) | 0.8878 (5) | 0.69680 (19) | 0.0940 (19) |
| O7 | 0.7729 (3) | 0.8381 (3) | 0.96887 (15) | 0.0365 (8) |
| O8 | 0.8331 (3) | 0.8287 (3) | 1.09201 (15) | 0.0452 (9) |
| O9 | 0.2665 (4) | 0.9682 (6) | 0.1236 (2) | 0.1102 (18) |
| H9A | 0.2637 | 0.9606 | 0.1631 | 0.132* |
| H9B | 0.2235 | 0.9014 | 0.1151 | 0.132* |
| O10 | 0.7423 (5) | 0.6893 (6) | 0.6157 (3) | 0.138 (2) |
| H10A | 0.7719 | 0.7625 | 0.6266 | 0.165* |
| H10B | 0.6913 | 0.7016 | 0.6410 | 0.165* |
| C1 | 0.2027 (5) | 0.7795 (6) | 0.2530 (3) | 0.0567 (16) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.3243 (4) | 0.8296 (6) | 0.2836 (2) | 0.0488 (13) |
| H2 | 0.3389 | 0.9148 | 0.2669 | 0.059* |
| C3 | 0.4194 (5) | 0.7354 (7) | 0.2679 (2) | 0.0638 (17) |
| H3A | 0.4072 | 0.7226 | 0.2223 | 0.077* |
| H3B | 0.4054 | 0.6536 | 0.2872 | 0.077* |
| C4 | 0.5513 (5) | 0.7724 (7) | 0.2886 (3) | 0.074 (2) |
| H4 | 0.5634 | 0.7897 | 0.3344 | 0.089* |
| C5 | 0.6332 (6) | 0.6615 (9) | 0.2758 (3) | 0.113 (3) |
| H5A | 0.6284 | 0.6492 | 0.2308 | 0.170* |
| H5B | 0.6078 | 0.5846 | 0.2948 | 0.170* |
| H5C | 0.7150 | 0.6809 | 0.2937 | 0.170* |
| C6 | 0.5864 (6) | 0.8914 (8) | 0.2545 (4) | 0.104 (3) |
| H6A | 0.6691 | 0.9128 | 0.2697 | 0.156* |
| H6B | 0.5353 | 0.9616 | 0.2626 | 0.156* |
| H6C | 0.5771 | 0.8750 | 0.2097 | 0.156* |
| C7 | 0.3970 (4) | 0.9105 (4) | 0.3880 (2) | 0.0404 (11) |
| H7 | 0.4420 | 0.9684 | 0.3678 | 0.048* |
| C8 | 0.4153 (4) | 0.9117 (4) | 0.4557 (2) | 0.0348 (10) |
| C9 | 0.3581 (4) | 0.8213 (4) | 0.4918 (2) | 0.0320 (10) |
| C10 | 0.3961 (4) | 0.8229 (4) | 0.5585 (2) | 0.0370 (11) |
| C11 | 0.4807 (4) | 0.9088 (5) | 0.5865 (2) | 0.0449 (12) |
| H11 | 0.5035 | 0.9078 | 0.6303 | 0.054* |
| C12 | 0.5327 (4) | 0.9974 (5) | 0.5497 (2) | 0.0473 (13) |
| H12 | 0.5887 | 1.0565 | 0.5689 | 0.057* |
| C13 | 0.5018 (4) | 0.9973 (5) | 0.4866 (3) | 0.0430 (14) |
| H13 | 0.5386 | 1.0556 | 0.4625 | 0.052* |
| C14 | 0.3722 (5) | 0.7327 (7) | 0.6588 (2) | 0.0672 (17) |
| H14A | 0.4585 | 0.7285 | 0.6694 | 0.101* |
| H14B | 0.3367 | 0.6597 | 0.6764 | 0.101* |
| H14C | 0.3432 | 0.8100 | 0.6759 | 0.101* |
| C15 | 0.0984 (4) | 0.4836 (5) | 0.4038 (2) | 0.0433 (13) |
| H15 | 0.1702 | 0.4536 | 0.3921 | 0.052* |
| C16 | 0.0177 (5) | 0.3962 (5) | 0.4217 (3) | 0.0496 (14) |
| H16 | 0.0361 | 0.3091 | 0.4220 | 0.060* |
| C17 | −0.0884 (5) | 0.4358 (5) | 0.4388 (3) | 0.0486 (14) |
| H17 | −0.1425 | 0.3767 | 0.4513 | 0.058* |
| C18 | −0.1149 (4) | 0.5669 (4) | 0.4373 (2) | 0.0348 (11) |
| C19 | −0.0288 (4) | 0.6520 (4) | 0.4180 (2) | 0.0301 (11) |
| C20 | −0.0515 (4) | 0.7856 (5) | 0.4158 (2) | 0.0358 (12) |
| C21 | −0.1618 (4) | 0.8341 (5) | 0.4321 (2) | 0.0410 (12) |
