

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

[4,4'-(Ethane-1,2-diylidinitrilo)bis(pent-2-en-2-olato)]copper(II) 0.25-hydrate

Muhammad Aslam,^{a,*} Itrat Anis,^b Nighat Afza,^a Ajaz Hussain,^c Waseem Ahmed^d and Muhammad Nadeem Arshad^{e*}

^aPakistan Council of Scientific and Industrial Research Laboratories Complex, Karachi 75280, Pakistan, ^bDepartment of Chemistry, University of Karachi, Karachi 75270, Pakistan, ^cDepartment of Chemistry, GC University, Faisalabad, Pakistan, ^dDepartment of Biochemistry, Federal Urdu University of Arts Science and Technology, Gulshan-e-Iqbal Campus, Karachi, Pakistan, and ^eDepartment of Chemistry, University of Gujrat (Hafiz Hayat campus), Gujrat 50781, Pakistan
Correspondence e-mail: maslamchemist@hotmail.com, mnchemist@hotmail.com

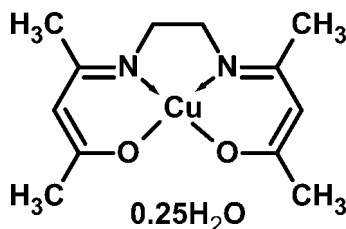
Received 12 April 2012; accepted 18 April 2012

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; disorder in solvent or counterion; R factor = 0.060; wR factor = 0.190; data-to-parameter ratio = 20.1.

In the title compound, $[\text{Cu}(\text{C}_{12}\text{H}_{18}\text{N}_2\text{O}_2)] \cdot 0.25\text{H}_2\text{O}$, the coordination of the O,N,N',O' -tetradentate ligand results in a *cis*- CuN_2O_2 square-planar geometry for the metal ion and the presence of two six-membered and one five-membered chelate rings. The complete complex molecule is close to planar (r.m.s. deviation = 0.047 Å). The uncoordinated water molecule (O-atom site symmetry 2) was modelled as half occupied. In the crystal, $\text{C}-\text{H} \cdots \text{O}_w$ and $\text{O}_w-\text{H} \cdots \text{O}$ ($w = \text{water}$) hydrogen bonds link the components into layers parallel to *ab* plane.

Related literature

For background to Schiff bases and their complexes, see: Aslam *et al.* (2012).



Experimental

Crystal data

$[\text{Cu}(\text{C}_{12}\text{H}_{18}\text{N}_2\text{O}_2)] \cdot 0.25\text{H}_2\text{O}$
 $M_r = 290.33$

Orthorhombic, *Pbcn*
 $a = 17.0029$ (7) Å

* Department of Chemistry, University of Karachi, Karachi 75270, Pakistan.

$b = 8.0198$ (3) Å
 $c = 19.6532$ (7) Å
 $V = 2679.91$ (18) Å³
 $Z = 8$

Mo $K\alpha$ radiation
 $\mu = 1.62$ mm⁻¹
 $T = 296$ K
 $0.24 \times 0.21 \times 0.13$ mm

Data collection

Bruker Kappa APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2007)
 $T_{\min} = 0.697$, $T_{\max} = 0.817$

22704 measured reflections
3338 independent reflections
1745 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$
 $wR(F^2) = 0.190$
 $S = 1.07$
3338 reflections
166 parameters
1 restraint

H atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{\max} = 0.56$ e Å⁻³
 $\Delta\rho_{\min} = -0.39$ e Å⁻³

Table 1

Selected bond lengths (Å).

| | | | |
|--------|-----------|--------|-----------|
| Cu1—O2 | 1.897 (4) | Cu1—N2 | 1.922 (4) |
| Cu1—O1 | 1.901 (4) | Cu1—N1 | 1.926 (4) |

Table 2

Hydrogen-bond geometry (Å, °).

| $D-\text{H} \cdots A$ | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|---|--------------|---------------------|--------------|-----------------------|
| $\text{C}12-\text{H}12A \cdots \text{O}1\text{W}^i$ | 0.96 | 2.58 | 3.466 (9) | 154 |
| $\text{C}6-\text{H}6B \cdots \text{O}1\text{W}^i$ | 0.97 | 2.44 | 3.303 (11) | 149 |
| $\text{O}1\text{W}-\text{H}1\text{WA} \cdots \text{O}2$ | 0.79 (2) | 2.29 (14) | 2.862 (8) | 130 (13) |

Symmetry code: (i) $x - \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

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: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

MA expresses his gratitude to the PCSIR Laboratories Complex, Karachi, the Department of Chemistry, University of Karachi, and the Department of Chemistry, GC University, Lahore, for providing financial support, research facilities and X-ray diffraction facilities, respectively. MNA also acknowledges Professor Helen Stoeckli-Evans, Switzerland, for guidance about the final refinement.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6739).

