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Bis(μ -2-phenylacetato- κ^2 O:O)bis[(2,2'-bipyridyl- κ^2 N,N')(2-phenylacetato- κ O)-copper(II)] dihydrate

Wei Xu,* Ling Jin and Bin-Bin Liu

Center of Applied Solid State Chemistry Research, Ningbo University, Ningbo, Zhejiang 315211, People's Republic of China

Correspondence e-mail: xuwei@nbu.edu.cn

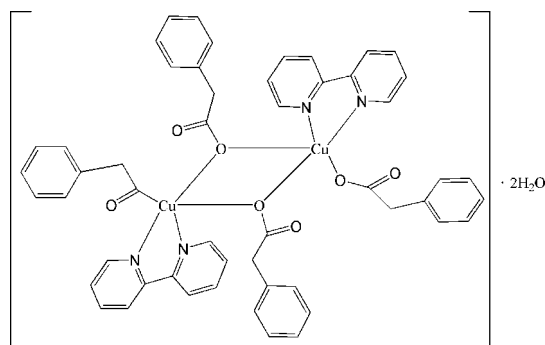
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.031; wR factor = 0.090; data-to-parameter ratio = 17.4.

The molecule of the binuclear title complex, $[\text{Cu}_2(\text{C}_8\text{H}_7\text{O}_2)_4(\text{C}_{10}\text{H}_8\text{N}_2)_2] \cdot 2\text{H}_2\text{O}$, is located on an inversion centre. The Cu atoms are bridged by two O atoms of the monodentate phenylacetate groups [$\text{Cu}-\text{O} = 1.9808(14)$ and $2.3668(14)$ Å]. The longer of the two bridging Cu—O bonds takes the apical position of the distorted square-pyramidal environment of the Cu atom, which is completed by two N atoms of the chelate 2,2'-bipyridine ligand [$\text{Cu}-\text{N} = 2.0107(17)$ and $2.0234(16)$ Å]. The molecules are assembled into stacks along [100] through π - π interactions with interplanar distances of 3.630(4) and 3.407(3) Å; the resulting stacks are further connected into a three-dimensional supramolecular architecture by $\text{O}-\text{H} \cdots \text{O}$ and $\text{C}-\text{H} \cdots \text{O}$ hydrogen-bonding interactions.

Related literature

For applications of inorganic-organic hybrid materials, see: Pan *et al.* (2003); Shibasaki & Yoshikawa (2002). For related structures, see: Addison & Rao (1984); Antolini *et al.* (1985); Zhang *et al.* (2006).



Experimental

Crystal data

$[\text{Cu}_2(\text{C}_8\text{H}_7\text{O}_2)_4(\text{C}_{10}\text{H}_8\text{N}_2)_2] \cdot 2\text{H}_2\text{O}$
 $M_r = 1016.02$
 Monoclinic, $P2_1/n$
 $a = 10.213(2)$ Å
 $b = 16.058(3)$ Å
 $c = 14.633(3)$ Å
 $\beta = 100.75(3)^\circ$
 $V = 2357.7(8)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.97$ mm⁻¹
 $T = 295$ K
 $0.17 \times 0.14 \times 0.11$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.678$, $T_{\max} = 0.784$
 22348 measured reflections
 5356 independent reflections
 4268 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.090$
 $S = 1.10$
 5356 reflections
 307 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.29$ e Å⁻³
 $\Delta\rho_{\min} = -0.56$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---|-------|--------------|--------------|----------------|
| $\text{O5}-\text{H51} \cdots \text{O4}$ | 0.85 | 2.05 | 2.781(3) | 143 |
| $\text{O5}-\text{H52} \cdots \text{O2}^i$ | 0.86 | 2.08 | 2.931(3) | 174 |
| $\text{C20}-\text{H20A} \cdots \text{O4}^{ii}$ | 0.93 | 2.38 | 3.245(3) | 156 |
| $\text{C24}-\text{H24A} \cdots \text{O2}^{iii}$ | 0.93 | 2.48 | 3.172(3) | 131 |
| $\text{C25}-\text{H25A} \cdots \text{O5}^{iv}$ | 0.93 | 2.50 | 3.201(3) | 132 |

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP II* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YA2144).