| C22 | −0.1788 (5) | 0.9677 (5) | 0.4294 (3) | 0.0559 (16) |
| H22 | −0.2489 | 1.0037 | 0.4403 | 0.067* |
| C23 | −0.0921 (5) | 1.0440 (5) | 0.4107 (3) | 0.0606 (17) |
| H23 | −0.1033 | 1.1324 | 0.4083 | 0.073* |
| C24 | 0.0125 (5) | 0.9904 (5) | 0.3953 (3) | 0.0566 (16) |
| H24 | 0.0702 | 1.0446 | 0.3823 | 0.068* |
| C25 | −0.2228 (4) | 0.6194 (6) | 0.4546 (2) | 0.0492 (14) |
| H25 | −0.2793 | 0.5644 | 0.4679 | 0.059* |

| | | | |
|---|---|---|---|
| C26 | −0.2453 (4) | 0.7458 (6) | 0.4521 (2) | 0.0486 (13) |
| H26 | −0.3169 | 0.7763 | 0.4637 | 0.058* |
| C27 | 0.7124 (5) | 0.8792 (7) | 0.7547 (3) | 0.0681 (19) |
| C28 | 0.8379 (4) | 0.9240 (6) | 0.7871 (2) | 0.0506 (13) |
| H28 | 0.8577 | 1.0083 | 0.7711 | 0.061* |
| C29 | 0.9290 (5) | 0.8203 (6) | 0.7707 (3) | 0.0612 (18) |
| H29A | 0.9089 | 0.7395 | 0.7893 | 0.073* |
| H29B | 0.9169 | 0.8090 | 0.7250 | 0.073* |
| C30 | 1.0599 (5) | 0.8464 (7) | 0.7920 (3) | 0.0636 (17) |
| H30 | 1.0732 | 0.8544 | 0.8384 | 0.076* |
| C31 | 1.1342 (6) | 0.7372 (9) | 0.7741 (3) | 0.094 (2) |
| H31A | 1.1273 | 0.7323 | 0.7287 | 0.141* |
| H31B | 1.1059 | 0.6586 | 0.7902 | 0.141* |
| H31C | 1.2172 | 0.7505 | 0.7919 | 0.141* |
| C32 | 1.1026 (6) | 0.9700 (8) | 0.7637 (4) | 0.100 (3) |
| H32A | 1.1055 | 0.9577 | 0.7193 | 0.150* |
| H32B | 1.1817 | 0.9918 | 0.7850 | 0.150* |
| H32C | 1.0474 | 1.0383 | 0.7691 | 0.150* |
| C33 | 0.9021 (4) | 1.0065 (5) | 0.8911 (2) | 0.0412 (11) |
| H33 | 0.9494 | 1.0630 | 0.8717 | 0.049* |
| C34 | 0.9109 (4) | 1.0140 (4) | 0.9588 (2) | 0.0368 (11) |
| C35 | 0.8521 (3) | 0.9214 (4) | 0.9934 (2) | 0.0326 (10) |
| C36 | 0.8865 (3) | 0.9238 (4) | 1.0618 (2) | 0.0332 (10) |
| C37 | 0.9640 (4) | 1.0140 (5) | 1.0907 (2) | 0.0430 (12) |
| H37 | 0.9846 | 1.0128 | 1.1346 | 0.052* |
| C38 | 1.0132 (4) | 1.1088 (5) | 1.0552 (3) | 0.0480 (13) |
| H38 | 1.0622 | 1.1730 | 1.0756 | 0.058* |
| C39 | 0.9887 (4) | 1.1058 (5) | 0.9915 (3) | 0.0434 (13) |
| H39 | 1.0245 | 1.1665 | 0.9682 | 0.052* |
| C40 | 0.8619 (5) | 0.8225 (6) | 1.1594 (2) | 0.0650 (18) |
| H40A | 0.9475 | 0.8123 | 1.1711 | 0.097* |
| H40B | 0.8211 | 0.7507 | 1.1749 | 0.097* |
| H40C | 0.8365 | 0.9003 | 1.1777 | 0.097* |
| C41 | 0.6150 (5) | 1.1534 (5) | 0.9030 (2) | 0.0462 (14) |
| H41 | 0.6885 | 1.1782 | 0.8914 | 0.055* |
| C42 | 0.5391 (4) | 1.2499 (5) | 0.9208 (2) | 0.0451 (13) |
| H42 | 0.5613 | 1.3359 | 0.9206 | 0.054* |
| C43 | 0.4313 (4) | 1.2134 (5) | 0.9384 (2) | 0.0476 (14) |
| H43 | 0.3795 | 1.2749 | 0.9509 | 0.057* |
| C44 | 0.3996 (4) | 1.0850 (5) | 0.9375 (2) | 0.0378 (12) |
| C45 | 0.4820 (4) | 0.9955 (5) | 0.9187 (2) | 0.0317 (11) |
| C46 | 0.4529 (4) | 0.8625 (5) | 0.9170 (2) | 0.0357 (12) |
| C47 | 0.3416 (4) | 0.8224 (5) | 0.9327 (2) | 0.0417 (13) |