References

- Aslam, M., Anis, I., Afza, N., Ali, B. & Shah, M. R. (2012). *J. Chem. Soc. Pak.* **34**, 391–395.
Bruker (2007). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2012). E68, m670 [doi:10.1107/S1600536812017102]

[4,4'-(Ethane-1,2-diylidinitrilo)bis(pent-2-en-2-olato)]copper(II) 0.25-hydrate

Muhammad Aslam, Itrat Anis, Nighat Afza, Ajaz Hussain, Waseem Ahmed and Muhammad Nadeem Arshad

S1. Comment

Herein we report the crystal structure of title compound, (I), which is a Cu complex of schiff base in continuation of our studies on synthesis and metal complexation of schiff bases (Aslam *et al.*, 2012). The copper metal bonded to the ligand 4,4'-(ethane-1,2-diylidinitrilo)bis(pent-2-en-2-ol) through Cu—O covalent & Cu—N coordinate covalent bonds in such a way that it causes to produce two six membered rings (C2/C3/C4/Cu1/N1/O1) "A" & (C7/C8/C9/Cu1/N2/O2) "B" and a five membered ring (C5/C6/N1/Cu1/N2) "C". All these three rings are almost planar with the r. m. s. deviation of 0.0114 Å, 0.0061 Å and 0.0273 Å respectively. The molecule as a whole is slightly twisted as the five membered ring is oriented at dihedral angle of 2.54 (23)° and 3.34 (23)° with respect to six membered rings "A" and "B". Both of six membered rings are twisted at angle of 3.47 (16)° which shows the slight nonplanar behaviour of the molecule.

Moreover, a half water molecule have also been identified during refinement which links the molecules in two dimensional network through O—H⋯O and C—H⋯O interactions along *a* & *b* axes (Table. 2, Fig. 2).

S2. Experimental

A methanolic solution of copper (II) chloride dihydrated (1 mol) (5 ml) was slowly added to a methanolic solution of 4-{[2-((1-methyl-3-oxobutylidene)amino)ethyl]imino}-2-pentanone (1 mol) (100 ml) and refluxed with stirring for 45 min. The pH was gradually raised to achieve the suitable pH for the formulation of the complex by the drop wise addition of 1 M NaOH solution. Now the reaction mixture was refluxed with stirring for 90 min. After cooling, the mixture was concentrated to one third under reduced pressure. The concentrated reaction mixture was kept at room temperature and black crystals were obtained after six days. The crystalline product was collected, washed with cooled methanol, recrystallized from ethylacetate and methanol (1:1) mixture and dried to afford the title compound in 73.1% yield. Slow evaporation of a methanol solution afforded dark brown blocks of (I).

S3. Refinement

All the C—H and H-atoms were positioned with idealized geometry with C—H = 0.93 Å for aromatic, C—H = 0.97 Å for methylene & C—H = 0.96 Å for methyl group and were refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for aromatic & methylene and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ for methyl carbon atoms. The O—H = 0.79 (2) Å & O—H 0.95 (2) Å H atoms were refined using fourier map with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$.

