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# {*N*′-[(2-Oxidonaphthalen-1-yl)methylidene]benzohydrazidato}(1,10-phenanthroline)copper(II) methanol monosolvate

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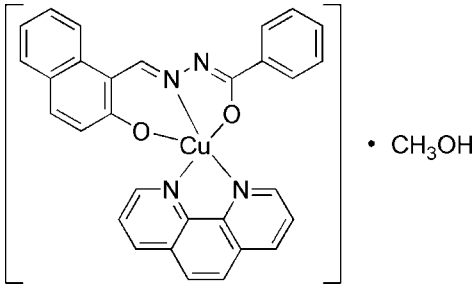
Key indicators: single-crystal X-ray study; $T$ = 185 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.042; $wR$ factor = 0.093; data-to-parameter ratio = 12.3.

The title mononuclear complex, $[Cu(C_{18}H_{12}N_2O_2)(C_{12}H_8N_2)]\cdot CH_3OH$, contains one *N*′-[(2-oxidonaphthalen-1-yl)methylidene]benzohydrazidate ligand ($L^{2-}$), a $Cu^{2+}$ cation, one 1,10-phenanthroline ligand and a methanol solvent molecule. The $Cu^{II}$ ion adopts a $CuO_2N_3$ distorted square-pyramidal coordination. An O—H···O hydrogen bond is formed between the methanol solvent molecule and the hydrazide O atom of the $L^{2-}$ ligand.

## Related literature

For details of the preparation of the Schiff base, see: Qiao *et al.* (2010). For applications of Schiff base compounds, see: Anford *et al.* (1998); Guo *et al.* (2010). For related structures, see: Huo *et al.* (2004); Liu *et al.* (2008); Sreeja *et al.* (2004).




## Experimental

### Crystal data

$[Cu(C_{18}H_{12}N_2O_2)(C_{12}H_8N_2)]\cdot CH_4O$
$M_r$ = 564.08
Monoclinic, $P2_1/c$
$a$ = 20.388 (2) Å
$b$ = 9.9707 (10) Å
$c$ = 12.5268 (12) Å
$\beta$ = 105.035 (2)°
$V$ = 2459.4 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.93 mm$^{-1}$
$T$ = 185 K
0.20 × 0.18 × 0.17 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.836, $T_{max}$ = 0.858
12077 measured reflections
4352 independent reflections
2950 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.059

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.093
$S$ = 1.02
4352 reflections
354 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Cu1—O2 | 1.913 (2) | Cu1—N4 | 2.023 (3) |
| Cu1—N2 | 1.914 (2) | Cu1—N3 | 2.321 (3) |
| Cu1—O1 | 1.984 (2) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3*A*···O1 | 0.84 | 1.99 | 2.820 (3) | 167 |

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2374).

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# supporting information

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# {*N*′-[(2-Oxidonaphthalen-1-yl)methylidene]benzohydrazidato}(1,10-phenanthroline)copper(II) methanol monosolvate