| C48 | 0.3171 (5) | 0.6905 (6) | 0.9303 (3) | 0.0559 (16) |
| H48 | 0.2445 | 0.6600 | 0.9407 | 0.067* |
| C49 | 0.3979 (5) | 0.6082 (5) | 0.9129 (3) | 0.0568 (15) |
| H49 | 0.3808 | 0.5208 | 0.9105 | 0.068* |
| C50 | 0.5081 (5) | 0.6536 (5) | 0.8984 (3) | 0.0539 (16) |

| | | | | |
|---|---|---|---|---|
| H50 | 0.5641 | 0.5955 | 0.8870 | 0.065* |
| C51 | 0.2882 (4) | 1.0414 (5) | 0.9544 (2) | 0.0494 (14) |
| H51 | 0.2347 | 1.1003 | 0.9676 | 0.059* |
| C52 | 0.2598 (4) | 0.9170 (6) | 0.9517 (3) | 0.0487 (15) |
| H52 | 0.1859 | 0.8907 | 0.9622 | 0.058* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0293 (4) | 0.0392 (4) | 0.0409 (4) | −0.0066 (3) | 0.0113 (3) | −0.0029 (3) |
| Cu2 | 0.0304 (4) | 0.0484 (4) | 0.0421 (4) | 0.0046 (3) | 0.0083 (3) | −0.0029 (3) |
| N1 | 0.034 (2) | 0.052 (3) | 0.038 (2) | −0.0060 (19) | 0.0152 (17) | 0.000 (2) |
| N2 | 0.032 (2) | 0.033 (2) | 0.038 (2) | −0.0035 (18) | 0.0112 (17) | −0.0033 (19) |
| N3 | 0.031 (2) | 0.033 (2) | 0.053 (3) | −0.009 (2) | 0.0092 (19) | 0.000 (2) |
| N4 | 0.032 (2) | 0.062 (3) | 0.035 (2) | 0.009 (2) | 0.0097 (17) | 0.008 (2) |
| N5 | 0.031 (2) | 0.034 (3) | 0.044 (3) | 0.0055 (18) | 0.0093 (18) | 0.002 (2) |
| N6 | 0.037 (3) | 0.043 (3) | 0.048 (3) | −0.0005 (19) | 0.008 (2) | −0.0031 (19) |
| O1 | 0.044 (2) | 0.071 (3) | 0.042 (2) | −0.021 (2) | 0.0089 (16) | −0.004 (2) |
| O2 | 0.063 (3) | 0.124 (4) | 0.038 (2) | −0.022 (2) | 0.0001 (19) | 0.011 (2) |
| O3 | 0.0316 (17) | 0.0334 (17) | 0.0404 (19) | −0.0082 (16) | 0.0088 (14) | −0.0032 (18) |
| O4 | 0.0490 (19) | 0.0399 (19) | 0.040 (2) | −0.0017 (17) | 0.0069 (15) | 0.0037 (18) |
| O5 | 0.038 (2) | 0.107 (4) | 0.046 (2) | −0.001 (2) | 0.0070 (18) | −0.005 (2) |
| O6 | 0.064 (3) | 0.177 (6) | 0.039 (2) | 0.017 (3) | 0.004 (2) | 0.007 (3) |
| O7 | 0.0317 (18) | 0.036 (2) | 0.042 (2) | −0.0040 (16) | 0.0067 (15) | 0.0003 (17) |
| O8 | 0.0455 (19) | 0.050 (2) | 0.041 (2) | −0.0049 (17) | 0.0096 (16) | 0.0081 (17) |
| O9 | 0.067 (3) | 0.128 (5) | 0.139 (4) | 0.008 (3) | 0.027 (3) | 0.050 (4) |
| O10 | 0.139 (5) | 0.098 (4) | 0.176 (6) | 0.000 (4) | 0.024 (4) | −0.028 (4) |
| C1 | 0.043 (3) | 0.076 (5) | 0.052 (4) | −0.007 (3) | 0.008 (3) | −0.002 (3) |
| C2 | 0.044 (3) | 0.065 (4) | 0.041 (3) | −0.012 (3) | 0.018 (2) | 0.000 (3) |
| C3 | 0.055 (3) | 0.095 (5) | 0.045 (3) | −0.010 (4) | 0.020 (3) | −0.019 (4) |
| C4 | 0.053 (4) | 0.121 (7) | 0.053 (4) | 0.001 (4) | 0.021 (3) | −0.015 (4) |
| C5 | 0.084 (5) | 0.166 (10) | 0.098 (6) | 0.035 (6) | 0.039 (4) | −0.003 (6) |
| C6 | 0.066 (5) | 0.138 (8) | 0.116 (6) | −0.029 (5) | 0.040 (4) | −0.023 (5) |
| C7 | 0.037 (3) | 0.036 (3) | 0.053 (3) | −0.008 (2) | 0.022 (2) | −0.002 (2) |
