# metal-organic compounds

# N,N′-Dimethylethylenediammonium dioxalatocuprate(II)

## Papa Aly Gaye,[a]* Aminata Diassé Sarr,[a] Mohamed Gaye,[a] Morgane Sanselme[b] and Peulon Valérie Agasse[b]

[a]Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop, Dakar, Senegal, and [b]Sciences et Méthodes Séparatives, UPRES EA 3233 IMR, IRCOF, F-76821, Mont-Saint-Aigan, Université de Rouen Cedex, France
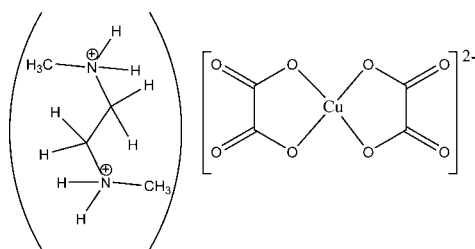Correspondence e-mail: mlgayeastou@yahoo.fr

The asymmetric unit of the title salt, $(C_4H_{14}N_2)[Cu(C_2O_4)_2]$, consists of one complex anion and two cationic half-molecules, the other halves being generated by inversion symmetry. The $Cu^{II}$ atom in the anion is coordinated by two bidentate oxalate ligands in a distorted square-planar geometry. Intermolecular hydrogen bonds, involving the NH groups as donors and O atoms as acceptors, are observed, which lead to the formation of a three-dimensional network structure.

## Related literature

For background to decomposition reactions leading to oxalate anions, see: Kelly *et al.* (2005); Diallo *et al.* (2008). For related structures, see: Androš *et al.* (2010); Fan *et al.* (2001); Zhang *et al.* (2009).



## Experimental

### Crystal data

$(C_4H_{14}N_2)[Cu(C_2O_4)_2]$
$M_r = 329.75$
Triclinic, $P\bar{1}$
$a = 5.7734$ (5) Å
$b = 8.4127$ (7) Å
$c = 12.5623$ (11) Å
$\alpha = 90.443$ (1)°
$\beta = 100.715$ (1)°

$\gamma = 107.188$ (1)°
$V = 571.46$ (8) Å$^3$
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.95$ mm$^{-1}$
$T = 293$ K
$0.15 \times 0.13 \times 0.10$ mm

### Data collection

Bruker SMART CCD diffractometer
4558 measured reflections

2292 independent reflections
2192 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.07$
$S = 1.12$
2292 reflections

174 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.35$ e Å$^{-3}$
$\Delta\rho_{min} = -0.43$ e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.9128 (13) | Cu1—O2A | 1.9184 (13) |
| Cu1—O2 | 1.9163 (13) | Cu1—O1A | 1.9572 (13) |

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| N1S—H2S1$\cdots$O3A[i] | 0.90 | 2.22 | 2.939 (2) | 137 |
| N1S—H2S2$\cdots$O1A[ii] | 0.90 | 2.13 | 3.018 (2) | 169 |
| N2S—H4S1$\cdots$O4A[ii] | 0.90 | 2.15 | 2.939 (2) | 145 |
| N2S—H4S1$\cdots$O3A[ii] | 0.90 | 2.31 | 3.004 (2) | 134 |
| N2S—H4S2$\cdots$O4[iii] | 0.90 | 2.11 | 2.861 (2) | 140 |
| N2S—H4S2$\cdots$O3[iv] | 0.90 | 2.58 | 3.131 (2) | 120 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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# supporting information

# *N,N′*-Dimethylethylenediammonium dioxalatocuprate(II)

## Papa Aly Gaye, Aminata Diassé Sarr, Mohamed Gaye, Morgane Sanselme and Peulon Valérie Agasse

### S1. Comment

The title salt, $(C_4H_{14}N_2)[Cu(C_2O_4)_2]$, was obtained as an unexpected product by reaction of the employed ligand $(C_6H_{10}N_2O_2)_n$, in a methanolic medium. The hydrolytically unstable cyclic ligand apparently is oxidatively hydrolyzed in the presence of metal ions, leading to the oxalate dianion (Diallo *et al.*, 2008; Kelly *et al.*, 2005). This species, which is generated *in situ*, acts with copper(II) ions resulting in the formation of the title compound. A similar reaction was found elsewhere (Zhang *et al.*, 2009).