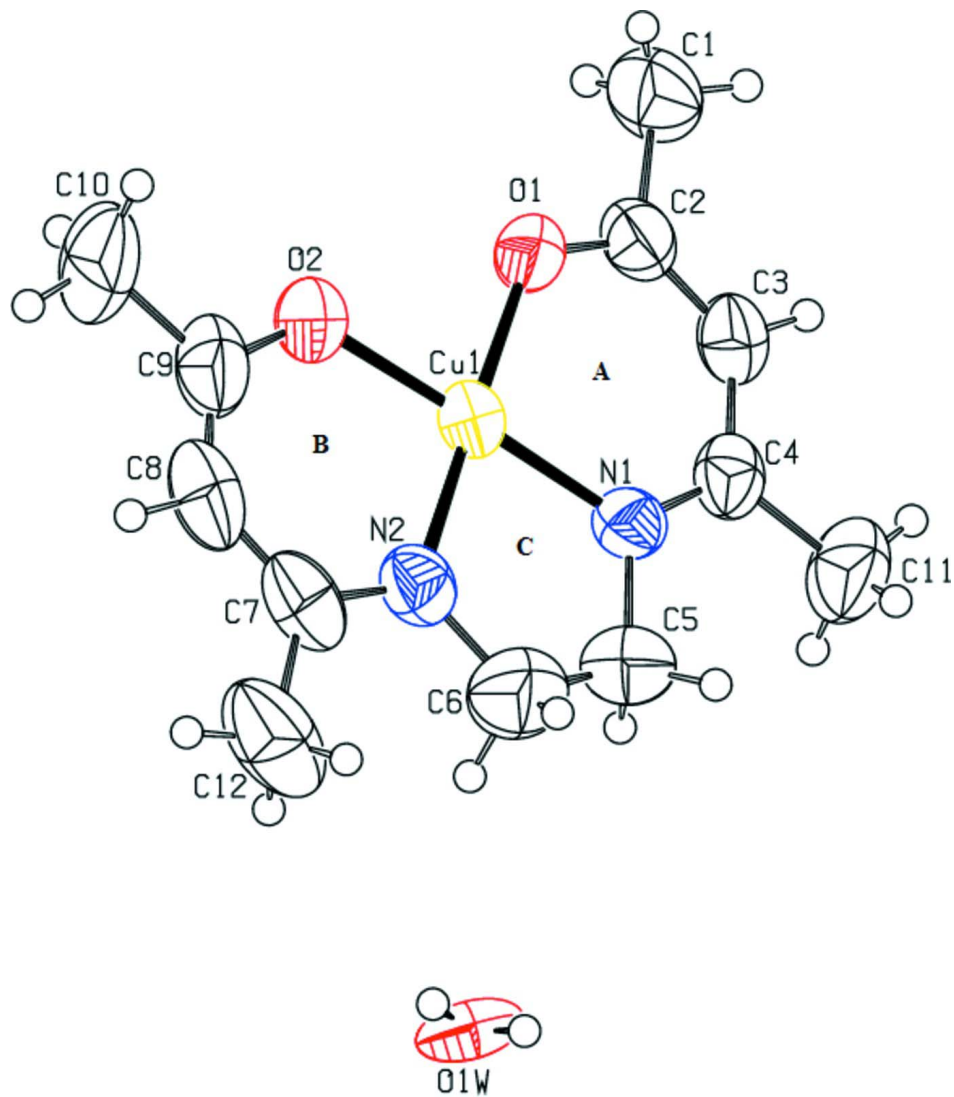


Figure 1

The molecular structure of (I) with 50% displacement ellipsoids.

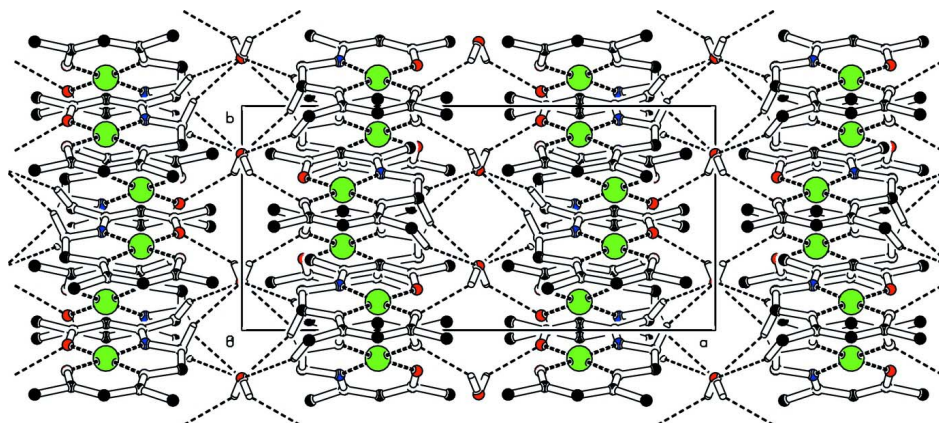


Figure 2

A view of the unit cell packing showing two dimensional hydrogen bonding network through dashed lines.