| C8 | 0.030 (2) | 0.030 (2) | 0.046 (3) | −0.0021 (19) | 0.013 (2) | −0.005 (2) |
| C9 | 0.027 (2) | 0.027 (3) | 0.045 (3) | 0.0041 (18) | 0.0135 (19) | −0.004 (2) |
| C10 | 0.033 (2) | 0.033 (3) | 0.045 (3) | 0.004 (2) | 0.007 (2) | 0.000 (2) |
| C11 | 0.036 (3) | 0.046 (3) | 0.051 (3) | 0.000 (2) | 0.002 (2) | −0.007 (2) |
| C12 | 0.033 (3) | 0.041 (3) | 0.065 (4) | −0.007 (2) | 0.001 (2) | −0.011 (3) |
| C13 | 0.027 (2) | 0.038 (3) | 0.066 (4) | −0.009 (2) | 0.012 (3) | −0.008 (3) |
| C14 | 0.083 (4) | 0.073 (4) | 0.047 (4) | −0.007 (4) | 0.015 (3) | 0.007 (3) |
| C15 | 0.039 (3) | 0.039 (3) | 0.053 (3) | −0.003 (2) | 0.010 (2) | −0.005 (3) |
| C16 | 0.054 (3) | 0.026 (3) | 0.070 (4) | −0.009 (2) | 0.012 (3) | −0.004 (2) |
| C17 | 0.042 (3) | 0.044 (4) | 0.060 (4) | −0.013 (3) | 0.012 (3) | −0.001 (3) |
| C18 | 0.029 (2) | 0.034 (3) | 0.041 (3) | −0.006 (2) | 0.003 (2) | 0.001 (2) |
| C19 | 0.026 (2) | 0.028 (3) | 0.036 (3) | −0.004 (2) | 0.006 (2) | −0.003 (2) |
| C20 | 0.034 (3) | 0.036 (3) | 0.038 (3) | −0.002 (2) | 0.007 (2) | 0.000 (2) |
| C21 | 0.033 (3) | 0.037 (3) | 0.055 (3) | 0.006 (2) | 0.012 (2) | −0.006 (3) |

| | | | | | |
|---|---|---|---|---|---|
| C22 | 0.042 (3) | 0.047 (4) | 0.078 (4) | 0.012 (3) | 0.006 (3) | −0.005 (3) |
| C23 | 0.049 (3) | 0.029 (3) | 0.104 (5) | 0.005 (3) | 0.011 (3) | 0.007 (3) |
| C24 | 0.053 (4) | 0.035 (3) | 0.083 (4) | −0.006 (3) | 0.014 (3) | 0.008 (3) |
| C25 | 0.034 (3) | 0.051 (4) | 0.067 (4) | −0.010 (3) | 0.022 (2) | 0.002 (3) |
| C26 | 0.033 (3) | 0.054 (4) | 0.063 (3) | 0.005 (3) | 0.018 (2) | 0.002 (3) |
| C27 | 0.048 (3) | 0.108 (6) | 0.046 (4) | 0.028 (3) | −0.002 (3) | −0.008 (3) |
| C28 | 0.044 (3) | 0.070 (4) | 0.039 (3) | 0.006 (3) | 0.012 (2) | 0.009 (3) |
| C29 | 0.045 (3) | 0.094 (5) | 0.049 (3) | 0.017 (3) | 0.021 (3) | 0.006 (3) |
| C30 | 0.045 (3) | 0.102 (5) | 0.045 (4) | 0.018 (4) | 0.014 (3) | 0.012 (4) |
| C31 | 0.064 (4) | 0.133 (6) | 0.091 (5) | 0.034 (5) | 0.031 (4) | 0.016 (5) |
| C32 | 0.061 (4) | 0.108 (6) | 0.139 (7) | −0.007 (4) | 0.039 (4) | 0.004 (6) |
| C33 | 0.029 (2) | 0.048 (3) | 0.050 (3) | 0.006 (2) | 0.017 (2) | 0.010 (2) |
| C34 | 0.029 (2) | 0.036 (3) | 0.046 (3) | 0.003 (2) | 0.0073 (19) | 0.004 (2) |
| C35 | 0.027 (2) | 0.027 (2) | 0.046 (3) | 0.0077 (19) | 0.0124 (19) | 0.004 (2) |
| C36 | 0.026 (2) | 0.030 (3) | 0.044 (3) | 0.0000 (19) | 0.0057 (19) | 0.004 (2) |
| C37 | 0.034 (2) | 0.050 (3) | 0.045 (3) | 0.000 (2) | 0.007 (2) | −0.009 (2) |
| C38 | 0.036 (3) | 0.040 (3) | 0.068 (4) | −0.008 (2) | 0.005 (2) | −0.011 (3) |
| C39 | 0.034 (3) | 0.038 (3) | 0.061 (4) | −0.007 (2) | 0.015 (3) | 0.004 (3) |