**Bao-Lin Liu, De-Ming Dong, Xiu-Yi Hua and Jian-Wei Zhu**

## S1. Comment

The study of transition metal-hydrazone compounds (Huo *et al.*, 2004), in which the acylhydrazone ligands are formed by condensing hydrazine with naphthaldehyde or their derivatives, has attracted considerable attention because of the magnetochemistry and chemical versatility of these compounds (Anford *et al.*, 1998; Guo *et al.*, 2010). We selected acyl-hydrazone ligand of 2-hydroxy-1-naphthaldehyde benzoylhydrazide ($H_2L$) to construct coordination polymers with defined geometry. We report here the preparation and crystal structure of the title Schiff base copper(II) compound (Fig. 1, Table 1). The title compound has a distorted square-pyramidal geometry and the central $Cu^{II}$ is five-coordinated with the two O atoms and one N atom from $H_2L$ and two N atoms from 1,10-phenanthroline. Several mononuclear compounds with similar structures have been reported previously (Sreeja *et al.*, 2004; Liu *et al.*, 2008). The square plane around the Cu1 atom is formed by $O_2N_2$ donor atoms (O1, O2, N2 and N4 ). The apical position occupied by the second nitrogen atom (N3) of 1,10-phenanthroline with a larger distance than N4. The four basal atoms are coplanar showing a significant distortion from square geometry indicated by the trans-bond angle O1—Cu1—O2 [162.81 (9)°]. $Cu^{II}$ is displaced from the basal plane in the direction of the axial nitrogen, which is evident from the bond angles of N2—Cu1—N4 [172.79 (11)°] and O1—Cu1—N2 [80.85 (10)°]. The maximum displacements from the least-squares plane through O1, O2, N2 and N4 are -0.0600 (21)Å and 0.1055 (27) Å for atoms O1 and N2, respectively; Cu1 is 0.2104 (4)Å below this plane. O3—H3A···O1 hydrogen bond is formed between the methanol solvent molecule and the O atom of the $L^{2-}$ ligand (Table 2).

## S2. Experimental

The 2-hydroxy-1-naphthaldehyde benzoylhydrazide ligand ($H_2L$) was prepared in a similar manner to the reported procedures (Qiao *et al.* 2010). The title compound was synthesised by adding $Cu(OAc)_2.H_2O$ (0.1 mmol) to a solution of $H_2L$ (0.1 mmol) and triethylamine (0.1 mmol) in methanol/dichloromethane (1:1 20 mL). After stirring for 3 h, 1,10-phenanthroline (0.1 mmol) was added to the resulting solution. Brown crystals of the title compound were isolated from the solution after two weeks.

## S3. Refinement

H atoms bonded to C atoms were placed in calculated positions and refined using a riding model [C$sp^2$–H = 0.95 Å; C$sp^3$–H = 0.98 Å and $U_{iso}$(H) = 1.2/1.5 *U*eq(C). H atoms bonded to methanol OH groups were located from difference Fourier series and then allowed to ride on their parent O atoms (AFIX 147) with $U_{iso}$(H) = 1.2*U*eq(C) refined.