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supporting information

Acta Cryst. (2011). E67, m1334 [https://doi.org/10.1107/S1600536811035483]

Bis(μ -2-phenylacetato- κ^2 O:O)bis[(2,2'-bipyridyl- κ^2 N,N')(2-phenylacetato- κ O)copper(II)] dihydrate

Wei Xu, Ling Jin and Bin-Bin Liu

S1. Comment

The use of metal centers for organizing of molecular building blocks into inorganic–organic hybrid materials have been studied for potential applications in catalysis, gas storage, and in molecular–based magnetic materials (Pan *et al.*, 2003; Shibasaki & Yoshikawa, 2002). As part of our investigations of self-assemblies of Cu²⁺ ions and bipy with phenylacetic acid, we prepared the title complex, [Cu₂(C₈H₇O₂)₄(C₁₀H₈N₂)₂].2H₂O.

The molecule of the complex occupies a special position in the inversion centre (Fig. 1). The square pyramidal coordination environment of the Cu atom is formed by the N atoms of 2,2'-bipyridine ligands (Cu—N1 2.0108 (17) Å and Cu—N2 2.0234 (16) Å), the O atom of terminal phenylacetato ligand (Cu—O3 1.9557 (16) Å), and two O atoms of bridging phenylacetato groups, the O1ⁱ atom [symmetry code (i): 1 - x, -y, -z] takes one of the equatorial positions, whereas the O1 atom occupies the apical site. As one would expect (Antolini *et al.*, 1985; Zhang *et al.*, 2006), the apical bond Cu—O1 2.3669 (14) Å is substantially longer than the equatorial Cu—O1ⁱ distance of 1.9807 (14) Å. The Cu atom is displaced by 0.078 (1) Å towards the apical vertex from the mean plane of the equatorial ligands [$\tau = 0.04$ according to Addison & Rao (1984)].

The molecules are assembled into stacks along [100] through $\pi \cdots \pi$ stacking interactions with the mean interplanar distance of 3.407 (3) Å between adjacent bipy ligands and 3.630 (4) Å between bipy ligands and phenylacetato groups, and the stacks are further stabilized by the weak C—H \cdots O hydrogen bonding interactions from the phenyl CH groups to the uncoordinating carboxylate O2 and O4 atoms (Table 1), as well O—H \cdots O bonds involving water molecule (Fig. 2). As a result, three-dimensional network is formed.

S2. Experimental

Phenylacetic acid (0.2726 g, 2.000 mmol) was completely dissolved in a mixture of 10 ml of ethanol, 10 ml of water, and bipy (0.1561 g, 1.000 mmol). 0.2602 g (1.084 mmol) of Cu(NO₃)₂.3H₂O were then added, and after dropwise addition of 2.0 ml (1M) NaOH to the resulting solution under continuous stirring for 1 h, the blue suspension was produced. The suspension was filtered and the filtrate (pH = 6.51) was allowed to stand at room temperature for several weeks; the precipitation of blue block crystals was observed.

S3. Refinement

H atoms bonded to C atoms were placed in geometrically calculated positions (C—H 0.93 Å and 0.97 Å for aromatic and methylene H atoms respectively) and were included in the refinement in a riding model approximation, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. H atoms attached to O atoms were found in a difference Fourier synthesis and were also included in the riding model approximation, with the O—H distances fixed as initially found and with $U_{\text{iso}}(\text{H})$ values set at 1.5 $U_{\text{eq}}(\text{O})$.