| C40 | 0.065 (4) | 0.090 (5) | 0.041 (3) | −0.016 (3) | 0.013 (3) | 0.006 (3) |
| C41 | 0.040 (3) | 0.046 (4) | 0.054 (3) | 0.004 (2) | 0.009 (2) | 0.014 (3) |
| C42 | 0.047 (3) | 0.034 (3) | 0.052 (3) | 0.007 (2) | 0.000 (2) | 0.001 (3) |
| C43 | 0.039 (3) | 0.047 (4) | 0.058 (3) | 0.015 (2) | 0.011 (2) | 0.004 (3) |
| C44 | 0.032 (3) | 0.040 (3) | 0.042 (3) | 0.003 (2) | 0.007 (2) | 0.000 (3) |
| C45 | 0.026 (2) | 0.038 (3) | 0.031 (3) | 0.003 (2) | 0.0031 (19) | 0.002 (2) |
| C46 | 0.022 (2) | 0.049 (3) | 0.035 (3) | 0.000 (2) | 0.0030 (19) | −0.001 (3) |
| C47 | 0.036 (3) | 0.040 (3) | 0.048 (3) | −0.002 (2) | 0.002 (2) | 0.002 (3) |
| C48 | 0.035 (3) | 0.064 (4) | 0.067 (4) | −0.005 (3) | 0.003 (3) | 0.012 (3) |
| C49 | 0.057 (4) | 0.029 (3) | 0.080 (4) | −0.009 (3) | −0.002 (3) | −0.001 (3) |
| C50 | 0.048 (3) | 0.044 (4) | 0.069 (4) | 0.002 (3) | 0.006 (3) | −0.011 (3) |
| C51 | 0.037 (3) | 0.052 (4) | 0.061 (4) | 0.010 (3) | 0.015 (2) | 0.001 (3) |
| C52 | 0.023 (3) | 0.068 (4) | 0.056 (4) | 0.000 (3) | 0.011 (2) | 0.008 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.919 (4) | C16—C17 | 1.358 (7) |
| Cu1—N2 | 2.010 (4) | C16—H16 | 0.9300 |
| Cu1—N3 | 2.298 (4) | C17—C18 | 1.398 (7) |
| Cu1—O1 | 1.960 (3) | C17—H17 | 0.9300 |
| Cu1—O3 | 1.929 (3) | C18—C19 | 1.414 (6) |
| Cu2—N4 | 1.934 (4) | C18—C25 | 1.424 (7) |
| Cu2—N5 | 2.268 (4) | C19—C20 | 1.415 (6) |
| Cu2—N6 | 2.039 (4) | C20—C21 | 1.425 (6) |
| Cu2—O5 | 1.953 (4) | C21—C22 | 1.405 (7) |
| Cu2—O7 | 1.945 (3) | C21—C26 | 1.421 (7) |
| N1—C7 | 1.291 (5) | C22—C23 | 1.360 (7) |
| N1—C2 | 1.461 (5) | C22—H22 | 0.9300 |
| N2—C15 | 1.319 (6) | C23—C24 | 1.380 (7) |
| N2—C19 | 1.361 (6) | C23—H23 | 0.9300 |

| | | | |
|---|---|---|---|
| N3—C24 | 1.341 (7) | C24—H24 | 0.9300 |
| N3—C20 | 1.360 (6) | C25—C26 | 1.340 (7) |
| N4—C33 | 1.273 (6) | C25—H25 | 0.9300 |
| N4—C28 | 1.458 (6) | C26—H26 | 0.9300 |
| N5—C41 | 1.300 (6) | C27—C28 | 1.543 (7) |
| N5—C45 | 1.359 (5) | C28—C29 | 1.560 (7) |
| N6—C50 | 1.319 (7) | C28—H28 | 0.9800 |
| N6—C46 | 1.357 (6) | C29—C30 | 1.494 (7) |
| O1—C1 | 1.286 (6) | C29—H29A | 0.9700 |
| O2—C1 | 1.249 (6) | C29—H29B | 0.9700 |
| O3—C9 | 1.303 (5) | C30—C31 | 1.492 (9) |
| O4—C10 | 1.379 (5) | C30—C32 | 1.529 (10) |
| O4—C14 | 1.431 (5) | C30—H30 | 0.9800 |
| O5—C27 | 1.258 (7) | C31—H31A | 0.9600 |
| O6—C27 | 1.223 (6) | C31—H31B | 0.9600 |
| O7—C35 | 1.293 (5) | C31—H31C | 0.9600 |
| O8—C36 | 1.366 (5) | C32—H32A | 0.9600 |
| O8—C40 | 1.426 (6) | C32—H32B | 0.9600 |
| O9—H9A | 0.8501 | C32—H32C | 0.9600 |
| O9—H9B | 0.8500 | C33—C34 | 1.432 (6) |
| O10—H10A | 0.8500 | C33—H33 | 0.9300 |
| O10—H10B | 0.8500 | C34—C39 | 1.406 (6) |
