Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Tetra-$\mu$-acetato-$\kappa^8O:O'$-bis{[2-(phenylsulfanylmethyl)pyridine-$\kappa N$]copper(II)}

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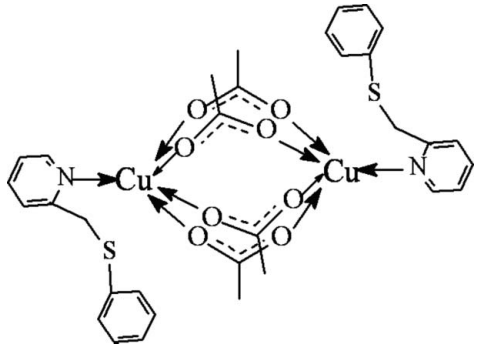
Received 25 May 2007; accepted 29 May 2007

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.028; $wR$ factor = 0.078; data-to-parameter ratio = 14.6.

The title compound, $[Cu_2(C_2H_3O_2)_4(C_{12}H_{11}NS)_2]$, is a centrosymmetric dimer. The Cu centre presents a $CuO_4N$ square-pyramidal geometry arising from four *syn*–syn bridging acetate anions and a 2-(phenylsulfanylmethyl)pyridine ligand N-coordinated in the apical position. The Cu···Cu separation is 2.6309 (6) Å.

## Related literature

For a related structure and background, see: Del Sesto *et al.* (2000).




## Experimental

### Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{12}H_{11}NS)_2]$
$M_r$ = 765.85
Triclinic, $P\overline{1}$
$a$ = 7.7587 (16) Å
$b$ = 7.9690 (16) Å
$c$ = 13.986 (3) Å
$\alpha$ = 102.51 (3)°
$\beta$ = 101.86 (2)°
$\gamma$ = 94.29 (3)°
$V$ = 819.7 (3) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 1.48 mm$^{-1}$
$T$ = 293 (2) K
0.34 × 0.33 × 0.30 mm

### Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.622, $T_{max}$ = 0.652
6775 measured reflections
3029 independent reflections
2859 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.078
$S$ = 1.05
3029 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Cu1—O3 | 1.9663 (15) | Cu1—O2 | 1.9746 (16) |
| Cu1—O1 | 1.9680 (16) | Cu1—N1 | 2.2227 (19) |
| Cu1—O4 | 1.9743 (16) | | |

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2004).

The authors gratefully acknowledge financial support from the National Natural Science Foundation of China (grant No. 20576089) and from Tianjin Natural Science Foundation (grant Nos. 05YFJZJC02000 and 05YFGHHZ01100).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2435).

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  doi:10.1107/S1600536807026189 

# supplementary materials

*Acta Cryst.* (2007). E**63**, m2172 [ **doi:10.1107/S1600536807026189** ]

# Tetra-$\mu$-acetato-$\kappa^8O:O'$-bis{[2-(phenylsulfanylmethyl)pyridine-$\kappa N$]copper(II)}

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## Comment

In the preparation of $Cu^{II}$ complex with the ligand, 2-(phenylsulfanyl)methylpyridine (*L*), we obtained the title compound, (I), (Fig. 1).

The complex consists of a centrosymmetric dicopper(II) core with four acetate anions bridging the two copper atoms and two monodentate *L* ligands. The intradimer $Cu\cdots Cu^{i}$ (i = $-x$, $1-y$, $-z$) distance is 2.6309 (6) Å, which is similar to that (2.63 Å) in $[Cu(O_2CPh)_2(DMF)]_2$ (Del Sesto *et al.*, 2000). The copper ion in (I) presents a nearly square pyramidal geometry with four oxygen atoms in a plane, at a mean distance of 1.971 (2) Å. The axial site is occupied by the pyridine N atom of a ligand molecule at 2.232 (2) Å. The $Cu^{II}$ ion is displaced from the basal plane towards the apical N atom by 0.199 (2) A. The *L* ligand takes a *gauche* conformation with a C6—S1—C7—C8 torsion angle of 76.8 (2)° between the two aryl groups.

## Experimental

Thiophenol (630 mg, 5.7 mmol) was added to a stirred solution of KOH (320 mg, 5.7 mmol) in ethanol (30 ml). The mixture was refluxed for 30 min and a solution of 2-bromomethylpyridine (986 mg, 5.7 mmol) in ethanol (25 ml) was slowly added to it. The mixture was refluxed for 4 h more. The KBr precipitate was filtered off, and the filtrate was washed by water and evaporated to obtain ligand *L* as a brown oil in 40% yield. A solution (5.0 ml) of $Cu(OAc)_2$ (0.1 mmol) and *L* (0.2 mmol) in methanol/chloroform (1:1 *v*/*v*) was stirred for 30 min at room temperature, and then filtered. Green single crystals of (I) were obtained from the filtrate.

## Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

## Figures

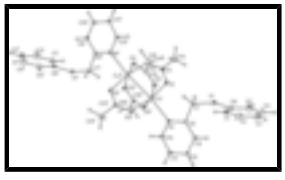


Fig. 1. View of (I) with 30% probability displacement ellipsoids (arbitrary spheres of H atoms). Symmetry code: (i) $-x$, $1-y$, $-z$.

## Tetra-μ-acetato-κ$^8$*O*:*O*'-bis{[2-(phenylsulfanylmethyl)pyridine-κ*N*]copper(II)}

*Crystal data*

| | |
|---|---|
| $[Cu_2(C_2H_3O_2)_4(C_{12}H_{11}NS)_2]$ | $Z = 1$ |
| $M_r = 765.85$ | $F_{000} = 394$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.551$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 7.7587$ (16) Å | Cell parameters from 7557 reflections |
| $b = 7.9690$ (16) Å | $\theta = 3.1$–$27.5°$ |
| $c = 13.986$ (3) Å | $\mu = 1.48$ mm$^{-1}$ |
| $\alpha = 102.51$ (3)° | $T = 293$ (2) K |
| $\beta = 101.86$ (2)° | Block, green |
| $\gamma = 94.29$ (3)° | 0.34 × 0.33 × 0.30 mm |
| $V = 819.7$ (3) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID IP area-detector diffractometer | 3029 independent reflections |
| Radiation source: rotating anode | 2859 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.029$ |
| $T = 293$(2) K | $\theta_{max} = 25.5°$ |
| ω scans | $\theta_{min} = 3.1°$ |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | $h = -9 \rightarrow 9$ |
| $T_{min} = 0.622$, $T_{max} = 0.652$ | $k = -9 \rightarrow 8$ |
| 6775 measured reflections | $l = -16 \rightarrow 16$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.028$ | H-atom parameters constrained |
| $wR(F^2) = 0.078$ | $w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 0.5716P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3029 reflections | $\Delta\rho_{max} = 0.41$ e Å$^{-3}$ |
| 208 parameters | $\Delta\rho_{min} = -0.37$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.15681 (7) | 1.02827 (7) | 0.41049 (4) | 0.02382 (14) |
| N1 | 0.3502 (2) | 0.7760 (2) | 0.18067 (12) | 0.0167 (3) |
| Cu1 | 0.12181 (3) | 0.60867 (3) | 0.069933 (16) | 0.01511 (10) |
| O1 | −0.0394 (2) | 0.78294 (19) | 0.04802 (11) | 0.0230 (3) |
| O2 | −0.2453 (2) | 0.59886 (19) | −0.07185 (12) | 0.0271 (4) |
| O3 | −0.0150 (2) | 0.5378 (2) | 0.16144 (11) | 0.0245 (3) |
| O4 | −0.2209 (2) | 0.3513 (2) | 0.04359 (11) | 0.0259 (3) |
| C1 | 0.2586 (3) | 1.3074 (3) | 0.33349 (17) | 0.0296 (5) |
| H1A | 0.2590 | 1.2289 | 0.2737 | 0.036* |
| C2 | 0.3046 (4) | 1.4820 (3) | 0.34379 (19) | 0.0377 (6) |
| H2A | 0.3354 | 1.5205 | 0.2906 | 0.045* |
| C3 | 0.3055 (4) | 1.5996 (3) | 0.4319 (2) | 0.0416 (6) |
| H3A | 0.3386 | 1.7170 | 0.4388 | 0.050* |
| C4 | 0.2570 (5) | 1.5422 (4) | 0.5097 (2) | 0.0471 (7) |
| H4A | 0.2558 | 1.6216 | 0.5690 | 0.057* |
| C5 | 0.2101 (4) | 1.3675 (3) | 0.50064 (19) | 0.0375 (6) |
| H5A | 0.1776 | 1.3298 | 0.5536 | 0.045* |
| C6 | 0.2118 (3) | 1.2487 (3) | 0.41206 (16) | 0.0236 (5) |
| C7 | 0.1672 (3) | 0.9108 (3) | 0.28692 (15) | 0.0213 (4) |
| H7A | 0.1012 | 0.7968 | 0.2738 | 0.026* |
| H7B | 0.1066 | 0.9697 | 0.2385 | 0.026* |
| C8 | 0.3503 (3) | 0.8875 (3) | 0.26746 (15) | 0.0168 (4) |
| C9 | 0.5058 (3) | 0.9744 (3) | 0.33319 (16) | 0.0236 (5) |
| H9A | 0.5022 | 1.0513 | 0.3929 | 0.028* |
| C10 | 0.6667 (3) | 0.9446 (3) | 0.30849 (17) | 0.0275 (5) |
| H10A | 0.7727 | 1.0007 | 0.3517 | 0.033* |
| C11 | 0.6675 (3) | 0.8307 (3) | 0.21884 (18) | 0.0268 (5) |
| H11A | 0.7737 | 0.8097 | 0.2002 | 0.032* |
| C12 | 0.5073 (3) | 0.7486 (3) | 0.15746 (16) | 0.0224 (4) |
| H12A | 0.5080 | 0.6710 | 0.0974 | 0.027* |
| C13 | −0.1833 (3) | 0.7472 (3) | −0.01779 (15) | 0.0185 (4) |
| C14 | −0.2888 (3) | 0.8945 (3) | −0.03217 (19) | 0.0287 (5) |
| H14A | −0.2322 | 0.9983 | 0.0167 | 0.043* |