The structure exhibits an ion-pair complex comprising two cationic half-molecules (the other halves being generated by inversion symmetry) and a $[Cu(C_2O_4)_2]^{2-}$ dianion (Fig. 1). The $Cu^{II}$ ion is four-coordinated in a slightly distorted square–planar $CuO_4$ environment, comprising four O donor atoms from two oxalate ligands [Cu–O, 1.9128 (13), 1.9163 (13), 1.9184 (13) and 1.9572 (13) Å]. The O(1)—Cu—O(2 A) and O(2)—Cu—O(1 A) angles are 179.52 (5) and 178.10 (5)°, respectively, which are slightly smaller than those observed in the complex $[K_2Cu(ox)_2]\cdot4H_2O$ (180 °), where ox is oxalate (Fan *et al.*, 2001). The other two oxygen atoms of each oxalate group are not involved in coordination. The two oxalate anions deviate slightly from planarity, with torsion angles of O(1)—C(1)—C(2)—O(2), O(4)—C(1)—C(2)—O(3), O(1A)—C(1A)—C(2A)—O(2A) and O(4A)—C(1A)—C(2A)—O(3A) -2.5 (2), -3.4 (3), 2.8 (2) and 3.8 (2)°, respectively. These values are similar to those found in $[Cu(bpy)(C_2O_4)(H_2O)]\cdot H_2C_2O_4$ (Androš *et al.*, 2010), where bpy is bipyridine.

N—H···O hydrogen-bonding interactions, part of which are bifurcated, between the cations and the complex anions lead to the formation of a three-dimensional network structure (Table 2; Figs. 2, 3).

### S2. Experimental

In a 50 ml round bottom flask dimethyl oxalate (2.36 g, 0.020 mol), dissolved in ethanol (10 ml), was reacted with *N,N′*-dimethyl-1,2-diaminoethane (1.77 g, 0.020 mol) in ethanol (10 ml), to yield immediately a quantitative precipitate. The white solid formed was separated by filtration, washed with methanol and ether and dried under vacuum (yield 3.32 g, 58.5%); m.p.= 513 K. $^1$H NMR in CDCl₃, $\delta$ (p.p.m.): 3.1, s, 12H, –CH3; 3.5, s, 8H, –CH₂–. $^{13}$C NMR in CDCl₃, $\delta$ (p.p.m.): 34.86, N—CH₃, 46.12, N—CH₂, 157.56, C=O. IR (cm⁻¹) 1598 (C=O), 1284 (C—N). Anal. Calc. for $C_{12}H_{20}N_4O_4$ (%): C, 50.62; H, 7.11; N, 19.68. Found: C, 50.60; H, 7.09; N, 19.71. Mass spectrum (m/*z*) 284, 162, 134, 106, 78. Into a methanolic solution (5 ml) of copper chloride dihydrate (0.2131 g, 1.25 mmol) was added a methanolic solution (10 ml) of the ligand prepared as described above (0.3554 g, 1.25 mmol). The resulting mixture was heated at 333 K for thirty minutes. The green solution was filtered and then allowed to evaporate slowly in open atmosphere. After one week, blue crystals suitable for X-ray analysis were obtained. The crystals were separated, washed with cold methanol and dried (yield: 65%); Anal. Calc. for $(C_4H_{14}N_2)[Cu(C_2O_4)_2]$(%): C, 29.14; H, 4.28; N, 8.50. Found: C, 29.16; H, 4.26; N, 8.46. Selected IR data (cm⁻¹, KBr pellet): 3300, 1637, 1600, 1582, 1197, 764.