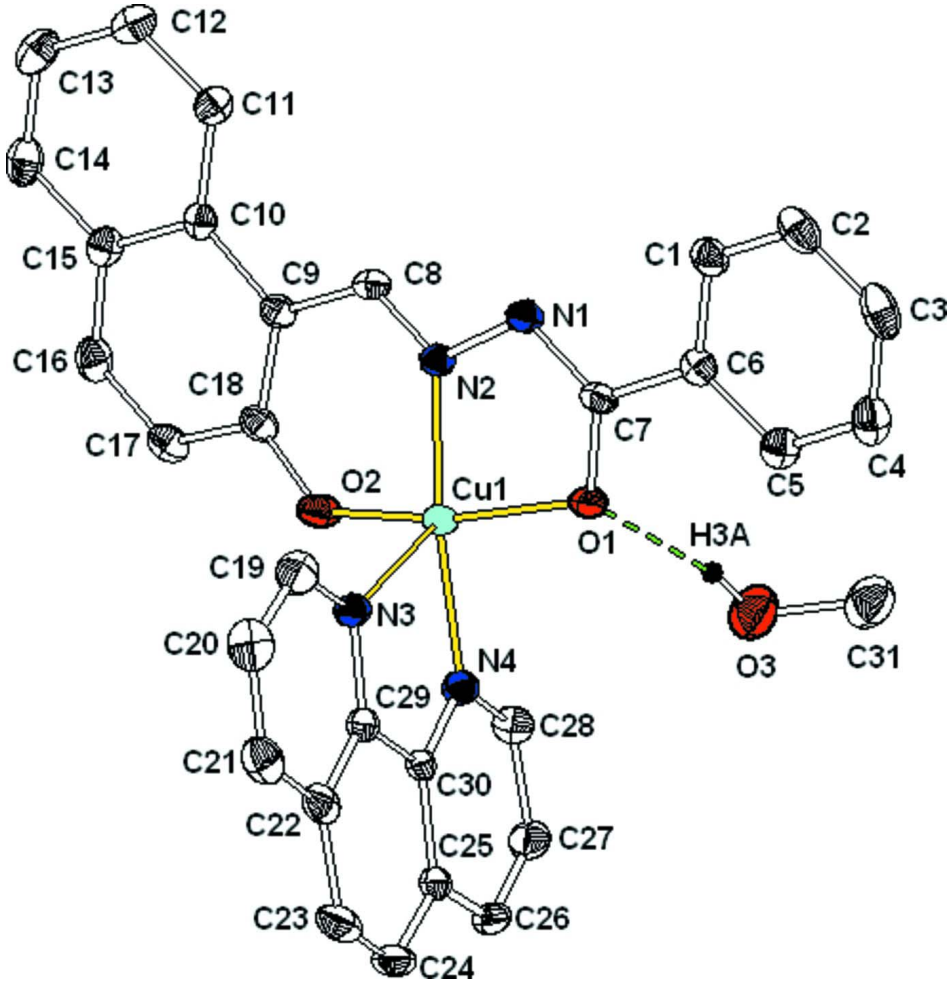


**Figure 1**

A view of the title organic compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

## {*N*′-[(2-Oxidonaphthalen-1-yl)methylidene]benzohydrazidato}(1,10- phenanthroline)copper(II) methanol monosolvate

*Crystal data*

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$M_r = 564.08$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 20.388$ (2) Å
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$c = 12.5268$ (12) Å
$\beta = 105.035$ (2)°
$V = 2459.4$ (4) Å$^3$
$Z = 4$
$F(000) = 1164$
$D_x = 1.523$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3881 reflections
$\theta = 2.3$–25.1°
$\mu = 0.93$ mm$^{-1}$
$T = 185$ K
Block, brown
0.20 × 0.18 × 0.17 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.836, $T_{max}$ = 0.858
12077 measured reflections
4352 independent reflections
2950 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.059
$\theta_{max}$ = 25.1°, $\theta_{min}$ = 2.1°
$h$ = −21→24
$k$ = −11→10
$l$ = −14→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.093
$S$ = 1.02
4352 reflections
354 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
$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 0.1098P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 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 | 0.25702 (2) | 0.62657 (4) | 0.14434 (3) | 0.02321 (13) |
| N2 | 0.22403 (12) | 0.6138 (3) | 0.2738 (2) | 0.0210 (6) |
| N4 | 0.30304 (13) | 0.6479 (3) | 0.0204 (2) | 0.0243 (7) |
| O1 | 0.32626 (11) | 0.5026 (2) | 0.23282 (18) | 0.0248 (5) |
| O2 | 0.20269 (11) | 0.7819 (2) | 0.09414 (18) | 0.0272 (5) |
| N1 | 0.25609 (13) | 0.5187 (3) | 0.3516 (2) | 0.0225 (6) |
| C22 | 0.21141 (17) | 0.3799 (3) | −0.1607 (3) | 0.0281 (8) |
| C10 | 0.08817 (15) | 0.8615 (3) | 0.2718 (3) | 0.0201 (7) |
| C30 | 0.28412 (16) | 0.5641 (3) | −0.0679 (3) | 0.0219 (8) |
| C18 | 0.15699 (16) | 0.8359 (3) | 0.1370 (3) | 0.0230 (8) |
| C17 | 0.12057 (16) | 0.9477 (3) | 0.0781 (3) | 0.0283 (8) |
| H17 | 0.1332 | 0.9819 | 0.0155 | 0.034* |
| C19 | 0.15462 (17) | 0.3786 (4) | 0.0142 (3) | 0.0334 (9) |
| H19 | 0.1345 | 0.3769 | 0.0747 | 0.040* |
| C29 | 0.23126 (16) | 0.4680 (3) | −0.0704 (3) | 0.0223 (8) |
| N3 | 0.20374 (13) | 0.4662 (3) | 0.0168 (2) | 0.0237 (7) |