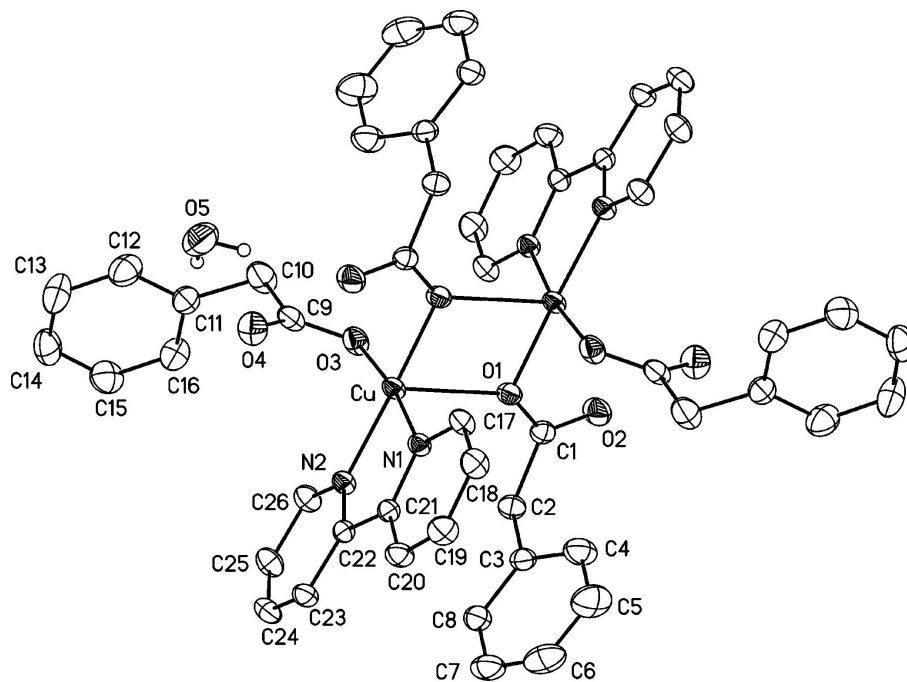


Figure 1

ORTEP view of the title compound. The displacement ellipsoids are drawn at 45% probability level; hydrogen atoms bonded to carbon were omitted.

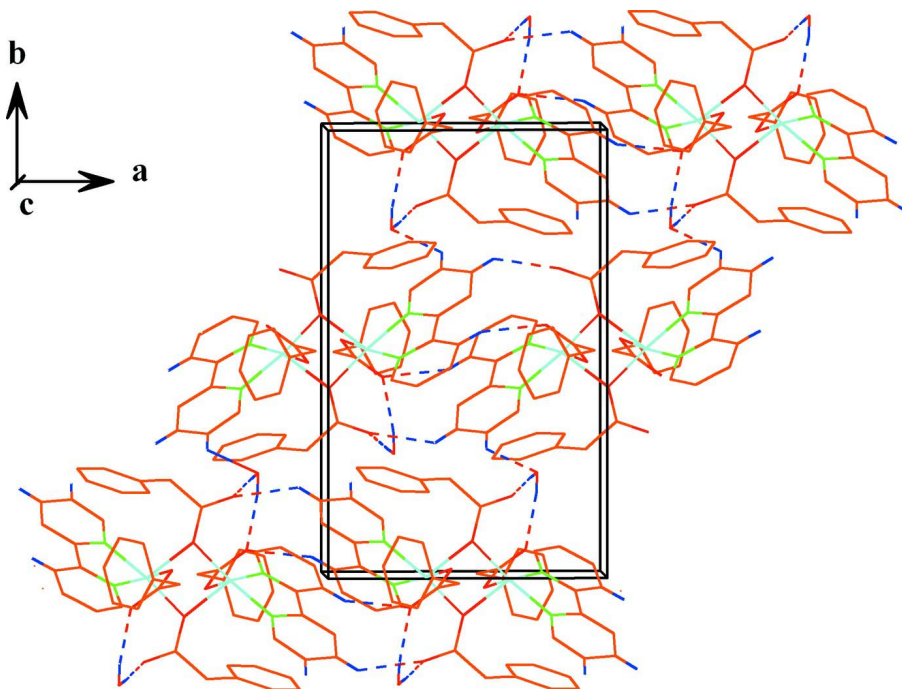


Figure 2

Crystal packing of the title complex viewed down the *c* axis. Hydrogen bonds are shown as dashed lines.

Bis(μ -2-phenylacetato- κ^2 O:O)bis[(2,2'-bipyridyl- κ^2 N,N')(2-phenylacetato- κ O)copper(II)] dihydrate

Crystal data

[Cu₂(C₈H₇O₂)₄(C₁₀H₈N₂)₂] \cdot 2H₂O
 $M_r = 1016.02$
 Monoclinic, $P2_1/n$
 Hall symbol: -P 2yn
 $a = 10.213$ (2) Å
 $b = 16.058$ (3) Å
 $c = 14.633$ (3) Å
 $\beta = 100.75$ (3)°
 $V = 2357.7$ (8) Å³
 $Z = 2$