[4,4'-(Ethane-1,2-diyldinitrilo)bis(pent-2-en-2-olato)]copper(II) 0.25-hydrate*Crystal data*[Cu(C₁₂H₁₈N₂O₂)]·0.25H₂O $M_r = 290.33$ Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

 $a = 17.0029 (7) \text{ \AA}$ $b = 8.0198 (3) \text{ \AA}$ $c = 19.6532 (7) \text{ \AA}$ $V = 2679.91 (18) \text{ \AA}^3$ $Z = 8$ $F(000) = 1212$ $D_x = 1.439 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 5532 reflections

 $\theta = 2.4\text{--}25.9^\circ$ $\mu = 1.62 \text{ mm}^{-1}$ $T = 296 \text{ K}$

Block, dark brown

 $0.24 \times 0.21 \times 0.13 \text{ mm}$ *Data collection*Bruker Kappa APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2007)

 $T_{\min} = 0.697$, $T_{\max} = 0.817$

22704 measured reflections

3338 independent reflections

1745 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.042$ $\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 2.8^\circ$ $h = -22 \rightarrow 22$ $k = -8 \rightarrow 10$ $l = -22 \rightarrow 26$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.060$ $wR(F^2) = 0.190$ $S = 1.07$

3338 reflections

166 parameters

1 restraint

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0608P)^2 + 6.2772P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.56 \text{ e \AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$ *Special details*

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|-------------|-------------|-------------|----------------------------------|-----------|
| Cu1 | 0.28720 (4) | 0.12613 (9) | 0.19272 (3) | 0.0578 (3) | |

| | | | | | |
|------|------------|--------------|--------------|-------------|------|
| O1 | 0.3694 (2) | 0.1823 (5) | 0.13133 (18) | 0.0729 (11) | |
| O2 | 0.3675 (2) | 0.0653 (6) | 0.25492 (19) | 0.0791 (12) | |
| N1 | 0.2057 (2) | 0.2001 (5) | 0.1317 (2) | 0.0557 (10) | |
| N2 | 0.2037 (3) | 0.0604 (5) | 0.2529 (2) | 0.0609 (11) | |
| C1 | 0.4377 (4) | 0.2870 (10) | 0.0361 (3) | 0.096 (2) | |
| H1A | 0.4698 | 0.1885 | 0.0365 | 0.144* | |
| H1B | 0.4650 | 0.3758 | 0.0589 | 0.144* | |
| H1C | 0.4272 | 0.3189 | -0.0101 | 0.144* | |
| C2 | 0.3606 (4) | 0.2520 (7) | 0.0726 (3) | 0.0662 (15) | |
| C3 | 0.2912 (4) | 0.2910 (7) | 0.0431 (3) | 0.0670 (15) | |
| H3 | 0.2932 | 0.3401 | 0.0002 | 0.080* | |
| C4 | 0.2160 (3) | 0.2638 (6) | 0.0715 (3) | 0.0596 (13) | |
| C5 | 0.1275 (4) | 0.1746 (10) | 0.1597 (4) | 0.094 (2) | |
| H5A | 0.1025 | 0.2822 | 0.1659 | 0.113* | |
| H5B | 0.0963 | 0.1117 | 0.1273 | 0.113* | |
| C6 | 0.1280 (4) | 0.0880 (11) | 0.2234 (4) | 0.109 (3) | |
| H6A | 0.0964 | 0.1507 | 0.2555 | 0.131* | |
| H6B | 0.1027 | -0.0193 | 0.2169 | 0.131* | |
| C7 | 0.2129 (4) | -0.0013 (8) | 0.3139 (3) | 0.0741 (17) | |
| C8 | 0.2866 (5) | -0.0314 (8) | 0.3429 (3) | 0.084 (2) | |
| H8 | 0.2871 | -0.0793 | 0.3859 | 0.100* | |
| C9 | 0.3573 (5) | 0.0023 (9) | 0.3145 (3) | 0.0825 (18) | |
| C10 | 0.4323 (5) | -0.0375 (12) | 0.3520 (4) | 0.126 (3) | |
| H10A | 0.4631 | 0.0622 | 0.3569 | 0.189* | |
| H10B | 0.4617 | -0.1189 | 0.3269 | 0.189* | |
| H10C | 0.4199 | -0.0811 | 0.3962 | 0.189* | |
| C11 | 0.1458 (4) | 0.3136 (9) | 0.0287 (3) | 0.094 (2) | |
| H11A | 0.1143 | 0.3925 | 0.0534 | 0.141* | |
| H11B | 0.1149 | 0.2166 | 0.0186 | 0.141* | |
| H11C | 0.1637 | 0.3633 | -0.0129 | 0.141* | |
| C12 | 0.1418 (5) | -0.0453 (10) | 0.3561 (4) | 0.116 (3) | |
| H12A | 0.1105 | -0.1259 | 0.3323 | 0.174* | |
| H12B | 0.1111 | 0.0533 | 0.3642 | 0.174* | |
| H12C | 0.1585 | -0.0912 | 0.3988 | 0.174* | |
| O1W | 0.5000 | 0.2851 (13) | 0.2500 | 0.070 (3) | 0.50 |
| H1WA | 0.484 (9) | 0.205 (9) | 0.269 (6) | 0.105* | 0.50 |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|------------|--------------|-------------|
| Cu1 | 0.0602 (4) | 0.0703 (5) | 0.0430 (4) | 0.0012 (4) | -0.0011 (3) | -0.0032 (3) |
| O1 | 0.054 (2) | 0.116 (3) | 0.049 (2) | -0.002 (2) | -0.0047 (17) | 0.005 (2) |
| O2 | 0.071 (2) | 0.117 (3) | 0.049 (2) | 0.011 (2) | -0.0059 (19) | 0.006 (2) |
| N1 | 0.053 (2) | 0.059 (2) | 0.056 (2) | 0.002 (2) | 0.003 (2) | -0.010 (2) |
| N2 | 0.068 (3) | 0.060 (3) | 0.055 (3) | -0.006 (2) | 0.004 (2) | -0.008 (2) |
| C1 | 0.088 (5) | 0.124 (6) | 0.075 (4) | -0.022 (5) | 0.017 (4) | 0.006 (4) |
| C2 | 0.069 (4) | 0.079 (4) | 0.051 (3) | -0.011 (3) | 0.007 (3) | -0.006 (3) |
| C3 | 0.081 (4) | 0.074 (4) | 0.047 (3) | -0.002 (3) | -0.004 (3) | 0.006 (3) |

