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# Bis(4-aminophenylhydroxamato-$\kappa^2O,O'$)copper(II) methanol disolvate

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**Keywords:** crystal structure; copper complex; 4-aminophenylhydroxamic acid; solvate; hydrogen bonds.

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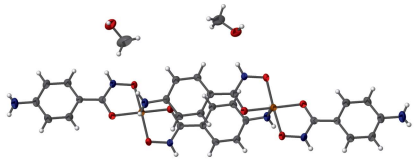
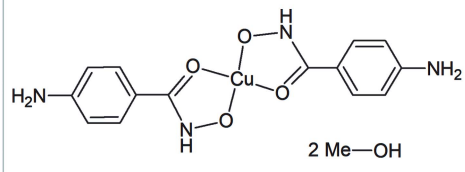
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title complex, $[Cu(C_7H_7N_2O_2)_2]\cdot 2CH_3OH$, the metal centre is coordinated by two 4-aminophenylhydroxamate bidentate ligands, in a distorted square-planar geometry. The asymmetric unit is completed by two methanol solvent molecules, which are involved in hydrogen bonding with N—H functionalities of the free hydroxamate groups. The crystal structure also features N—H···O bonds formed by the $NH_2$ groups, and O—H···O hydrogen bonds with the methanol solvent molecules as donors.

**3D view**



**Chemical scheme**




## Structure description

The asymmetric unit of the title compound consists of a $Cu^{II}$ metal centre bound to two bidentate 4-Apha$^-$ ligands (4-AphaH is 4-aminophenylhydroxamic acid) in a distorted square-planar geometry, to form $[Cu(4\text{-Apha})_2]$. A weak interaction exists between two neighbouring $[Cu(4\text{-Apha})_2]$ molecules, forming a contact between the metal and the free amino $NH_2$ group of the ligand 4-Apha$^-$ (Fig. 1). The compound crystallizes with two methanol molecules for each $[Cu(4\text{-Apha})_2]$ complex in the crystal. The Cu—O bond lengths range from 1.9208 (13) to 1.9583 (14) Å, which agrees well with the values observed in related structures (*e.g.* Chen *et al.*, 2015; Gaynor *et al.*, 2001). The apical Cu···N contact is 2.487 (2) Å, which is larger than that reported for five-coordinated $Cu^{II}$ complexes (*e.g.* Applegate *et al.*, 2003). It may be thus be considered as a weak interaction between the $Cu^{II}$ ion and the $NH_2$ group, which was not observed in the hydrate of the same complex (Gaynor *et al.*, 2001). The Cu···Cu distance in the centrosymmetric pseudo-dimers resulting from these contacts is 8.8174 (8) Å.

In the crystal, N—H···O hydrogen bonds are formed between the $NH_2$ groups of 4-Apha$^-$ as hydrogen-bond donors and O atoms of the O—N(H)– hydroxamate groups as hydrogen-bond acceptors. The methanol solvent molecules are connected to the

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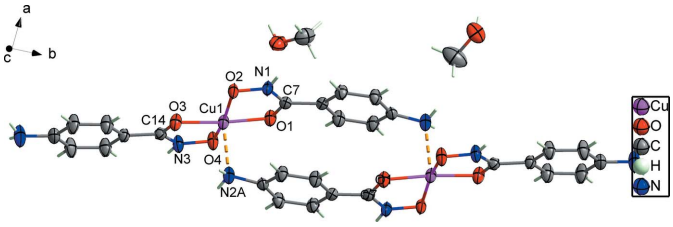


**Figure 1**
The structure of title complex, with displacement ellipsoids drawn at the 30% probability level. Two complexes are represented, in order to emphasize contacts involving the $NH_2$ group in the ligand (dashed bonds). [Symmetry code: (A) $-x, 1-y, 1-z$.]

[Cu(4-Apha)$_2$] complex molecules through N—H···O and O—H···O hydrogen bonds, forming a three-dimensional supramolecular network structure (Table 1 and Fig. 2).