$F(000) = 1052$
 $D_x = 1.431$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 22348 reflections
 $\theta = 3.1$ – 27.4 °
 $\mu = 0.97$ mm⁻¹
 $T = 295$ K
 Block, blue
 $0.17 \times 0.14 \times 0.11$ mm

Data collection

Rigaku R-AXIS RAPID
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 0 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.678$, $T_{\max} = 0.784$

22348 measured reflections
 5356 independent reflections
 4268 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\max} = 27.4$ °, $\theta_{\min} = 3.1$ °
 $h = -13 \rightarrow 13$
 $k = -20 \rightarrow 20$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.090$
 $S = 1.10$
 5356 reflections
 307 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
 $w = 1/[\sigma^2(F_o^2) + (0.0357P)^2 + 1.1037P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.29$ e Å⁻³
 $\Delta\rho_{\min} = -0.56$ e Å⁻³

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 (Å²)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|--------------|---------------|---------------|----------------------------------|
| Cu | 0.34936 (2) | 0.003603 (15) | 0.032956 (16) | 0.03079 (8) |
| O1 | 0.51708 (12) | 0.08258 (8) | -0.01885 (10) | 0.0349 (3) |
| O2 | 0.65975 (14) | 0.18355 (10) | -0.03382 (12) | 0.0509 (4) |
| C1 | 0.54722 (19) | 0.15958 (13) | -0.02762 (13) | 0.0335 (4) |

| | | | | |
|------|---------------|---------------|---------------|------------|
| C2 | 0.4344 (2) | 0.22176 (13) | -0.03118 (15) | 0.0390 (5) |
| H2A | 0.3904 | 0.2116 | 0.0211 | 0.047* |
| H2B | 0.4716 | 0.2775 | -0.0244 | 0.047* |
| C3 | 0.33151 (19) | 0.21773 (12) | -0.12042 (15) | 0.0371 (4) |
| C4 | 0.3645 (3) | 0.18987 (17) | -0.20253 (17) | 0.0583 (7) |
| H4A | 0.4507 | 0.1714 | -0.2029 | 0.070* |
| C5 | 0.2707 (3) | 0.1891 (2) | -0.2844 (2) | 0.0775 (9) |
| H5A | 0.2943 | 0.1704 | -0.3393 | 0.093* |
| C6 | 0.1426 (3) | 0.2159 (2) | -0.2846 (2) | 0.0747 (9) |
| H6A | 0.0796 | 0.2149 | -0.3394 | 0.090* |
| C7 | 0.1079 (2) | 0.24395 (17) | -0.2039 (2) | 0.0633 (8) |
| H7A | 0.0213 | 0.2620 | -0.2039 | 0.076* |