| | | | | |
|---|---|---|---|---|
| H14B | −0.4067 | 0.8675 | −0.0238 | 0.043* |
| H14C | −0.2948 | 0.9117 | −0.0986 | 0.043* |
| C15 | −0.1492 (3) | 0.4248 (3) | 0.13311 (15) | 0.0201 (4) |
| C16 | −0.2312 (4) | 0.3755 (3) | 0.21380 (18) | 0.0355 (6) |
| H16A | −0.3240 | 0.2808 | 0.1837 | 0.053* |
| H16B | −0.2796 | 0.4730 | 0.2471 | 0.053* |
| H16C | −0.1419 | 0.3412 | 0.2618 | 0.053* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0221 (3) | 0.0269 (3) | 0.0200 (3) | −0.0009 (2) | 0.0070 (2) | −0.0002 (2) |
| N1 | 0.0151 (8) | 0.0168 (8) | 0.0174 (8) | 0.0000 (6) | 0.0027 (6) | 0.0037 (7) |
| Cu1 | 0.01397 (14) | 0.01466 (15) | 0.01485 (14) | −0.00007 (9) | 0.00168 (9) | 0.00172 (10) |
| O1 | 0.0225 (8) | 0.0181 (7) | 0.0248 (8) | 0.0029 (6) | 0.0003 (6) | 0.0020 (6) |
| O2 | 0.0206 (8) | 0.0187 (8) | 0.0350 (9) | 0.0029 (6) | −0.0038 (6) | 0.0006 (7) |
| O3 | 0.0280 (8) | 0.0255 (8) | 0.0175 (7) | −0.0063 (6) | 0.0046 (6) | 0.0036 (6) |
| O4 | 0.0232 (8) | 0.0316 (9) | 0.0193 (7) | −0.0075 (6) | 0.0058 (6) | 0.0011 (6) |
| C1 | 0.0370 (13) | 0.0312 (13) | 0.0189 (10) | 0.0094 (10) | 0.0038 (9) | 0.0031 (9) |
| C2 | 0.0503 (16) | 0.0350 (14) | 0.0304 (13) | 0.0098 (12) | 0.0052 (11) | 0.0156 (11) |
| C3 | 0.0603 (18) | 0.0260 (13) | 0.0348 (14) | 0.0091 (12) | 0.0001 (12) | 0.0083 (11) |
| C4 | 0.081 (2) | 0.0278 (14) | 0.0295 (13) | 0.0116 (13) | 0.0139 (14) | −0.0016 (11) |
| C5 | 0.0564 (17) | 0.0329 (13) | 0.0252 (12) | 0.0099 (12) | 0.0141 (11) | 0.0049 (11) |
| C6 | 0.0198 (10) | 0.0258 (11) | 0.0218 (10) | 0.0062 (8) | 0.0000 (8) | 0.0020 (9) |
| C7 | 0.0146 (10) | 0.0241 (11) | 0.0201 (10) | −0.0004 (8) | 0.0025 (8) | −0.0037 (8) |
| C8 | 0.0144 (9) | 0.0170 (10) | 0.0177 (9) | −0.0007 (7) | 0.0021 (7) | 0.0042 (8) |
| C9 | 0.0191 (10) | 0.0262 (11) | 0.0196 (10) | 0.0005 (8) | 0.0005 (8) | −0.0026 (9) |
| C10 | 0.0134 (10) | 0.0337 (13) | 0.0296 (12) | −0.0013 (9) | −0.0013 (8) | 0.0021 (10) |
| C11 | 0.0147 (10) | 0.0329 (12) | 0.0315 (12) | 0.0028 (9) | 0.0060 (9) | 0.0040 (10) |
| C12 | 0.0177 (10) | 0.0248 (11) | 0.0233 (10) | 0.0024 (8) | 0.0050 (8) | 0.0023 (9) |
| C13 | 0.0186 (10) | 0.0187 (10) | 0.0214 (10) | 0.0041 (8) | 0.0091 (8) | 0.0067 (8) |
| C14 | 0.0270 (12) | 0.0231 (11) | 0.0358 (12) | 0.0074 (9) | 0.0037 (10) | 0.0088 (10) |
| C15 | 0.0235 (11) | 0.0178 (10) | 0.0209 (10) | 0.0040 (8) | 0.0081 (8) | 0.0054 (8) |
| C16 | 0.0446 (15) | 0.0380 (14) | 0.0252 (12) | −0.0083 (11) | 0.0165 (11) | 0.0065 (10) |