### S3. Refinement

All H atoms were located from the Fourier electron density maps, then placed according to their geometrical environment and refined isotropically. They were refined using a riding model with 0.96 Å for methyl H atoms and $U_{iso}(H) =$ $1.5U_{eq}(C)$, with 0.97 Å for methylene H atoms and $U_{iso}(H) = 1.2U_{eq}(C)$, and with 0.90 Å for ammonium H atoms and $U_{iso}(H) = 1.2U_{eq}(N)$. In addition, a rotating-group model was applied for methyl groups.
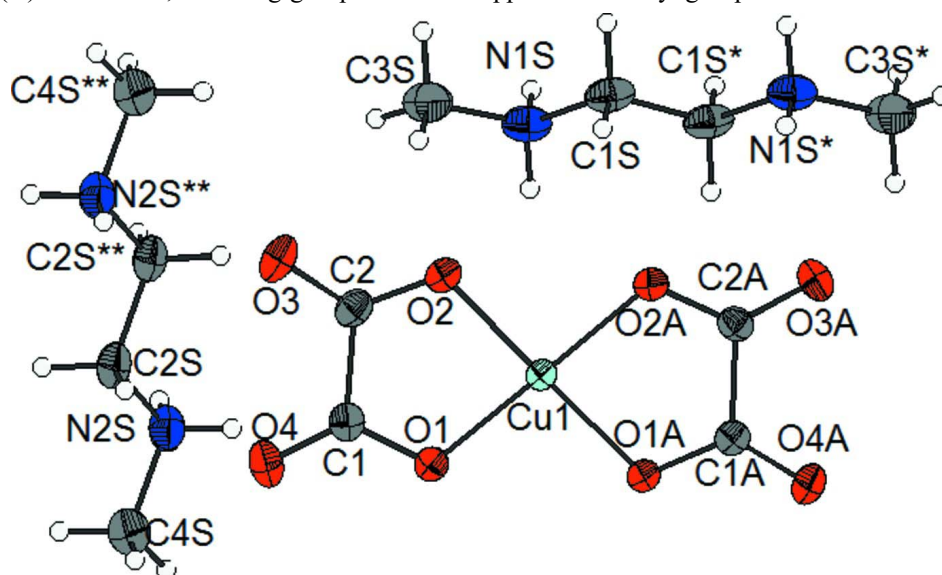


**Figure 1**

An *ORTEP* view of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 50% probability level. [Symmetry codes: *) -x + 1, -y + 1, -z; **) -x + 1, -y, -z + 1].
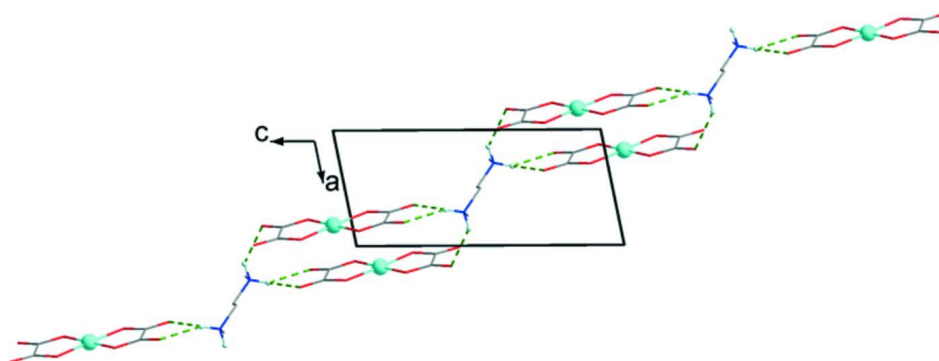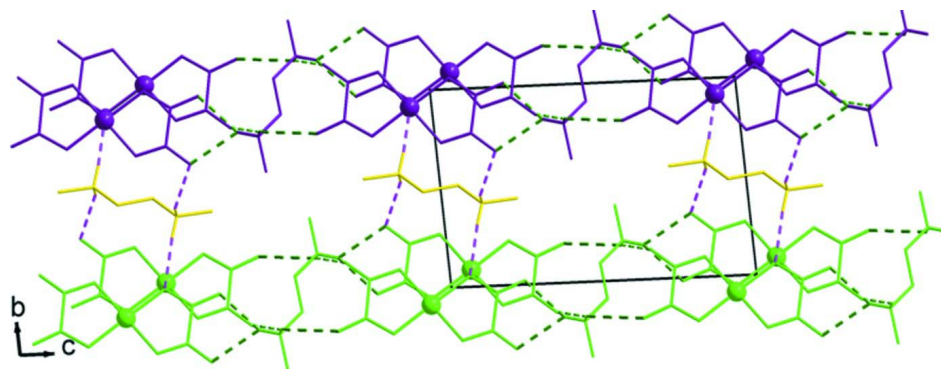