| C1—C2 | 1.512 (7) | C34—C35 | 1.433 (6) |
| C2—C3 | 1.521 (8) | C35—C36 | 1.449 (6) |
| C2—H2 | 0.9800 | C36—C37 | 1.363 (6) |
| C3—C4 | 1.527 (7) | C37—C38 | 1.405 (7) |
| C3—H3A | 0.9700 | C37—H37 | 0.9300 |
| C3—H3B | 0.9700 | C38—C39 | 1.346 (7) |
| C4—C6 | 1.518 (10) | C38—H38 | 0.9300 |
| C4—C5 | 1.525 (9) | C39—H39 | 0.9300 |
| C4—H4 | 0.9800 | C40—H40A | 0.9600 |
| C5—H5A | 0.9600 | C40—H40B | 0.9600 |
| C5—H5B | 0.9600 | C40—H40C | 0.9600 |
| C5—H5C | 0.9600 | C41—C42 | 1.405 (7) |
| C6—H6A | 0.9600 | C41—H41 | 0.9300 |
| C6—H6B | 0.9600 | C42—C43 | 1.370 (7) |
| C6—H6C | 0.9600 | C42—H42 | 0.9300 |
| C7—C8 | 1.426 (6) | C43—C44 | 1.384 (7) |
| C7—H7 | 0.9300 | C43—H43 | 0.9300 |
| C8—C13 | 1.406 (6) | C44—C45 | 1.411 (6) |
| C8—C9 | 1.427 (6) | C44—C51 | 1.423 (7) |
| C9—C10 | 1.422 (6) | C45—C46 | 1.423 (7) |
| C10—C11 | 1.373 (6) | C46—C47 | 1.400 (6) |
| C11—C12 | 1.394 (7) | C47—C48 | 1.401 (8) |
| C11—H11 | 0.9300 | C47—C52 | 1.444 (7) |
| C12—C13 | 1.336 (7) | C48—C49 | 1.338 (7) |
| C12—H12 | 0.9300 | C48—H48 | 0.9300 |
| C13—H13 | 0.9300 | C49—C50 | 1.398 (8) |

| | | | |
|---|---|---|---|
| C14—H14A | 0.9600 | C49—H49 | 0.9300 |
| C14—H14B | 0.9600 | C50—H50 | 0.9300 |
| C14—H14C | 0.9600 | C51—C52 | 1.334 (7) |
| C15—C16 | 1.376 (7) | C51—H51 | 0.9300 |
| C15—H15 | 0.9300 | C52—H52 | 0.9300 |
| | | | |
| N1—Cu1—O3 | 92.92 (14) | N2—C19—C20 | 118.7 (4) |
| N1—Cu1—O1 | 83.54 (15) | C18—C19—C20 | 120.0 (4) |
| O3—Cu1—O1 | 172.26 (15) | N3—C20—C19 | 118.0 (4) |
| N1—Cu1—N2 | 168.34 (16) | N3—C20—C21 | 122.1 (5) |
| O3—Cu1—N2 | 90.15 (15) | C19—C20—C21 | 119.9 (4) |
| O1—Cu1—N2 | 92.01 (16) | C22—C21—C26 | 124.2 (5) |
| N1—Cu1—N3 | 113.34 (16) | C22—C21—C20 | 117.3 (5) |
| O3—Cu1—N3 | 95.04 (14) | C26—C21—C20 | 118.5 (5) |
| O1—Cu1—N3 | 92.68 (15) | C23—C22—C21 | 119.5 (5) |
| N2—Cu1—N3 | 77.54 (14) | C23—C22—H22 | 120.2 |
| N4—Cu2—O7 | 91.66 (14) | C21—C22—H22 | 120.2 |
| N4—Cu2—O5 | 83.18 (16) | C22—C23—C24 | 120.1 (5) |
| O7—Cu2—O5 | 167.25 (17) | C22—C23—H23 | 119.9 |
| N4—Cu2—N6 | 174.25 (17) | C24—C23—H23 | 119.9 |
| O7—Cu2—N6 | 94.02 (16) | N3—C24—C23 | 123.0 (5) |
| O5—Cu2—N6 | 91.43 (18) | N3—C24—H24 | 118.5 |
| N4—Cu2—N5 | 100.62 (15) | C23—C24—H24 | 118.5 |
| O7—Cu2—N5 | 93.51 (15) | C26—C25—C18 | 121.9 (5) |
| O5—Cu2—N5 | 98.88 (17) | C26—C25—H25 | 119.0 |
| N6—Cu2—N5 | 78.18 (15) | C18—C25—H25 | 119.0 |
| C7—N1—C2 | 121.6 (4) | C25—C26—C21 | 121.3 (5) |
| C7—N1—Cu1 | 124.3 (3) | C25—C26—H26 | 119.4 |
| C2—N1—Cu1 | 113.9 (3) | C21—C26—H26 | 119.4 |
| C15—N2—C19 | 118.8 (4) | O6—C27—O5 | 126.1 (6) |
| C15—N2—Cu1 | 123.8 (3) | O6—C27—C28 | 116.9 (6) |
| C19—N2—Cu1 | 117.4 (3) | O5—C27—C28 | 117.0 (5) |