| | | | | |
|---|---|---|---|---|
| C28 | 0.35071 (17) | 0.7391 (3) | 0.0217 (3) | 0.0298 (8) |
| H28 | 0.3632 | 0.7984 | 0.0830 | 0.036* |
| C7 | 0.30846 (16) | 0.4681 (3) | 0.3224 (3) | 0.0218 (8) |
| C6 | 0.34865 (15) | 0.3646 (3) | 0.3957 (3) | 0.0224 (7) |
| C5 | 0.40428 (16) | 0.3049 (3) | 0.3705 (3) | 0.0283 (8) |
| H5 | 0.4179 | 0.3337 | 0.3073 | 0.034* |
| C8 | 0.17973 (15) | 0.6886 (3) | 0.3031 (3) | 0.0211 (7) |
| H8 | 0.1713 | 0.6720 | 0.3730 | 0.025* |
| C15 | 0.04909 (16) | 0.9624 (3) | 0.2047 (3) | 0.0253 (8) |
| C27 | 0.38318 (17) | 0.7519 (4) | −0.0626 (3) | 0.0327 (9) |
| H27 | 0.4168 | 0.8190 | −0.0590 | 0.039* |
| C25 | 0.31509 (16) | 0.5700 (3) | −0.1560 (3) | 0.0252 (8) |
| C9 | 0.14253 (16) | 0.7951 (3) | 0.2367 (3) | 0.0213 (7) |
| C24 | 0.29397 (18) | 0.4778 (4) | −0.2454 (3) | 0.0337 (9) |
| H24 | 0.3152 | 0.4805 | −0.3046 | 0.040* |
| C16 | 0.06880 (17) | 1.0053 (3) | 0.1098 (3) | 0.0294 (8) |
| H16 | 0.0448 | 1.0770 | 0.0670 | 0.035* |
| C4 | 0.44030 (18) | 0.2036 (3) | 0.4365 (3) | 0.0346 (9) |
| H4 | 0.4786 | 0.1642 | 0.4187 | 0.042* |
| C23 | 0.24477 (18) | 0.3873 (4) | −0.2479 (3) | 0.0343 (9) |
| H23 | 0.2319 | 0.3271 | −0.3086 | 0.041* |
| C12 | 0.01612 (16) | 0.8884 (3) | 0.3977 (3) | 0.0322 (9) |
| H12 | 0.0051 | 0.8635 | 0.4642 | 0.039* |
| C20 | 0.13060 (19) | 0.2883 (3) | −0.0727 (3) | 0.0377 (10) |
| H20 | 0.0950 | 0.2275 | −0.0711 | 0.045* |
| C21 | 0.15930 (17) | 0.2894 (3) | −0.1600 (3) | 0.0352 (9) |
| H21 | 0.1438 | 0.2289 | −0.2198 | 0.042* |
| C13 | −0.02362 (18) | 0.9835 (3) | 0.3284 (3) | 0.0353 (9) |
| H13 | −0.0619 | 1.0222 | 0.3466 | 0.042* |
| C11 | 0.07096 (16) | 0.8301 (3) | 0.3714 (3) | 0.0251 (8) |
| H11 | 0.0979 | 0.7675 | 0.4211 | 0.030* |
| C2 | 0.36495 (18) | 0.2189 (3) | 0.5537 (3) | 0.0336 (9) |
| H2 | 0.3510 | 0.1889 | 0.6164 | 0.040* |
| C1 | 0.32968 (17) | 0.3206 (3) | 0.4892 (3) | 0.0274 (8) |
| H1 | 0.2922 | 0.3612 | 0.5084 | 0.033* |
| C14 | −0.00667 (17) | 1.0199 (3) | 0.2342 (3) | 0.0331 (9) |
| H14 | −0.0332 | 1.0856 | 0.1873 | 0.040* |
| C26 | 0.36606 (17) | 0.6671 (3) | −0.1501 (3) | 0.0300 (9) |
| H26 | 0.3885 | 0.6732 | −0.2076 | 0.036* |
| C3 | 0.42037 (19) | 0.1600 (3) | 0.5282 (3) | 0.0381 (10) |
| H3 | 0.4446 | 0.0903 | 0.5733 | 0.046* |
| O3 | 0.45503 (12) | 0.6073 (3) | 0.2347 (2) | 0.0496 (7) |
| H3A | 0.4200 | 0.5690 | 0.2430 | 0.074* |
| C31 | 0.51281 (18) | 0.5443 (4) | 0.3014 (4) | 0.0487 (11) |
| H31A | 0.5537 | 0.5877 | 0.2906 | 0.073* |
| H31B | 0.5128 | 0.4494 | 0.2810 | 0.073* |
| H31C | 0.5122 | 0.5518 | 0.3792 | 0.073* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0281 (2) | 0.0251 (2) | 0.0184 (2) | 0.0030 (2) | 0.00950 (17) | 0.0013 (2) |
| N2 | 0.0245 (14) | 0.0205 (15) | 0.0193 (15) | 0.0015 (13) | 0.0081 (12) | 0.0036 (13) |
| N4 | 0.0260 (15) | 0.0254 (16) | 0.0228 (17) | 0.0045 (13) | 0.0087 (13) | 0.0020 (13) |
| O1 | 0.0274 (12) | 0.0288 (13) | 0.0199 (14) | 0.0057 (10) | 0.0090 (11) | 0.0031 (10) |
| O2 | 0.0360 (13) | 0.0264 (13) | 0.0220 (14) | 0.0046 (11) | 0.0124 (11) | 0.0042 (10) |
| N1 | 0.0271 (16) | 0.0227 (15) | 0.0187 (16) | 0.0027 (12) | 0.0079 (13) | 0.0015 (13) |