| C8 | 0.2023 (2) | 0.24547 (14) | -0.12211 (17) | 0.0467 (5) |
| H8A | 0.1786 | 0.2654 | -0.0678 | 0.056* |
| O3 | 0.43667 (14) | 0.02350 (11) | 0.16182 (10) | 0.0444 (4) |
| O4 | 0.28773 (16) | -0.06110 (11) | 0.20372 (11) | 0.0555 (4) |
| C9 | 0.3872 (2) | -0.01680 (15) | 0.22212 (14) | 0.0411 (5) |
| C10 | 0.4592 (2) | -0.00598 (19) | 0.32311 (16) | 0.0596 (7) |
| H10A | 0.5128 | -0.0550 | 0.3420 | 0.071* |
| H10B | 0.5188 | 0.0414 | 0.3269 | 0.071* |
| C11 | 0.3641 (2) | 0.00710 (15) | 0.38924 (15) | 0.0456 (5) |
| C12 | 0.3061 (3) | -0.05839 (18) | 0.42846 (19) | 0.0650 (7) |
| H12A | 0.3274 | -0.1128 | 0.4152 | 0.078* |
| C13 | 0.2172 (3) | -0.0439 (2) | 0.4869 (2) | 0.0742 (8) |
| H13A | 0.1795 | -0.0887 | 0.5129 | 0.089* |
| C14 | 0.1839 (3) | 0.0353 (2) | 0.50716 (18) | 0.0636 (7) |
| H14A | 0.1238 | 0.0447 | 0.5467 | 0.076* |
| C15 | 0.2394 (3) | 0.10011 (19) | 0.46888 (19) | 0.0631 (7) |
| H15A | 0.2170 | 0.1543 | 0.4821 | 0.076* |
| C16 | 0.3284 (3) | 0.08655 (17) | 0.41081 (18) | 0.0563 (6) |
| H16A | 0.3655 | 0.1319 | 0.3854 | 0.068* |
| N1 | 0.23495 (15) | -0.01459 (10) | -0.09298 (11) | 0.0314 (3) |
| N2 | 0.19920 (15) | 0.08350 (10) | 0.04221 (11) | 0.0325 (3) |
| C17 | 0.2643 (2) | -0.06336 (14) | -0.16069 (14) | 0.0391 (5) |
| H17A | 0.3461 | -0.0906 | -0.1511 | 0.047* |
| C18 | 0.1775 (2) | -0.07459 (15) | -0.24405 (15) | 0.0466 (5) |
| H18A | 0.2003 | -0.1090 | -0.2898 | 0.056* |
| C19 | 0.0565 (2) | -0.03411 (16) | -0.25860 (16) | 0.0495 (6) |
| H19A | -0.0037 | -0.0413 | -0.3141 | 0.059* |
| C20 | 0.0255 (2) | 0.01729 (14) | -0.18992 (15) | 0.0427 (5) |
| H20A | -0.0553 | 0.0456 | -0.1988 | 0.051* |
| C21 | 0.11684 (18) | 0.02584 (12) | -0.10760 (13) | 0.0312 (4) |
| C22 | 0.09470 (17) | 0.07952 (12) | -0.02961 (13) | 0.0306 (4) |
| C23 | -0.02197 (19) | 0.12337 (13) | -0.02906 (15) | 0.0383 (5) |
| H23A | -0.0940 | 0.1183 | -0.0781 | 0.046* |
| C24 | -0.0295 (2) | 0.17477 (14) | 0.04555 (16) | 0.0440 (5) |
| H24A | -0.1070 | 0.2047 | 0.0473 | 0.053* |
| C25 | 0.0786 (2) | 0.18136 (14) | 0.11732 (16) | 0.0452 (5) |