| | | | | | | |
|-----|-----------|-----------|------------|------------|------------|------------|
| C4 | 0.072 (3) | 0.052 (3) | 0.055 (3) | 0.005 (3) | -0.010 (3) | -0.010 (2) |
| C5 | 0.064 (4) | 0.131 (6) | 0.088 (5) | 0.002 (4) | 0.009 (4) | -0.012 (4) |
| C6 | 0.074 (5) | 0.156 (8) | 0.097 (5) | -0.013 (5) | 0.007 (4) | 0.009 (5) |
| C7 | 0.111 (5) | 0.057 (3) | 0.055 (3) | -0.013 (4) | 0.016 (4) | -0.009 (3) |
| C8 | 0.131 (6) | 0.075 (4) | 0.045 (3) | 0.003 (4) | -0.001 (4) | 0.004 (3) |
| C9 | 0.105 (5) | 0.087 (4) | 0.055 (4) | 0.014 (4) | -0.017 (4) | -0.001 (3) |
| C10 | 0.133 (7) | 0.167 (8) | 0.076 (5) | 0.032 (6) | -0.043 (5) | 0.014 (5) |
| C11 | 0.097 (5) | 0.103 (5) | 0.082 (4) | 0.014 (4) | -0.029 (4) | 0.009 (4) |
| C12 | 0.156 (7) | 0.120 (6) | 0.073 (4) | -0.041 (6) | 0.037 (5) | -0.003 (4) |
| O1W | 0.033 (5) | 0.055 (6) | 0.122 (10) | 0.000 | -0.007 (6) | 0.000 |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|------------|-----------|
| Cu1—O2 | 1.897 (4) | C5—H5A | 0.9700 |
| Cu1—O1 | 1.901 (4) | C5—H5B | 0.9700 |
| Cu1—N2 | 1.922 (4) | C6—H6A | 0.9700 |
| Cu1—N1 | 1.926 (4) | C6—H6B | 0.9700 |
| O1—C2 | 1.291 (6) | C7—C8 | 1.398 (8) |
| O2—C9 | 1.287 (7) | C7—C12 | 1.509 (9) |
| N1—C4 | 1.301 (7) | C8—C9 | 1.352 (9) |
| N1—C5 | 1.454 (7) | C8—H8 | 0.9300 |
| N2—C7 | 1.307 (7) | C9—C10 | 1.506 (9) |
| N2—C6 | 1.429 (8) | C10—H10A | 0.9600 |
| C1—C2 | 1.521 (8) | C10—H10B | 0.9600 |
| C1—H1A | 0.9600 | C10—H10C | 0.9600 |
| C1—H1B | 0.9600 | C11—H11A | 0.9600 |
| C1—H1C | 0.9600 | C11—H11B | 0.9600 |
| C2—C3 | 1.351 (7) | C11—H11C | 0.9600 |
| C3—C4 | 1.412 (7) | C12—H12A | 0.9600 |
| C3—H3 | 0.9300 | C12—H12B | 0.9600 |
| C4—C11 | 1.514 (7) | C12—H12C | 0.9600 |
| C5—C6 | 1.431 (10) | O1W—H1WA | 0.79 (2) |
| O2—Cu1—O1 | 86.59 (16) | H5A—C5—H5B | 107.7 |
| O2—Cu1—N2 | 93.75 (19) | N2—C6—C5 | 115.8 (6) |
| O1—Cu1—N2 | 177.56 (18) | N2—C6—H6A | 108.3 |
| O2—Cu1—N1 | 176.84 (19) | C5—C6—H6A | 108.3 |
| O1—Cu1—N1 | 93.48 (17) | N2—C6—H6B | 108.3 |
| N2—Cu1—N1 | 86.31 (19) | C5—C6—H6B | 108.3 |
| C2—O1—Cu1 | 125.8 (4) | H6A—C6—H6B | 107.4 |
| C9—O2—Cu1 | 126.2 (5) | N2—C7—C8 | 123.2 (6) |
| C4—N1—C5 | 121.5 (5) | N2—C7—C12 | 119.8 (7) |
| C4—N1—Cu1 | 126.2 (4) | C8—C7—C12 | 117.0 (6) |
| C5—N1—Cu1 | 112.3 (4) | C9—C8—C7 | 126.5 (6) |
| C7—N2—C6 | 122.7 (6) | C9—C8—H8 | 116.8 |
| C7—N2—Cu1 | 125.4 (4) | C7—C8—H8 | 116.8 |
| C6—N2—Cu1 | 112.0 (4) | O2—C9—C8 | 124.9 (6) |
| C2—C1—H1A | 109.5 | O2—C9—C10 | 114.5 (7) |