## Synthesis and crystallization

A mixture of 4-AphaH (0.0306 g, 0.2 mmol), Cu(CH$_3$COO)$_2$·H$_2$O (0.0199 g, 0.1 mmol) and methanol (1 ml) was sealed in a 6 ml Pyrex tube. The tube was heated to 323 K for a day under autogenous pressure. Slow cooling of the resultant solution to room temperature gave green rod-shaped crystals [yield 0.0230 g (56% based on Cu)].

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Funding information

This research was supported by the Natural Science Foundation of Hubei Province (No. 2016CFB147), the Foundation of Hubei Educational Committee (No. D20172904) and Doctoral Fund Project of Huanggang Normal University (grant No. 2015001803).

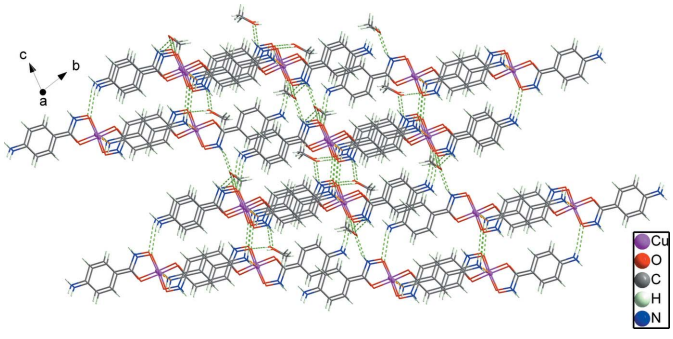


**Figure 2**
Crystal packing of title complex, viewed down the *a* axis, with hydrogen bonds drawn as dashed lines.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O5 | 0.86 | 2.05 | 2.848 (2) | 154 |
| N3—H3···O6$^{i}$ | 0.86 | 2.03 | 2.840 (2) | 157 |
| N2—H2$B$···O2$^{ii}$ | 0.85 (3) | 2.30 (3) | 3.147 (3) | 175 (2) |
| N4—H4$A$···O4$^{iii}$ | 0.81 (3) | 2.34 (3) | 3.149 (3) | 171 (3) |
| O5—H5$A$···O2$^{iv}$ | 0.82 | 1.93 | 2.745 (2) | 179 |
| O6—H6$A$···O4$^{v}$ | 0.82 | 1.94 | 2.756 (2) | 173 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | [Cu(C$_7$H$_7$N$_2$O$_2$)$_2$]·2CH$_4$O |
| $M_r$ | 429.92 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 288 |
| $a, b, c$ (Å) | 7.3969 (7), 9.7196 (10), 13.6589 (14) |
| $\alpha, \beta, \gamma$ (°) | 75.309 (1), 82.904 (1), 83.066 (1) |
| $V$ (Å$^3$) | 938.53 (16) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.20 |
| Crystal size (mm) | 0.30 × 0.24 × 0.20 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2005) |
| $T_{min}$, $T_{max}$ | 0.714, 0.795 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 6568, 3301, 2962 |
| $R_{int}$ | 0.016 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.594 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.027, 0.071, 1.03 |
| No. of reflections | 3301 |
| No. of parameters | 264 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.25, −0.29 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2005), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *DIAMOND* (Brandenburg, 1999).

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# full crystallographic data

*IUCrData* (2018). **3**, x180033 [https://doi.org/10.1107/S2414314618000330]

## Bis(4-aminophenylhydroxamato-$\kappa^2O,O'$)copper(II) methanol disolvate

**Yansi Zhao and Yanmei Chen**

### Bis(4-aminobenzhydroxamato-$\kappa^2O,O'$)copper(II) methanol disolvate

*Crystal data*

$[Cu(C_7H_7N_2O_2)_2]\cdot 2CH_4O$
$M_r = 429.92$
Triclinic, $P\overline{1}$
$a = 7.3969$ (7) Å
$b = 9.7196$ (10) Å
$c = 13.6589$ (14) Å
$\alpha = 75.309$ (1)°
$\beta = 82.904$ (1)°
$\gamma = 83.066$ (1)°
$V = 938.53$ (16) Å$^3$
$Z = 2$
$F(000) = 446$
$D_x = 1.521$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3706 reflections
$\theta = 2.8$–27.3°
$\mu = 1.20$ mm$^{-1}$
$T = 288$ K
Rod, green
0.30 × 0.24 × 0.20 mm