| | | | | |
|------|------------|---------------|--------------|------------|
| H25A | 0.0763 | 0.2170 | 0.1671 | 0.054* |
| C26 | 0.1906 (2) | 0.13390 (14) | 0.11387 (15) | 0.0405 (5) |
| H26A | 0.2626 | 0.1371 | 0.1631 | 0.049* |
| O5 | 0.2460 (2) | -0.23227 (13) | 0.20341 (15) | 0.0773 (6) |
| H51 | 0.2485 | -0.1839 | 0.2272 | 0.116* |
| H52 | 0.2711 | -0.2215 | 0.1520 | 0.116* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|---------------|
| Cu | 0.02265 (12) | 0.03791 (15) | 0.03088 (13) | 0.00331 (9) | 0.00258 (8) | -0.00214 (10) |
| O1 | 0.0285 (6) | 0.0323 (7) | 0.0433 (8) | 0.0024 (5) | 0.0051 (6) | 0.0023 (6) |
| O2 | 0.0342 (8) | 0.0455 (9) | 0.0739 (11) | -0.0039 (7) | 0.0121 (7) | 0.0069 (8) |
| C1 | 0.0320 (10) | 0.0356 (11) | 0.0312 (10) | 0.0014 (8) | 0.0019 (8) | -0.0005 (8) |
| C2 | 0.0400 (11) | 0.0334 (11) | 0.0426 (11) | 0.0032 (9) | 0.0055 (9) | -0.0029 (9) |
| C3 | 0.0351 (10) | 0.0321 (10) | 0.0428 (11) | 0.0030 (8) | 0.0039 (8) | 0.0058 (9) |
| C4 | 0.0551 (14) | 0.0698 (18) | 0.0468 (14) | 0.0191 (13) | 0.0007 (11) | -0.0008 (13) |
| C5 | 0.090 (2) | 0.090 (2) | 0.0448 (15) | 0.0176 (18) | -0.0081 (14) | -0.0041 (15) |
| C6 | 0.0710 (19) | 0.075 (2) | 0.0636 (19) | 0.0014 (16) | -0.0254 (15) | 0.0121 (15) |
| C7 | 0.0376 (12) | 0.0606 (17) | 0.086 (2) | 0.0029 (11) | -0.0042 (13) | 0.0222 (15) |
| C8 | 0.0377 (11) | 0.0428 (12) | 0.0599 (14) | 0.0023 (9) | 0.0099 (10) | 0.0093 (11) |
| O3 | 0.0309 (7) | 0.0674 (10) | 0.0337 (8) | 0.0018 (7) | 0.0031 (6) | -0.0036 (7) |
| O4 | 0.0500 (9) | 0.0661 (11) | 0.0491 (10) | -0.0099 (8) | 0.0062 (7) | -0.0053 (8) |
| C9 | 0.0315 (10) | 0.0574 (14) | 0.0335 (11) | 0.0116 (10) | 0.0037 (8) | -0.0074 (10) |
| C10 | 0.0410 (12) | 0.100 (2) | 0.0355 (12) | 0.0106 (13) | 0.0012 (9) | -0.0053 (13) |
| C11 | 0.0457 (12) | 0.0607 (15) | 0.0286 (10) | 0.0041 (11) | 0.0024 (9) | 0.0002 (10) |
| C12 | 0.090 (2) | 0.0494 (15) | 0.0579 (16) | 0.0079 (14) | 0.0187 (15) | 0.0018 (13) |
| C13 | 0.096 (2) | 0.071 (2) | 0.0629 (18) | -0.0154 (18) | 0.0345 (16) | 0.0074 (16) |
| C14 | 0.0631 (16) | 0.085 (2) | 0.0467 (15) | -0.0023 (15) | 0.0211 (12) | -0.0068 (15) |
| C15 | 0.0716 (18) | 0.0637 (17) | 0.0549 (16) | 0.0097 (14) | 0.0144 (13) | -0.0113 (13) |
| C16 | 0.0660 (16) | 0.0532 (15) | 0.0509 (14) | -0.0050 (12) | 0.0140 (12) | 0.0018 (12) |
| N1 | 0.0259 (7) | 0.0354 (9) | 0.0325 (8) | 0.0004 (6) | 0.0044 (6) | -0.0008 (7) |
| N2 | 0.0259 (7) | 0.0372 (9) | 0.0340 (8) | 0.0012 (7) | 0.0046 (6) | -0.0020 (7) |
| C17 | 0.0321 (10) | 0.0462 (12) | 0.0395 (11) | 0.0043 (9) | 0.0080 (8) | -0.0070 (9) |
| C18 | 0.0477 (12) | 0.0546 (14) | 0.0372 (11) | 0.0004 (11) | 0.0071 (9) | -0.0115 (10) |
| C19 | 0.0462 (13) | 0.0617 (15) | 0.0358 (12) | 0.0001 (11) | -0.0044 (9) | -0.0055 (11) |
| C20 | 0.0333 (10) | 0.0501 (13) | 0.0413 (12) | 0.0052 (9) | -0.0018 (9) | 0.0010 (10) |
| C21 | 0.0260 (9) | 0.0332 (10) | 0.0341 (10) | -0.0011 (7) | 0.0048 (7) | 0.0023 (8) |
| C22 | 0.0256 (8) | 0.0330 (10) | 0.0330 (10) | -0.0009 (8) | 0.0052 (7) | 0.0034 (8) |
| C23 | 0.0282 (9) | 0.0416 (11) | 0.0440 (11) | 0.0037 (8) | 0.0040 (8) | 0.0025 (9) |
| C24 | 0.0323 (10) | 0.0449 (12) | 0.0565 (14) | 0.0080 (9) | 0.0125 (9) | -0.0031 (10) |
| C25 | 0.0416 (11) | 0.0467 (13) | 0.0492 (13) | 0.0034 (10) | 0.0135 (10) | -0.0125 (10) |
| C26 | 0.0339 (10) | 0.0462 (12) | 0.0405 (11) | 0.0011 (9) | 0.0046 (8) | -0.0085 (10) |
| O5 | 0.0807 (14) | 0.0718 (13) | 0.0769 (14) | -0.0005 (11) | 0.0082 (11) | 0.0222 (11) |