*Geometric parameters (Å, °)*

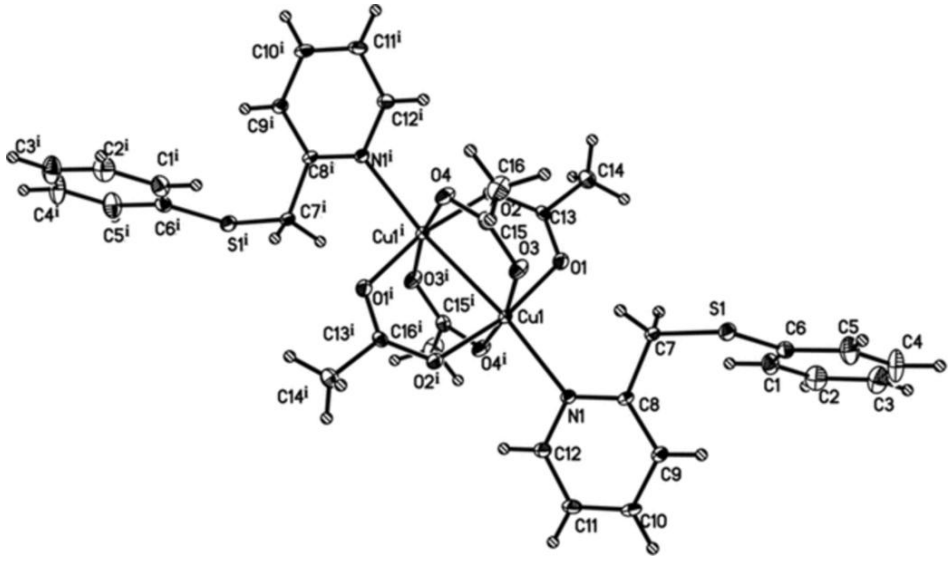
| | | | |
|---|---|---|---|
| S1—C6 | 1.771 (2) | C4—C5 | 1.384 (4) |
| S1—C7 | 1.799 (2) | C4—H4A | 0.9300 |
| N1—C8 | 1.340 (3) | C5—C6 | 1.390 (3) |
| N1—C12 | 1.345 (3) | C5—H5A | 0.9300 |
| Cu1—O3 | 1.9663 (15) | C7—C8 | 1.517 (3) |
| Cu1—O1 | 1.9680 (16) | C7—H7A | 0.9700 |
| Cu1—N1 | 2.2227 (19) | C7—H7B | 0.9700 |
| Cu1—O4$^{i}$ | 1.9743 (16) | C8—C9 | 1.387 (3) |
| Cu1—O2$^{i}$ | 1.9746 (16) | C9—C10 | 1.385 (3) |
| Cu1—Cu1$^{i}$ | 2.6309 (13) | C9—H9A | 0.9300 |
| O1—C13 | 1.262 (3) | C10—C11 | 1.381 (3) |