*Data collection*

Bruker APEXII CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2005)
$T_{min} = 0.714$, $T_{max} = 0.795$
6568 measured reflections
3301 independent reflections
2962 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -8\rightarrow 8$
$k = -11\rightarrow 11$
$l = -16\rightarrow 16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.071$
$S = 1.03$
3301 reflections
264 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 0.4758P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$

*Special details*

**Refinement**. Hydrogen atoms of the non-coordinating amine group N4 were found in a difference map and refined with free coordinates and isotropic displacement parameters. Other H atoms were placed geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.96 (methyl), O—H = 0.82 and N—H = 0.86 Å. For these H atoms, isotropic displacement parameters were based on $U_{eq}$ parameters of their carrier atoms.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.03678 (3) | 0.05781 (2) | 0.68807 (2) | 0.02744 (10) |
| N1 | 0.2586 (2) | 0.17752 (17) | 0.52451 (13) | 0.0308 (4) |
| H1 | 0.3254 | 0.1947 | 0.4674 | 0.037* |
| C1 | 0.2397 (3) | 0.4293 (2) | 0.52501 (14) | 0.0243 (4) |
| O1 | 0.1102 (2) | 0.24819 (14) | 0.65777 (10) | 0.0308 (3) |
| O2 | 0.2065 (2) | 0.04134 (14) | 0.56879 (11) | 0.0315 (3) |
| C2 | 0.1814 (3) | 0.5281 (2) | 0.58312 (15) | 0.0322 (5) |
| H2 | 0.1354 | 0.4959 | 0.6506 | 0.039* |
| N2 | 0.2485 (3) | 0.87055 (19) | 0.39870 (17) | 0.0351 (4) |
| H2A | 0.322 (3) | 0.894 (3) | 0.355 (2) | 0.037 (8)* |
| H2B | 0.233 (3) | 0.920 (3) | 0.442 (2) | 0.044 (7)* |
| N3 | −0.1200 (2) | −0.07629 (17) | 0.87137 (13) | 0.0317 (4) |
| H3 | −0.1720 | −0.0961 | 0.9325 | 0.038* |
| C3 | 0.1903 (3) | 0.6722 (2) | 0.54304 (16) | 0.0327 (5) |
| H3A | 0.1496 | 0.7361 | 0.5833 | 0.039* |
| O3 | −0.0158 (2) | −0.13922 (14) | 0.72716 (10) | 0.0326 (3) |
| O4 | −0.0667 (2) | 0.05964 (14) | 0.82653 (10) | 0.0336 (3) |
| C4 | 0.2600 (3) | 0.7229 (2) | 0.44265 (15) | 0.0265 (4) |
| N4 | −0.2531 (4) | −0.7465 (2) | 0.9708 (2) | 0.0553 (6) |
| H4A | −0.212 (4) | −0.803 (3) | 0.937 (2) | 0.068 (10)* |
| H4B | −0.278 (4) | −0.772 (3) | 1.024 (2) | 0.059 (11)* |
| C5 | 0.3258 (3) | 0.6242 (2) | 0.38504 (16) | 0.0328 (5) |
| H5 | 0.3774 | 0.6561 | 0.3187 | 0.039* |
| O5 | 0.5020 (2) | 0.13785 (19) | 0.35327 (13) | 0.0499 (4) |
| H5A | 0.5889 | 0.0848 | 0.3772 | 0.075* |
| C6 | 0.3151 (3) | 0.4798 (2) | 0.42554 (16) | 0.0312 (5) |
| H6 | 0.3586 | 0.4156 | 0.3860 | 0.037* |
| O6 | 0.7664 (3) | 0.9217 (2) | 0.07809 (12) | 0.0518 (5) |
| H6A | 0.8534 | 0.9208 | 0.1102 | 0.078* |
| C7 | 0.2038 (3) | 0.2796 (2) | 0.57141 (14) | 0.0244 (4) |
| C8 | −0.1372 (3) | −0.3207 (2) | 0.86329 (15) | 0.0258 (4) |
| C9 | −0.1021 (3) | −0.4174 (2) | 0.80218 (17) | 0.0403 (5) |
| H9 | −0.0533 | −0.3859 | 0.7351 | 0.048* |
| C10 | −0.1370 (4) | −0.5572 (2) | 0.83750 (18) | 0.0427 (6) |
| H10 | −0.1086 | −0.6197 | 0.7952 | 0.051* |
| C11 | −0.2148 (3) | −0.6064 (2) | 0.93641 (17) | 0.0343 (5) |
| C12 | −0.2552 (3) | −0.5096 (2) | 0.99779 (17) | 0.0420 (6) |
| H12 | −0.3089 | −0.5402 | 1.0639 | 0.050* |
| C13 | −0.2166 (3) | −0.3693 (2) | 0.96193 (16) | 0.0378 (5) |
| H13 | −0.2439 | −0.3066 | 1.0042 | 0.045* |
| C14 | −0.0894 (3) | −0.1740 (2) | 0.81866 (15) | 0.0254 (4) |
| C15 | 0.5618 (4) | 0.2259 (3) | 0.25923 (19) | 0.0568 (7) |
| H15A | 0.4602 | 0.2883 | 0.2313 | 0.085* |
| H15B | 0.6123 | 0.1678 | 0.2134 | 0.085* |
| H15C | 0.6537 | 0.2818 | 0.2687 | 0.085* |