| C22 | 0.0337 (19) | 0.0243 (19) | 0.024 (2) | 0.0075 (18) | 0.0038 (16) | 0.0030 (17) |
| C10 | 0.0194 (16) | 0.0169 (17) | 0.0224 (19) | −0.0027 (14) | 0.0026 (14) | −0.0041 (15) |
| C30 | 0.0228 (18) | 0.0262 (19) | 0.0174 (19) | 0.0095 (15) | 0.0065 (16) | 0.0066 (15) |
| C18 | 0.0289 (19) | 0.0201 (19) | 0.0185 (19) | −0.0016 (14) | 0.0032 (16) | −0.0031 (14) |
| C17 | 0.036 (2) | 0.026 (2) | 0.022 (2) | −0.0012 (16) | 0.0056 (18) | 0.0032 (16) |
| C19 | 0.034 (2) | 0.031 (2) | 0.036 (2) | 0.0011 (19) | 0.0110 (18) | 0.0088 (19) |
| C29 | 0.0224 (18) | 0.0227 (19) | 0.022 (2) | 0.0086 (15) | 0.0055 (16) | 0.0038 (15) |
| N3 | 0.0268 (16) | 0.0256 (16) | 0.0210 (17) | 0.0045 (13) | 0.0104 (14) | 0.0041 (12) |
| C28 | 0.032 (2) | 0.033 (2) | 0.026 (2) | 0.0006 (17) | 0.0095 (17) | 0.0021 (17) |
| C7 | 0.0259 (19) | 0.0244 (19) | 0.0153 (19) | −0.0037 (15) | 0.0059 (16) | −0.0025 (14) |
| C6 | 0.0232 (17) | 0.0203 (17) | 0.0228 (19) | −0.0037 (16) | 0.0041 (15) | −0.0006 (16) |
| C5 | 0.0295 (19) | 0.0247 (19) | 0.031 (2) | 0.0005 (16) | 0.0073 (17) | −0.0022 (16) |
| C8 | 0.0247 (18) | 0.0218 (18) | 0.0187 (19) | −0.0035 (15) | 0.0089 (16) | −0.0026 (15) |
| C15 | 0.0241 (19) | 0.0218 (19) | 0.030 (2) | 0.0010 (15) | 0.0062 (17) | −0.0016 (16) |
| C27 | 0.029 (2) | 0.040 (2) | 0.032 (2) | 0.0010 (17) | 0.0136 (18) | 0.0117 (18) |
| C25 | 0.0258 (19) | 0.0297 (19) | 0.021 (2) | 0.0111 (16) | 0.0067 (17) | 0.0051 (16) |
| C9 | 0.0244 (18) | 0.0197 (18) | 0.0193 (19) | −0.0012 (15) | 0.0050 (15) | −0.0006 (15) |
| C24 | 0.042 (2) | 0.041 (2) | 0.022 (2) | 0.0164 (19) | 0.0154 (19) | 0.0033 (17) |
| C16 | 0.0294 (19) | 0.0234 (19) | 0.032 (2) | 0.0071 (16) | 0.0024 (18) | 0.0030 (16) |
| C4 | 0.032 (2) | 0.030 (2) | 0.037 (2) | 0.0038 (17) | 0.0012 (19) | −0.0067 (18) |
| C23 | 0.047 (2) | 0.034 (2) | 0.021 (2) | 0.008 (2) | 0.0072 (18) | −0.0025 (18) |
| C12 | 0.032 (2) | 0.033 (2) | 0.036 (2) | −0.0023 (18) | 0.0159 (18) | −0.0052 (18) |
| C20 | 0.040 (2) | 0.026 (2) | 0.045 (3) | −0.0039 (18) | 0.007 (2) | 0.0040 (19) |
| C21 | 0.039 (2) | 0.028 (2) | 0.033 (2) | 0.0024 (18) | 0.0009 (19) | −0.0030 (17) |
| C13 | 0.029 (2) | 0.032 (2) | 0.048 (3) | 0.0073 (18) | 0.016 (2) | −0.0036 (19) |
| C11 | 0.0256 (18) | 0.0216 (19) | 0.029 (2) | 0.0011 (15) | 0.0090 (17) | 0.0004 (15) |
| C2 | 0.037 (2) | 0.033 (2) | 0.026 (2) | −0.0103 (18) | −0.0001 (18) | 0.0073 (17) |
| C1 | 0.0255 (19) | 0.032 (2) | 0.023 (2) | −0.0059 (16) | 0.0034 (17) | −0.0017 (16) |
| C14 | 0.028 (2) | 0.027 (2) | 0.041 (3) | 0.0077 (16) | 0.0046 (19) | 0.0043 (17) |
| C26 | 0.029 (2) | 0.040 (2) | 0.025 (2) | 0.0100 (17) | 0.0146 (18) | 0.0105 (17) |
| C3 | 0.041 (2) | 0.027 (2) | 0.037 (2) | 0.0005 (17) | −0.008 (2) | 0.0085 (17) |
| O3 | 0.0353 (15) | 0.0576 (19) | 0.057 (2) | −0.0004 (15) | 0.0143 (15) | 0.0074 (15) |
| C31 | 0.035 (2) | 0.056 (3) | 0.056 (3) | −0.007 (2) | 0.014 (2) | −0.009 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O2 | 1.913 (2) | C8—C9 | 1.437 (4) |
| Cu1—N2 | 1.914 (2) | C8—H8 | 0.9500 |
| Cu1—O1 | 1.984 (2) | C15—C14 | 1.405 (4) |