| | | | |
|---|---|---|---|
| O2—C13 | 1.257 (3) | C10—H10A | 0.9300 |
| O2—Cu1$^{i}$ | 1.9746 (16) | C11—C12 | 1.381 (3) |
| O3—C15 | 1.260 (3) | C11—H11A | 0.9300 |
| O4—C15 | 1.252 (3) | C12—H12A | 0.9300 |
| O4—Cu1$^{i}$ | 1.9743 (16) | C13—C14 | 1.505 (3) |
| C1—C2 | 1.379 (4) | C14—H14A | 0.9600 |
| C1—C6 | 1.385 (3) | C14—H14B | 0.9600 |
| C1—H1A | 0.9300 | C14—H14C | 0.9600 |
| C2—C3 | 1.376 (4) | C15—C16 | 1.511 (3) |
| C2—H2A | 0.9300 | C16—H16A | 0.9600 |
| C3—C4 | 1.376 (4) | C16—H16B | 0.9600 |
| C3—H3A | 0.9300 | C16—H16C | 0.9600 |
| C6—S1—C7 | 104.84 (11) | C1—C6—S1 | 124.78 (17) |
| C8—N1—C12 | 118.22 (17) | C8—C7—S1 | 117.10 (14) |
| C8—N1—Cu1 | 128.57 (13) | C8—C7—H7A | 108.0 |
| C12—N1—Cu1 | 113.04 (13) | S1—C7—H7A | 108.0 |
| O3—Cu1—O1 | 89.29 (7) | C8—C7—H7B | 108.0 |
| O3—Cu1—O4$^{i}$ | 168.33 (6) | S1—C7—H7B | 108.0 |
| O1—Cu1—O4$^{i}$ | 89.15 (7) | H7A—C7—H7B | 107.3 |
| O3—Cu1—O2$^{i}$ | 88.87 (7) | N1—C8—C9 | 122.23 (18) |
| O1—Cu1—O2$^{i}$ | 168.47 (6) | N1—C8—C7 | 114.47 (17) |
| O4$^{i}$—Cu1—O2$^{i}$ | 90.36 (8) | C9—C8—C7 | 123.30 (18) |
| O3—Cu1—N1 | 100.28 (6) | C10—C9—C8 | 118.96 (19) |
| O1—Cu1—N1 | 100.09 (7) | C10—C9—H9A | 120.5 |
| O4$^{i}$—Cu1—N1 | 91.38 (6) | C8—C9—H9A | 120.5 |
| O2$^{i}$—Cu1—N1 | 91.44 (7) | C11—C10—C9 | 119.1 (2) |
| O3—Cu1—Cu1$^{i}$ | 83.62 (5) | C11—C10—H10A | 120.4 |
| O1—Cu1—Cu1$^{i}$ | 85.08 (5) | C9—C10—H10A | 120.4 |
| O4$^{i}$—Cu1—Cu1$^{i}$ | 84.73 (5) | C12—C11—C10 | 118.6 (2) |
| O2$^{i}$—Cu1—Cu1$^{i}$ | 83.41 (5) | C12—C11—H11A | 120.7 |
| N1—Cu1—Cu1$^{i}$ | 173.51 (5) | C10—C11—H11A | 120.7 |
| C13—O1—Cu1 | 122.22 (14) | N1—C12—C11 | 122.9 (2) |
| C13—O2—Cu1$^{i}$ | 124.00 (14) | N1—C12—H12A | 118.6 |
| C15—O3—Cu1 | 123.84 (14) | C11—C12—H12A | 118.6 |
| C15—O4—Cu1$^{i}$ | 122.33 (14) | O2—C13—O1 | 125.2 (2) |
| C2—C1—C6 | 120.1 (2) | O2—C13—C14 | 117.68 (19) |
| C2—C1—H1A | 120.0 | O1—C13—C14 | 117.14 (19) |
| C6—C1—H1A | 120.0 | C13—C14—H14A | 109.5 |
| C1—C2—C3 | 120.7 (2) | C13—C14—H14B | 109.5 |
| C1—C2—H2A | 119.7 | H14A—C14—H14B | 109.5 |
| C3—C2—H2A | 119.7 | C13—C14—H14C | 109.5 |
| C4—C3—C2 | 119.5 (3) | H14A—C14—H14C | 109.5 |
| C4—C3—H3A | 120.3 | H14B—C14—H14C | 109.5 |
| C2—C3—H3A | 120.3 | O4—C15—O3 | 125.3 (2) |
| C3—C4—C5 | 120.7 (2) | O4—C15—C16 | 117.43 (19) |