| | | | | |
|---|---|---|---|---|
| C16 | 0.6166 (4) | 0.8733 (4) | 0.1456 (2) | 0.0762 (10) |
| H16A | 0.6445 | 0.7751 | 0.1798 | 0.114* |
| H16B | 0.5120 | 0.8814 | 0.1085 | 0.114* |
| H16C | 0.5902 | 0.9300 | 0.1947 | 0.114* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.03733 (16) | 0.01877 (14) | 0.02422 (14) | −0.00400 (10) | 0.00401 (10) | −0.00424 (10) |
| N1 | 0.0383 (10) | 0.0180 (8) | 0.0316 (9) | −0.0039 (7) | 0.0101 (8) | −0.0033 (7) |
| C1 | 0.0237 (10) | 0.0219 (10) | 0.0266 (10) | −0.0018 (8) | −0.0026 (8) | −0.0046 (8) |
| O1 | 0.0421 (8) | 0.0229 (7) | 0.0264 (7) | −0.0064 (6) | 0.0054 (6) | −0.0065 (6) |
| O2 | 0.0414 (8) | 0.0165 (7) | 0.0334 (8) | −0.0046 (6) | 0.0078 (6) | −0.0047 (6) |
| C2 | 0.0443 (13) | 0.0260 (10) | 0.0240 (10) | −0.0043 (9) | 0.0061 (9) | −0.0058 (8) |
| N2 | 0.0472 (12) | 0.0221 (9) | 0.0344 (11) | −0.0087 (8) | 0.0006 (10) | −0.0037 (8) |
| N3 | 0.0467 (11) | 0.0220 (8) | 0.0255 (9) | −0.0121 (8) | 0.0085 (8) | −0.0056 (7) |
| C3 | 0.0428 (12) | 0.0244 (10) | 0.0320 (11) | −0.0025 (9) | 0.0020 (9) | −0.0121 (9) |
| O3 | 0.0487 (9) | 0.0214 (7) | 0.0249 (7) | −0.0038 (6) | 0.0081 (6) | −0.0061 (6) |
| O4 | 0.0534 (9) | 0.0203 (7) | 0.0268 (7) | −0.0119 (6) | 0.0078 (7) | −0.0064 (6) |
| C4 | 0.0269 (10) | 0.0218 (10) | 0.0305 (11) | −0.0053 (8) | −0.0046 (8) | −0.0038 (8) |
| N4 | 0.0826 (18) | 0.0269 (11) | 0.0549 (16) | −0.0194 (11) | 0.0102 (14) | −0.0085 (12) |
| C5 | 0.0405 (12) | 0.0287 (11) | 0.0265 (11) | −0.0062 (9) | 0.0054 (9) | −0.0042 (9) |
| O5 | 0.0409 (10) | 0.0530 (11) | 0.0472 (10) | 0.0031 (8) | 0.0088 (8) | −0.0060 (8) |