**Figure 2**

Projection of the structure along the *b* axis showing the anions connected by organics cations. Broken lines stand for hydrogen bonds.

**Figure 3**

Projection of the structure along the *a* axis showing the anions connected by organics cations. Broken lines stand for hydrogen bonds.

**N,N′-Dimethylethylenediammonium dioxalatocuprate(II)**

*Crystal data*

| | |
|---|---|
| $(C_4H_{14}N_2)[Cu(C_2O_4)_2]$ | $Z = 2$ |
| $M_r = 329.75$ | $F(000) = 338$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.916$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 5.7734$ (5) Å | Cell parameters from 2192 reflections |
| $b = 8.4127$ (7) Å | $\theta = 1.7–26.4°$ |
| $c = 12.5623$ (11) Å | $\mu = 1.95$ mm$^{-1}$ |
| $\alpha = 90.443$ (1)° | $T = 293$ K |
| $\beta = 100.715$ (1)° | Prism, blue |
| $\gamma = 107.188$ (1)° | $0.15 \times 0.13 \times 0.10$ mm |
| $V = 571.46$ (8) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 2192 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.014$ |
| $\omega$ scans | $\theta_{max} = 26.4°$, $\theta_{min} = 1.7°$ |
| 4558 measured reflections | $h = -7 \rightarrow 7$ |
| 2292 independent reflections | $k = -10 \rightarrow 10$ |
| | $l = -15 \rightarrow 15$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.024$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.07$ | |
| $S = 1.12$ | H-atom parameters constrained |
| 2292 reflections | $w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.2106P]$ |
| 174 parameters | where $P = (F_o^2 + 2F_c^2)/3$ |
| 0 restraints | $(\Delta/\sigma)_{max} < 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.35$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.43$ 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)*