| C24—N3—C20 | 117.9 (4) | N4—C28—C27 | 107.7 (4) |
| C24—N3—Cu1 | 133.8 (4) | N4—C28—C29 | 111.2 (4) |
| C20—N3—Cu1 | 108.3 (3) | C27—C28—C29 | 105.8 (5) |
| C33—N4—C28 | 121.6 (4) | N4—C28—H28 | 110.6 |
| C33—N4—Cu2 | 121.5 (3) | C27—C28—H28 | 110.6 |
| C28—N4—Cu2 | 114.4 (3) | C29—C28—H28 | 110.6 |
| C41—N5—C45 | 117.9 (4) | C30—C29—C28 | 116.8 (5) |
| C41—N5—Cu2 | 133.3 (4) | C30—C29—H29A | 108.1 |
| C45—N5—Cu2 | 108.7 (3) | C28—C29—H29A | 108.1 |
| C50—N6—C46 | 119.5 (5) | C30—C29—H29B | 108.1 |
| C50—N6—Cu2 | 124.7 (4) | C28—C29—H29B | 108.1 |
| C46—N6—Cu2 | 115.8 (3) | H29A—C29—H29B | 107.3 |
| C1—O1—Cu1 | 115.1 (3) | C31—C30—C29 | 110.1 (6) |
| C9—O3—Cu1 | 125.4 (3) | C31—C30—C32 | 108.9 (5) |
| C10—O4—C14 | 116.0 (4) | C29—C30—C32 | 112.6 (5) |
| C27—O5—Cu2 | 116.7 (4) | C31—C30—H30 | 108.4 |

| | | | |
|---|---|---|---|
| C35—O7—Cu2 | 121.5 (3) | C29—C30—H30 | 108.4 |
| C36—O8—C40 | 117.3 (4) | C32—C30—H30 | 108.4 |
| H9A—O9—H9B | 91.9 | C30—C31—H31A | 109.5 |
| H10A—O10—H10B | 88.0 | C30—C31—H31B | 109.5 |
| O2—C1—O1 | 123.4 (5) | H31A—C31—H31B | 109.5 |
| O2—C1—C2 | 119.5 (5) | C30—C31—H31C | 109.5 |
| O1—C1—C2 | 116.9 (5) | H31A—C31—H31C | 109.5 |
| N1—C2—C1 | 108.1 (4) | H31B—C31—H31C | 109.5 |
| N1—C2—C3 | 111.0 (4) | C30—C32—H32A | 109.5 |
| C1—C2—C3 | 107.3 (4) | C30—C32—H32B | 109.5 |
| N1—C2—H2 | 110.1 | H32A—C32—H32B | 109.5 |
| C1—C2—H2 | 110.1 | C30—C32—H32C | 109.5 |
| C3—C2—H2 | 110.1 | H32A—C32—H32C | 109.5 |
| C2—C3—C4 | 116.9 (5) | H32B—C32—H32C | 109.5 |
| C2—C3—H3A | 108.1 | N4—C33—C34 | 125.7 (4) |
| C4—C3—H3A | 108.1 | N4—C33—H33 | 117.1 |
| C2—C3—H3B | 108.1 | C34—C33—H33 | 117.1 |
| C4—C3—H3B | 108.1 | C39—C34—C33 | 118.7 (4) |
| H3A—C3—H3B | 107.3 | C39—C34—C35 | 120.1 (4) |
| C6—C4—C5 | 109.1 (6) | C33—C34—C35 | 120.9 (4) |
| C6—C4—C3 | 112.1 (6) | O7—C35—C34 | 125.7 (4) |
| C5—C4—C3 | 109.8 (6) | O7—C35—C36 | 118.8 (4) |
| C6—C4—H4 | 108.6 | C34—C35—C36 | 115.5 (4) |
| C5—C4—H4 | 108.6 | C37—C36—O8 | 125.5 (4) |
| C3—C4—H4 | 108.6 | C37—C36—C35 | 121.5 (4) |
| C4—C5—H5A | 109.5 | O8—C36—C35 | 113.0 (4) |
| C4—C5—H5B | 109.5 | C36—C37—C38 | 121.1 (4) |
| H5A—C5—H5B | 109.5 | C36—C37—H37 | 119.4 |
| C4—C5—H5C | 109.5 | C38—C37—H37 | 119.4 |
| H5A—C5—H5C | 109.5 | C39—C38—C37 | 119.2 (5) |
| H5B—C5—H5C | 109.5 | C39—C38—H38 | 120.4 |
| C4—C6—H6A | 109.5 | C37—C38—H38 | 120.4 |
| C4—C6—H6B | 109.5 | C38—C39—C34 | 122.2 (5) |
| H6A—C6—H6B | 109.5 | C38—C39—H39 | 118.9 |
| C4—C6—H6C | 109.5 | C34—C39—H39 | 118.9 |
| H6A—C6—H6C | 109.5 | O8—C40—H40A | 109.5 |
| H6B—C6—H6C | 109.5 | O8—C40—H40B | 109.5 |
| N1—C7—C8 | 125.9 (4) | H40A—C40—H40B | 109.5 |
| N1—C7—H7 | 117.0 | O8—C40—H40C | 109.5 |
| C8—C7—H7 | 117.0 | H40A—C40—H40C | 109.5 |