| | | | |
|------------|-----------|---------------|-----------|
| C2—C1—H1B | 109.5 | C8—C9—C10 | 120.6 (6) |
| H1A—C1—H1B | 109.5 | C9—C10—H10A | 109.5 |
| C2—C1—H1C | 109.5 | C9—C10—H10B | 109.5 |
| H1A—C1—H1C | 109.5 | H10A—C10—H10B | 109.5 |
| H1B—C1—H1C | 109.5 | C9—C10—H10C | 109.5 |
| O1—C2—C3 | 125.9 (5) | H10A—C10—H10C | 109.5 |
| O1—C2—C1 | 113.6 (5) | H10B—C10—H10C | 109.5 |
| C3—C2—C1 | 120.5 (5) | C4—C11—H11A | 109.5 |
| C2—C3—C4 | 125.8 (5) | C4—C11—H11B | 109.5 |
| C2—C3—H3 | 117.1 | H11A—C11—H11B | 109.5 |
| C4—C3—H3 | 117.1 | C4—C11—H11C | 109.5 |
| N1—C4—C3 | 122.8 (5) | H11A—C11—H11C | 109.5 |
| N1—C4—C11 | 120.2 (5) | H11B—C11—H11C | 109.5 |
| C3—C4—C11 | 117.0 (5) | C7—C12—H12A | 109.5 |
| C6—C5—N1 | 113.2 (6) | C7—C12—H12B | 109.5 |
| C6—C5—H5A | 108.9 | H12A—C12—H12B | 109.5 |
| N1—C5—H5A | 108.9 | C7—C12—H12C | 109.5 |
| C6—C5—H5B | 108.9 | H12A—C12—H12C | 109.5 |
| N1—C5—H5B | 108.9 | H12B—C12—H12C | 109.5 |

Hydrogen-bond geometry (Å, °)

| <i>D—H...A</i> | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|-----------------------------|------------|--------------|--------------|----------------|
| C12—H12A...O1W ^a | 0.96 | 2.58 | 3.466 (9) | 154 |
| C6—H6B...O1W ^a | 0.97 | 2.44 | 3.303 (11) | 149 |
| O1W—H1WA...O2 | 0.79 (2) | 2.29 (14) | 2.862 (8) | 130 (13) |

Symmetry code: (i) $x-1/2, y-1/2, -z+1/2$.