| C6 | 0.0376 (12) | 0.0251 (10) | 0.0305 (11) | −0.0028 (9) | 0.0050 (9) | −0.0101 (9) |
| O6 | 0.0601 (11) | 0.0650 (12) | 0.0333 (9) | −0.0213 (10) | 0.0019 (8) | −0.0134 (8) |
| C7 | 0.0245 (10) | 0.0219 (10) | 0.0258 (10) | −0.0022 (8) | −0.0025 (8) | −0.0043 (8) |
| C8 | 0.0304 (11) | 0.0207 (10) | 0.0256 (10) | −0.0024 (8) | 0.0003 (8) | −0.0058 (8) |
| C9 | 0.0583 (15) | 0.0292 (11) | 0.0310 (11) | −0.0080 (10) | 0.0111 (10) | −0.0083 (9) |
| C10 | 0.0638 (16) | 0.0254 (11) | 0.0402 (13) | −0.0071 (10) | 0.0067 (11) | −0.0147 (10) |
| C11 | 0.0383 (12) | 0.0236 (10) | 0.0403 (12) | −0.0067 (9) | −0.0038 (10) | −0.0049 (9) |
| C12 | 0.0600 (16) | 0.0318 (12) | 0.0312 (12) | −0.0154 (11) | 0.0106 (11) | −0.0043 (10) |
| C13 | 0.0547 (14) | 0.0274 (11) | 0.0323 (12) | −0.0099 (10) | 0.0074 (10) | −0.0115 (9) |
| C14 | 0.0266 (10) | 0.0230 (10) | 0.0260 (10) | −0.0009 (8) | −0.0008 (8) | −0.0062 (8) |
| C15 | 0.0502 (16) | 0.0701 (19) | 0.0414 (14) | 0.0071 (14) | −0.0022 (12) | −0.0045 (13) |
| C16 | 0.065 (2) | 0.114 (3) | 0.0594 (19) | −0.0310 (19) | 0.0109 (16) | −0.0355 (19) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.9208 (13) | N4—H4B | 0.72 (3) |
| Cu1—O3 | 1.9271 (14) | C5—C6 | 1.379 (3) |
| Cu1—O4 | 1.9543 (14) | C5—H5 | 0.9300 |
| Cu1—O2 | 1.9583 (14) | O5—C15 | 1.404 (3) |
| N1—C7 | 1.311 (2) | O5—H5A | 0.8200 |
| N1—O2 | 1.387 (2) | C6—H6 | 0.9300 |
| N1—H1 | 0.8600 | O6—C16 | 1.397 (3) |
| C1—C6 | 1.392 (3) | O6—H6A | 0.8200 |
| C1—C2 | 1.394 (3) | C8—C13 | 1.390 (3) |
| C1—C7 | 1.474 (3) | C8—C9 | 1.390 (3) |