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|---|---|---|---|
| Cu1—N4 | 2.023 (3) | C15—C16 | 1.417 (5) |
| Cu1—N3 | 2.321 (3) | C27—C26 | 1.357 (5) |
| N2—C8 | 1.296 (4) | C27—H27 | 0.9500 |
| N2—N1 | 1.396 (3) | C25—C26 | 1.408 (4) |
| N4—C28 | 1.328 (4) | C25—C24 | 1.427 (5) |
| N4—C30 | 1.360 (4) | C24—C23 | 1.344 (4) |
| O1—C7 | 1.312 (4) | C24—H24 | 0.9500 |
| O2—C18 | 1.306 (3) | C16—H16 | 0.9500 |
| N1—C7 | 1.315 (4) | C4—C3 | 1.384 (5) |
| C22—C21 | 1.395 (4) | C4—H4 | 0.9500 |
| C22—C29 | 1.406 (4) | C23—H23 | 0.9500 |
| C22—C23 | 1.431 (4) | C12—C11 | 1.374 (4) |
| C10—C11 | 1.416 (4) | C12—C13 | 1.395 (5) |
| C10—C15 | 1.416 (4) | C12—H12 | 0.9500 |
| C10—C9 | 1.454 (4) | C20—C21 | 1.367 (5) |
| C30—C25 | 1.407 (4) | C20—H20 | 0.9500 |
| C30—C29 | 1.436 (4) | C21—H21 | 0.9500 |
| C18—C9 | 1.416 (4) | C13—C14 | 1.362 (5) |
| C18—C17 | 1.433 (4) | C13—H13 | 0.9500 |
| C17—C16 | 1.349 (4) | C11—H11 | 0.9500 |
| C17—H17 | 0.9500 | C2—C1 | 1.378 (4) |
| C19—N3 | 1.323 (4) | C2—C3 | 1.382 (5) |
| C19—C20 | 1.400 (5) | C2—H2 | 0.9500 |
| C19—H19 | 0.9500 | C1—H1 | 0.9500 |
| C29—N3 | 1.352 (4) | C14—H14 | 0.9500 |
| C28—C27 | 1.390 (4) | C26—H26 | 0.9500 |
| C28—H28 | 0.9500 | C3—H3 | 0.9500 |
| C7—C6 | 1.480 (4) | O3—C31 | 1.403 (4) |
| C6—C5 | 1.387 (4) | O3—H3A | 0.8400 |
| C6—C1 | 1.396 (4) | C31—H31A | 0.9800 |
| C5—C4 | 1.388 (5) | C31—H31B | 0.9800 |
| C5—H5 | 0.9500 | C31—H31C | 0.9800 |