| | | | |
|---|---|---|---|
| C3—C4—H4A | 119.7 | O3—C15—C16 | 117.25 (19) |
| C5—C4—H4A | 119.7 | C15—C16—H16A | 109.5 |
| C4—C5—C6 | 119.7 (2) | C15—C16—H16B | 109.5 |
| C4—C5—H5A | 120.1 | H16A—C16—H16B | 109.5 |
| C6—C5—H5A | 120.1 | C15—C16—H16C | 109.5 |
| C5—C6—C1 | 119.4 (2) | H16A—C16—H16C | 109.5 |
| C5—C6—S1 | 115.81 (19) | H16B—C16—H16C | 109.5 |
| C8—N1—Cu1—O3 | −38.69 (18) | C2—C1—C6—S1 | −177.9 (2) |
| C12—N1—Cu1—O3 | 136.51 (15) | C7—S1—C6—C5 | 179.03 (18) |
| C8—N1—Cu1—O1 | 52.42 (18) | C7—S1—C6—C1 | −2.4 (2) |
| C12—N1—Cu1—O1 | −132.38 (15) | C6—S1—C7—C8 | 76.80 (19) |
| C8—N1—Cu1—O4$^{i}$ | 141.80 (18) | C12—N1—C8—C9 | 0.0 (3) |
| C12—N1—Cu1—O4$^{i}$ | −43.00 (16) | Cu1—N1—C8—C9 | 175.01 (15) |
| C8—N1—Cu1—O2$^{i}$ | −127.81 (18) | C12—N1—C8—C7 | 179.67 (19) |
| C12—N1—Cu1—O2$^{i}$ | 47.39 (16) | Cu1—N1—C8—C7 | −5.3 (3) |
| O3—Cu1—O1—C13 | −86.13 (16) | S1—C7—C8—N1 | 169.58 (15) |
| O4$^{i}$—Cu1—O1—C13 | 82.31 (16) | S1—C7—C8—C9 | −10.8 (3) |
| O2$^{i}$—Cu1—O1—C13 | −5.3 (4) | N1—C8—C9—C10 | −0.2 (3) |
| N1—Cu1—O1—C13 | 173.56 (15) | C7—C8—C9—C10 | −179.8 (2) |
| Cu1$^{i}$—Cu1—O1—C13 | −2.47 (15) | C8—C9—C10—C11 | 0.6 (4) |
| O1—Cu1—O3—C15 | 88.00 (18) | C9—C10—C11—C12 | −0.8 (4) |
| O4$^{i}$—Cu1—O3—C15 | 5.7 (4) | C8—N1—C12—C11 | −0.3 (3) |
| O2$^{i}$—Cu1—O3—C15 | −80.62 (18) | Cu1—N1—C12—C11 | −176.01 (18) |
| N1—Cu1—O3—C15 | −171.88 (17) | C10—C11—C12—N1 | 0.7 (4) |
| Cu1$^{i}$—Cu1—O3—C15 | 2.87 (17) | Cu1$^{i}$—O2—C13—O1 | −3.6 (3) |
| C6—C1—C2—C3 | 0.3 (4) | Cu1$^{i}$—O2—C13—C14 | 176.56 (15) |
| C1—C2—C3—C4 | −1.1 (4) | Cu1—O1—C13—O2 | 4.3 (3) |
| C2—C3—C4—C5 | 0.9 (5) | Cu1—O1—C13—C14 | −175.83 (14) |
| C3—C4—C5—C6 | 0.0 (5) | Cu1$^{i}$—O4—C15—O3 | 4.3 (3) |
| C4—C5—C6—C1 | −0.7 (4) | Cu1$^{i}$—O4—C15—C16 | −176.35 (16) |
| C4—C5—C6—S1 | 177.9 (2) | Cu1—O3—C15—O4 | −5.1 (3) |
| C2—C1—C6—C5 | 0.6 (4) | Cu1—O3—C15—C16 | 175.48 (16) |

Symmetry codes: (i) −*x*, −*y*+1, −*z*.

**Fig. 1**


C10i
C11i
C9i
C12i
C3i
C2i
C1i
C8i
N1i
O4
C16
C14
C4i
C5i
C6i
S1i
C7i
Cu1i
O2
C13
C15
O3
O1
O1i
O3i
C15i
Cu1
S1
C6
C5
C4
C13i
C16i
C7
O4i
O2i
C1
C2
C3
C14i
N1
C8
C12
C9
C11
C10