| | | | |
|---|---|---|---|
| O1—C7 | 1.277 (2) | C8—C14 | 1.468 (3) |
| C2—C3 | 1.375 (3) | C9—C10 | 1.366 (3) |
| C2—H2 | 0.9300 | C9—H9 | 0.9300 |
| N2—C4 | 1.405 (3) | C10—C11 | 1.390 (3) |
| N2—H2A | 0.76 (3) | C10—H10 | 0.9300 |
| N2—H2B | 0.85 (3) | C11—C12 | 1.395 (3) |
| N3—C14 | 1.314 (2) | C12—C13 | 1.379 (3) |
| N3—O4 | 1.390 (2) | C12—H12 | 0.9300 |
| N3—H3 | 0.8600 | C13—H13 | 0.9300 |
| C3—C4 | 1.390 (3) | C15—H15A | 0.9600 |
| C3—H3A | 0.9300 | C15—H15B | 0.9600 |
| O3—C14 | 1.279 (2) | C15—H15C | 0.9600 |
| C4—C5 | 1.397 (3) | C16—H16A | 0.9600 |
| N4—C11 | 1.375 (3) | C16—H16B | 0.9600 |
| N4—H4A | 0.81 (3) | C16—H16C | 0.9600 |

| | | | |
|---|---|---|---|
| O1—Cu1—O3 | 173.99 (6) | C5—C6—H6 | 119.6 |
| O1—Cu1—O4 | 94.34 (6) | C1—C6—H6 | 119.6 |
| O3—Cu1—O4 | 84.02 (6) | C16—O6—H6A | 109.5 |
| O1—Cu1—O2 | 83.76 (5) | O1—C7—N1 | 118.48 (17) |
| O3—Cu1—O2 | 96.14 (5) | O1—C7—C1 | 119.60 (17) |
| O4—Cu1—O2 | 163.24 (6) | N1—C7—C1 | 121.86 (17) |
| C7—N1—O2 | 118.74 (16) | C13—C8—C9 | 117.67 (19) |
| C7—N1—H1 | 120.6 | C13—C8—C14 | 124.68 (18) |
| O2—N1—H1 | 120.6 | C9—C8—C14 | 117.64 (18) |
| C6—C1—C2 | 118.05 (18) | C10—C9—C8 | 122.1 (2) |
| C6—C1—C7 | 124.74 (17) | C10—C9—H9 | 119.0 |
| C2—C1—C7 | 117.04 (17) | C8—C9—H9 | 119.0 |
| C7—O1—Cu1 | 111.62 (12) | C9—C10—C11 | 120.3 (2) |
| N1—O2—Cu1 | 106.16 (10) | C9—C10—H10 | 119.8 |
| C3—C2—C1 | 121.52 (19) | C11—C10—H10 | 119.8 |
| C3—C2—H2 | 119.2 | N4—C11—C10 | 120.0 (2) |
| C1—C2—H2 | 119.2 | N4—C11—C12 | 121.8 (2) |
| C4—N2—H2A | 114.5 (19) | C10—C11—C12 | 118.23 (19) |
| C4—N2—H2B | 113.1 (17) | C13—C12—C11 | 121.0 (2) |
| H2A—N2—H2B | 114 (3) | C13—C12—H12 | 119.5 |
| C14—N3—O4 | 118.81 (16) | C11—C12—H12 | 119.5 |
| C14—N3—H3 | 120.6 | C12—C13—C8 | 120.7 (2) |
| O4—N3—H3 | 120.6 | C12—C13—H13 | 119.7 |
| C2—C3—C4 | 120.31 (19) | C8—C13—H13 | 119.7 |
| C2—C3—H3A | 119.8 | O3—C14—N3 | 118.59 (17) |
| C4—C3—H3A | 119.8 | O3—C14—C8 | 120.23 (17) |
| C14—O3—Cu1 | 111.93 (12) | N3—C14—C8 | 121.17 (17) |
| N3—O4—Cu1 | 106.62 (10) | O5—C15—H15A | 109.5 |
| C3—C4—C5 | 118.57 (18) | O5—C15—H15B | 109.5 |
| C3—C4—N2 | 119.88 (19) | H15A—C15—H15B | 109.5 |
| C5—C4—N2 | 121.31 (19) | O5—C15—H15C | 109.5 |
| C11—N4—H4A | 119 (2) | H15A—C15—H15C | 109.5 |