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|---|---|---|---|
| O2—Cu1—N2 | 91.80 (10) | C10—C15—C16 | 118.3 (3) |
| O2—Cu1—O1 | 162.81 (9) | C26—C27—C28 | 118.9 (3) |
| N2—Cu1—O1 | 80.85 (10) | C26—C27—H27 | 120.6 |
| O2—Cu1—N4 | 90.39 (10) | C28—C27—H27 | 120.6 |
| N2—Cu1—N4 | 172.79 (11) | C30—C25—C26 | 117.6 (3) |
| O1—Cu1—N4 | 95.16 (9) | C30—C25—C24 | 118.9 (3) |
| O2—Cu1—N3 | 101.75 (9) | C26—C25—C24 | 123.5 (3) |
| N2—Cu1—N3 | 109.43 (10) | C18—C9—C8 | 121.6 (3) |
| O1—Cu1—N3 | 95.36 (9) | C18—C9—C10 | 119.0 (3) |
| N4—Cu1—N3 | 76.80 (10) | C8—C9—C10 | 119.4 (3) |
| C8—N2—N1 | 115.4 (3) | C23—C24—C25 | 121.5 (3) |
| C8—N2—Cu1 | 128.7 (2) | C23—C24—H24 | 119.3 |
| N1—N2—Cu1 | 115.65 (18) | C25—C24—H24 | 119.3 |
| C28—N4—C30 | 118.9 (3) | C17—C16—C15 | 122.2 (3) |
| C28—N4—Cu1 | 123.1 (2) | C17—C16—H16 | 118.9 |