| C13—C8—C7 | 117.7 (4) | H40B—C40—H40C | 109.5 |
| C13—C8—C9 | 120.0 (4) | N5—C41—C42 | 124.3 (5) |
| C7—C8—C9 | 122.0 (4) | N5—C41—H41 | 117.9 |
| O3—C9—C10 | 119.4 (4) | C42—C41—H41 | 117.9 |
| O3—C9—C8 | 124.6 (4) | C43—C42—C41 | 117.9 (5) |
| C10—C9—C8 | 116.0 (4) | C43—C42—H42 | 121.0 |
| C11—C10—O4 | 124.4 (4) | C41—C42—H42 | 121.0 |
| C11—C10—C9 | 121.7 (4) | C42—C43—C44 | 119.9 (5) |

| | | | |
|---|---|---|---|
| O4—C10—C9 | 113.8 (4) | C42—C43—H43 | 120.0 |
| C10—C11—C12 | 120.5 (4) | C44—C43—H43 | 120.0 |
| C10—C11—H11 | 119.8 | C43—C44—C45 | 117.8 (4) |
| C12—C11—H11 | 119.8 | C43—C44—C51 | 122.5 (5) |
| C13—C12—C11 | 119.8 (5) | C45—C44—C51 | 119.7 (5) |
| C13—C12—H12 | 120.1 | N5—C45—C44 | 122.2 (4) |
| C11—C12—H12 | 120.1 | N5—C45—C46 | 118.2 (4) |
| C12—C13—C8 | 121.9 (5) | C44—C45—C46 | 119.6 (4) |
| C12—C13—H13 | 119.0 | N6—C46—C47 | 121.5 (5) |
| C8—C13—H13 | 119.0 | N6—C46—C45 | 119.0 (4) |
| O4—C14—H14A | 109.5 | C47—C46—C45 | 119.5 (4) |
| O4—C14—H14B | 109.5 | C46—C47—C48 | 117.4 (5) |
| H14A—C14—H14B | 109.5 | C46—C47—C52 | 119.1 (5) |
| O4—C14—H14C | 109.5 | C48—C47—C52 | 123.4 (5) |
| H14A—C14—H14C | 109.5 | C49—C48—C47 | 120.1 (5) |
| H14B—C14—H14C | 109.5 | C49—C48—H48 | 120.0 |
| N2—C15—C16 | 122.4 (5) | C47—C48—H48 | 120.0 |
| N2—C15—H15 | 118.8 | C48—C49—C50 | 120.0 (5) |
| C16—C15—H15 | 118.8 | C48—C49—H49 | 120.0 |
| C17—C16—C15 | 120.7 (5) | C50—C49—H49 | 120.0 |
| C17—C16—H16 | 119.7 | N6—C50—C49 | 121.5 (5) |
| C15—C16—H16 | 119.7 | N6—C50—H50 | 119.2 |
| C16—C17—C18 | 118.8 (5) | C49—C50—H50 | 119.2 |
| C16—C17—H17 | 120.6 | C52—C51—C44 | 120.7 (5) |
| C18—C17—H17 | 120.6 | C52—C51—H51 | 119.6 |
| C17—C18—C19 | 117.9 (4) | C44—C51—H51 | 119.6 |
| C17—C18—C25 | 123.7 (5) | C51—C52—C47 | 121.3 (5) |
| C19—C18—C25 | 118.4 (4) | C51—C52—H52 | 119.4 |
| N2—C19—C18 | 121.3 (4) | C47—C52—H52 | 119.4 |
| | | | |
| C1—C2—C3—C4 | 174.4 (5) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C8–C13 ring.

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| O9—H9*A*···O2 | 0.85 | 2.22 | 2.715 (7) | 117 |
| O9—H9*B*···O2 | 0.85 | 2.20 | 2.715 (7) | 119 |
| O10—H10*A*···O6 | 0.85 | 2.27 | 2.805 (8) | 121 |
| O10—H10*B*···O6 | 0.85 | 2.27 | 2.805 (8) | 121 |
| C24—H24···O10[i] | 0.93 | 2.58 | 3.476 (8) | 162 |
| C40—H40*A*···O2[ii] | 0.96 | 2.53 | 3.486 (7) | 176 |
| C43—H43···O8[iii] | 0.93 | 2.48 | 3.172 (6) | 131 |
| C50—H50···O9[iv] | 0.93 | 2.35 | 3.268 (7) | 168 |
| C25—H25···*Cg*1[v] | 0.93 | 2.51 | 3.426 (6) | 168 |

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1; (ii) *x*+1, *y*, *z*+1; (iii) −*x*+1, *y*+1/2, −*z*+2; (iv) −*x*+1, *y*−1/2, −*z*+1; (v) −*x*, *y*−1/2, −*z*+1.