| | | | |
|---|---|---|---|
| C11—N4—H4B | 117 (3) | H15B—C15—H15C | 109.5 |
| H4A—N4—H4B | 119 (3) | O6—C16—H16A | 109.5 |
| C6—C5—C4 | 120.75 (19) | O6—C16—H16B | 109.5 |
| C6—C5—H5 | 119.6 | H16A—C16—H16B | 109.5 |
| C4—C5—H5 | 119.6 | O6—C16—H16C | 109.5 |
| C15—O5—H5A | 109.5 | H16A—C16—H16C | 109.5 |
| C5—C6—C1 | 120.71 (18) | H16B—C16—H16C | 109.5 |
| | | | |
| C7—N1—O2—Cu1 | 5.9 (2) | C2—C1—C7—N1 | −177.68 (19) |
| C6—C1—C2—C3 | 2.6 (3) | C13—C8—C9—C10 | −2.4 (4) |
| C7—C1—C2—C3 | −172.86 (19) | C14—C8—C9—C10 | 178.2 (2) |
| C1—C2—C3—C4 | −0.5 (3) | C8—C9—C10—C11 | 1.9 (4) |
| C14—N3—O4—Cu1 | 1.8 (2) | C9—C10—C11—N4 | 178.6 (2) |
| C2—C3—C4—C5 | −2.1 (3) | C9—C10—C11—C12 | −0.2 (4) |
| C2—C3—C4—N2 | 172.4 (2) | N4—C11—C12—C13 | −179.7 (2) |
| C3—C4—C5—C6 | 2.6 (3) | C10—C11—C12—C13 | −0.9 (4) |
| N2—C4—C5—C6 | −171.8 (2) | C11—C12—C13—C8 | 0.3 (4) |
| C4—C5—C6—C1 | −0.5 (3) | C9—C8—C13—C12 | 1.3 (3) |
| C2—C1—C6—C5 | −2.1 (3) | C14—C8—C13—C12 | −179.4 (2) |
| C7—C1—C6—C5 | 173.02 (19) | Cu1—O3—C14—N3 | 0.6 (2) |
| Cu1—O1—C7—N1 | −9.8 (2) | Cu1—O3—C14—C8 | −179.01 (14) |
| Cu1—O1—C7—C1 | 167.22 (13) | O4—N3—C14—O3 | −1.7 (3) |
| O2—N1—C7—O1 | 2.5 (3) | O4—N3—C14—C8 | 177.93 (17) |
| O2—N1—C7—C1 | −174.52 (16) | C13—C8—C14—O3 | 179.6 (2) |
| C6—C1—C7—O1 | −169.77 (19) | C9—C8—C14—O3 | −1.0 (3) |
| C2—C1—C7—O1 | 5.4 (3) | C13—C8—C14—N3 | 0.0 (3) |
| C6—C1—C7—N1 | 7.2 (3) | C9—C8—C14—N3 | 179.4 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O5 | 0.86 | 2.05 | 2.848 (2) | 154 |
| N3—H3···O6$^{i}$ | 0.86 | 2.03 | 2.840 (2) | 157 |
| N2—H2*B*···O2$^{ii}$ | 0.85 (3) | 2.30 (3) | 3.147 (3) | 175 (2) |
| N4—H4*A*···O4$^{iii}$ | 0.81 (3) | 2.34 (3) | 3.149 (3) | 171 (3) |
| O5—H5*A*···O2$^{iv}$ | 0.82 | 1.93 | 2.745 (2) | 179 |
| O6—H6*A*···O4$^{v}$ | 0.82 | 1.94 | 2.756 (2) | 173 |
| O6—H6*A*···N3$^{v}$ | 0.82 | 2.70 | 3.391 (2) | 143 |

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