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|---|---|---|---|
| C30—N4—Cu1 | 118.0 (2) | C15—C16—H16 | 118.9 |
| C7—O1—Cu1 | 109.05 (19) | C3—C4—C5 | 119.9 (3) |
| C18—O2—Cu1 | 127.8 (2) | C3—C4—H4 | 120.1 |
| C7—N1—N2 | 109.5 (2) | C5—C4—H4 | 120.1 |
| C21—C22—C29 | 117.3 (3) | C24—C23—C22 | 121.1 (3) |
| C21—C22—C23 | 123.5 (3) | C24—C23—H23 | 119.4 |
| C29—C22—C23 | 119.2 (3) | C22—C23—H23 | 119.4 |
| C11—C10—C15 | 116.7 (3) | C11—C12—C13 | 121.0 (3) |
| C11—C10—C9 | 123.3 (3) | C11—C12—H12 | 119.5 |
| C15—C10—C9 | 120.0 (3) | C13—C12—H12 | 119.5 |
| N4—C30—C25 | 121.4 (3) | C21—C20—C19 | 118.8 (3) |
| N4—C30—C29 | 118.7 (3) | C21—C20—H20 | 120.6 |
| C25—C30—C29 | 119.9 (3) | C19—C20—H20 | 120.6 |
| O2—C18—C9 | 125.3 (3) | C20—C21—C22 | 119.7 (3) |
| O2—C18—C17 | 116.0 (3) | C20—C21—H21 | 120.2 |
| C9—C18—C17 | 118.6 (3) | C22—C21—H21 | 120.2 |
| C16—C17—C18 | 121.4 (3) | C14—C13—C12 | 118.9 (3) |
| C16—C17—H17 | 119.3 | C14—C13—H13 | 120.5 |
| C18—C17—H17 | 119.3 | C12—C13—H13 | 120.5 |
| N3—C19—C20 | 123.6 (3) | C12—C11—C10 | 121.4 (3) |
| N3—C19—H19 | 118.2 | C12—C11—H11 | 119.3 |
| C20—C19—H19 | 118.2 | C10—C11—H11 | 119.3 |
| N3—C29—C22 | 123.3 (3) | C1—C2—C3 | 120.7 (3) |
| N3—C29—C30 | 117.2 (3) | C1—C2—H2 | 119.7 |
| C22—C29—C30 | 119.5 (3) | C3—C2—H2 | 119.7 |
| C19—N3—C29 | 117.3 (3) | C2—C1—C6 | 120.5 (3) |
| C19—N3—Cu1 | 133.5 (2) | C2—C1—H1 | 119.8 |
| C29—N3—Cu1 | 109.2 (2) | C6—C1—H1 | 119.8 |
| N4—C28—C27 | 123.0 (3) | C13—C14—C15 | 121.6 (3) |
| N4—C28—H28 | 118.5 | C13—C14—H14 | 119.2 |
| C27—C28—H28 | 118.5 | C15—C14—H14 | 119.2 |
| O1—C7—N1 | 124.2 (3) | C27—C26—C25 | 120.2 (3) |
| O1—C7—C6 | 118.8 (3) | C27—C26—H26 | 119.9 |
| N1—C7—C6 | 117.0 (3) | C25—C26—H26 | 119.9 |
| C5—C6—C1 | 118.5 (3) | C2—C3—C4 | 119.5 (3) |
| C5—C6—C7 | 120.8 (3) | C2—C3—H3 | 120.2 |
| C1—C6—C7 | 120.7 (3) | C4—C3—H3 | 120.2 |
| C6—C5—C4 | 121.0 (3) | C31—O3—H3A | 109.5 |
| C6—C5—H5 | 119.5 | O3—C31—H31A | 109.5 |
| C4—C5—H5 | 119.5 | O3—C31—H31B | 109.5 |
| N2—C8—C9 | 124.3 (3) | H31A—C31—H31B | 109.5 |
| N2—C8—H8 | 117.9 | O3—C31—H31C | 109.5 |
| C9—C8—H8 | 117.9 | H31A—C31—H31C | 109.5 |
| C14—C15—C10 | 120.2 (3) | H31B—C31—H31C | 109.5 |
| C14—C15—C16 | 121.5 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3*A*···O1 | 0.84 | 1.99 | 2.820 (3) | 167 |