Geometric parameters (Å, °)

| | | | |
|------------------------|-------------|--------------|-----------|
| Cu—O3 | 1.9558 (15) | C12—H12A | 0.9300 |
| Cu—O1 ⁱ | 1.9808 (14) | C13—C14 | 1.363 (4) |
| Cu—N1 | 2.0107 (17) | C13—H13A | 0.9300 |
| Cu—N2 | 2.0234 (16) | C14—C15 | 1.356 (4) |
| Cu—O1 | 2.3668 (14) | C14—H14A | 0.9300 |
| O1—C1 | 1.286 (2) | C15—C16 | 1.372 (4) |
| O1—Cu ⁱ | 1.9808 (14) | C15—H15A | 0.9300 |
| O2—C1 | 1.231 (2) | C16—H16A | 0.9300 |
| C1—C2 | 1.518 (3) | N1—C17 | 1.340 (3) |
| C2—C3 | 1.517 (3) | N1—C21 | 1.351 (2) |
| C2—H2A | 0.9700 | N2—C26 | 1.340 (3) |
| C2—H2B | 0.9700 | N2—C22 | 1.352 (2) |
| C3—C4 | 1.381 (3) | C17—C18 | 1.380 (3) |
| C3—C8 | 1.389 (3) | C17—H17A | 0.9300 |
| C4—C5 | 1.388 (4) | C18—C19 | 1.377 (3) |
| C4—H4A | 0.9300 | C18—H18A | 0.9300 |
| C5—C6 | 1.377 (4) | C19—C20 | 1.382 (3) |
| C5—H5A | 0.9300 | C19—H19A | 0.9300 |
| C6—C7 | 1.371 (4) | C20—C21 | 1.386 (3) |
| C6—H6A | 0.9300 | C20—H20A | 0.9300 |
| C7—C8 | 1.390 (3) | C21—C22 | 1.481 (3) |
| C7—H7A | 0.9300 | C22—C23 | 1.385 (3) |
| C8—H8A | 0.9300 | C23—C24 | 1.382 (3) |
| O3—C9 | 1.272 (3) | C23—H23A | 0.9300 |
| O4—C9 | 1.228 (3) | C24—C25 | 1.379 (3) |
| C9—C10 | 1.533 (3) | C24—H24A | 0.9300 |
| C10—C11 | 1.508 (3) | C25—C26 | 1.383 (3) |
| C10—H10A | 0.9700 | C25—H25A | 0.9300 |
| C10—H10B | 0.9700 | C26—H26A | 0.9300 |
| C11—C16 | 1.380 (3) | O5—H51 | 0.8494 |
| C11—C12 | 1.383 (4) | O5—H52 | 0.8560 |
| C12—C13 | 1.379 (4) | | |
| O3—Cu—O1 ⁱ | 90.90 (6) | C13—C12—C11 | 120.8 (3) |
| O3—Cu—N1 | 171.79 (6) | C13—C12—H12A | 119.6 |
| O1 ⁱ —Cu—N1 | 95.55 (6) | C11—C12—H12A | 119.6 |
| O3—Cu—N2 | 92.68 (7) | C14—C13—C12 | 120.8 (3) |
| O1 ⁱ —Cu—N2 | 174.44 (6) | C14—C13—H13A | 119.6 |
| N1—Cu—N2 | 80.52 (7) | C12—C13—H13A | 119.6 |
| O3—Cu—O1 | 89.67 (6) | C15—C14—C13 | 119.1 (3) |
| O1 ⁱ —Cu—O1 | 77.72 (6) | C15—C14—H14A | 120.5 |
| N1—Cu—O1 | 96.65 (6) | C13—C14—H14A | 120.5 |
| N2—Cu—O1 | 106.54 (6) | C14—C15—C16 | 120.7 (3) |
| C1—O1—Cu ⁱ | 118.61 (12) | C14—C15—H15A | 119.7 |
| C1—O1—Cu | 138.41 (12) | C16—C15—H15A | 119.7 |
| Cu ⁱ —O1—Cu | 102.28 (6) | C15—C16—C11 | 121.5 (3) |

| | | | |
|---------------|-------------|--------------|-------------|
| O2—C1—O1 | 123.49 (18) | C15—C16—H16A | 119.3 |
| O2—C1—C2 | 120.32 (19) | C11—C16—H16A | 119.3 |
| O1—C1—C2 | 116.18 (17) | C17—N1—C21 | 118.68 (17) |
| C3—C2—C1 | 113.63 (17) | C17—N1—Cu | 126.20 (13) |
| C3—C2—H2A | 108.8 | C21—N1—Cu | 115.11 (13) |
| C1—C2—H2A | 108.8 | C26—N2—C22 | 118.62 (16) |
| C3—C2—H2B | 108.8 | C26—N2—Cu | 126.61 (13) |
| C1—C2—H2B | 108.8 | C22—N2—Cu | 114.59 (13) |
| H2A—C2—H2B | 107.7 | N1—C17—C18 | 122.32 (19) |
| C4—C3—C8 | 118.3 (2) | N1—C17—H17A | 118.8 |
| C4—C3—C2 | 121.36 (19) | C18—C17—H17A | 118.8 |
| C8—C3—C2 | 120.3 (2) | C19—C18—C17 | 119.0 (2) |
| C3—C4—C5 | 120.9 (2) | C19—C18—H18A | 120.5 |
| C3—C4—H4A | 119.6 | C17—C18—H18A | 120.5 |
| C5—C4—H4A | 119.6 | C18—C19—C20 | 119.4 (2) |
| C6—C5—C4 | 120.1 (3) | C18—C19—H19A | 120.3 |
| C6—C5—H5A | 120.0 | C20—C19—H19A | 120.3 |
| C4—C5—H5A | 120.0 | C19—C20—C21 | 118.9 (2) |
| C7—C6—C5 | 120.0 (2) | C19—C20—H20A | 120.6 |
| C7—C6—H6A | 120.0 | C21—C20—H20A | 120.6 |
| C5—C6—H6A | 120.0 | N1—C21—C20 | 121.75 (19) |
| C6—C7—C8 | 119.9 (2) | N1—C21—C22 | 114.69 (16) |
| C6—C7—H7A | 120.1 | C20—C21—C22 | 123.56 (18) |
| C8—C7—H7A | 120.1 | N2—C22—C23 | 121.76 (18) |
| C3—C8—C7 | 120.9 (2) | N2—C22—C21 | 114.49 (16) |
| C3—C8—H8A | 119.5 | C23—C22—C21 | 123.75 (17) |
| C7—C8—H8A | 119.5 | C24—C23—C22 | 118.88 (19) |
| C9—O3—Cu | 114.65 (14) | C24—C23—H23A | 120.6 |
| O4—C9—O3 | 124.2 (2) | C22—C23—H23A | 120.6 |
| O4—C9—C10 | 120.3 (2) | C25—C24—C23 | 119.50 (19) |
| O3—C9—C10 | 115.5 (2) | C25—C24—H24A | 120.3 |
| C11—C10—C9 | 112.61 (19) | C23—C24—H24A | 120.3 |
| C11—C10—H10A | 109.1 | C24—C25—C26 | 118.7 (2) |
| C9—C10—H10A | 109.1 | C24—C25—H25A | 120.6 |
| C11—C10—H10B | 109.1 | C26—C25—H25A | 120.6 |
| C9—C10—H10B | 109.1 | N2—C26—C25 | 122.46 (19) |
| H10A—C10—H10B | 107.8 | N2—C26—H26A | 118.8 |
| C16—C11—C12 | 117.1 (2) | C25—C26—H26A | 118.8 |
| C16—C11—C10 | 120.3 (2) | H51—O5—H52 | 100.6 |
| C12—C11—C10 | 122.5 (2) | | |

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

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------------|-------|-------------|-------------|---------------|
| O5—H51 \cdots O4 | 0.85 | 2.05 | 2.781 (3) | 143 |
| O5—H52 \cdots O2 ⁱ | 0.86 | 2.08 | 2.931 (3) | 174 |

| | | | | |
|------------------------------|------|------|-----------|-----|
| C20—H20A···O4 ⁱⁱ | 0.93 | 2.38 | 3.245 (3) | 156 |
| C24—H24A···O2 ⁱⁱⁱ | 0.93 | 2.48 | 3.172 (3) | 131 |
| C25—H25A···O5 ^{iv} | 0.93 | 2.50 | 3.201 (3) | 132 |

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $-x, -y, -z$; (iii) $x-1, y, z$; (iv) $-x+1/2, y+1/2, -z+1/2$.