|  | *x* | *y* | *z* | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.81900 (4) | 0.08511 (2) | 0.071311 (15) | 0.02027 (10) |
| O1 | 0.7688 (2) | −0.09898 (16) | 0.16179 (10) | 0.0236 (3) |
| O2 | 0.9414 (3) | 0.22323 (16) | 0.20393 (11) | 0.0273 (3) |
| O3 | 0.9874 (3) | 0.1983 (2) | 0.38225 (12) | 0.0400 (4) |
| O4 | 0.8221 (3) | −0.14792 (19) | 0.33674 (12) | 0.0346 (3) |
| O1A | 0.7045 (2) | −0.05261 (16) | −0.06558 (10) | 0.0244 (3) |
| O2A | 0.8699 (3) | 0.27099 (16) | −0.01838 (11) | 0.0274 (3) |
| O3A | 0.7987 (3) | 0.32433 (18) | −0.19228 (12) | 0.0325 (3) |
| O4A | 0.6466 (2) | −0.01666 (17) | −0.24263 (10) | 0.0271 (3) |
| C1 | 0.8324 (3) | −0.0538 (2) | 0.26338 (15) | 0.0230 (4) |
| C2 | 0.9307 (3) | 0.1394 (2) | 0.28879 (15) | 0.0249 (4) |
| C1A | 0.7074 (3) | 0.0373 (2) | −0.14883 (14) | 0.0201 (3) |
| C2A | 0.8000 (3) | 0.2289 (2) | −0.11968 (15) | 0.0221 (4) |
| C1S | 0.5705 (4) | 0.5131 (2) | 0.05810 (18) | 0.0323 (4) |
| H1S1 | 0.7161 | 0.4764 | 0.0631 | 0.039* |
| H1S2 | 0.6244 | 0.6309 | 0.0809 | 0.039* |
| N1S | 0.4111 (3) | 0.4180 (2) | 0.13069 (15) | 0.0328 (4) |
| H2S1 | 0.2785 | 0.4547 | 0.1272 | 0.039* |
| H2S2 | 0.3564 | 0.3094 | 0.1074 | 0.039* |
| C2S | 0.4947 (4) | −0.0903 (3) | 0.50540 (16) | 0.0302 (4) |
| H3S1 | 0.6487 | −0.1056 | 0.4941 | 0.036* |
| H3S2 | 0.4737 | −0.1213 | 0.578 | 0.036* |
| N2S | 0.2872 (3) | −0.1980 (2) | 0.42503 (13) | 0.0329 (4) |
| H4S1 | 0.313 | −0.1731 | 0.3578 | 0.039* |
| H4S2 | 0.1467 | −0.177 | 0.4324 | 0.039* |
| C3S | 0.5449 (4) | 0.4354 (3) | 0.24519 (18) | 0.0394 (5) |
| H1S3 | 0.6805 | 0.3899 | 0.25 | 0.059* |
| H1S4 | 0.434 | 0.3762 | 0.2898 | 0.059* |
| H1S5 | 0.6069 | 0.5512 | 0.2698 | 0.059* |
| C4S | 0.2574 (5) | −0.3766 (3) | 0.4373 (2) | 0.0484 (6) |
| H2S3 | 0.4075 | −0.3993 | 0.4303 | 0.073* |
| H2S4 | 0.124 | −0.4417 | 0.382 | 0.073* |
| H2S5 | 0.2213 | −0.4051 | 0.5075 | 0.073* |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.02469 (14) | 0.01821 (14) | 0.01732 (14) | 0.00556 (9) | 0.00424 (9) | 0.00003 (9) |
| O1 | 0.0270 (7) | 0.0220 (6) | 0.0214 (6) | 0.0065 (5) | 0.0054 (5) | 0.0008 (5) |
| O2 | 0.0344 (7) | 0.0231 (6) | 0.0228 (7) | 0.0070 (6) | 0.0046 (5) | −0.0023 (5) |
| O3 | 0.0505 (9) | 0.0451 (9) | 0.0212 (7) | 0.0126 (7) | 0.0027 (6) | −0.0065 (6) |
| O4 | 0.0398 (8) | 0.0394 (8) | 0.0268 (7) | 0.0139 (7) | 0.0089 (6) | 0.0120 (6) |
| O1A | 0.0326 (7) | 0.0193 (6) | 0.0194 (6) | 0.0060 (5) | 0.0034 (5) | −0.0003 (5) |
| O2A | 0.0389 (8) | 0.0198 (6) | 0.0229 (7) | 0.0069 (6) | 0.0075 (6) | 0.0005 (5) |
| O3A | 0.0419 (8) | 0.0299 (7) | 0.0280 (7) | 0.0139 (6) | 0.0071 (6) | 0.0104 (6) |
| O4A | 0.0284 (7) | 0.0331 (7) | 0.0189 (7) | 0.0097 (6) | 0.0022 (5) | −0.0022 (5) |
| C1 | 0.0189 (8) | 0.0285 (9) | 0.0243 (9) | 0.0101 (7) | 0.0063 (7) | 0.0032 (7) |
| C2 | 0.0221 (9) | 0.0290 (9) | 0.0236 (9) | 0.0092 (7) | 0.0024 (7) | −0.0032 (7) |
| C1A | 0.0160 (8) | 0.0235 (9) | 0.0226 (9) | 0.0084 (7) | 0.0047 (6) | 0.0006 (7) |
| C2A | 0.0212 (8) | 0.0224 (8) | 0.0254 (9) | 0.0095 (7) | 0.0063 (7) | 0.0033 (7) |
| C1S | 0.0270 (10) | 0.0234 (9) | 0.0457 (12) | 0.0029 (8) | 0.0135 (9) | −0.0064 (8) |
| N1S | 0.0272 (8) | 0.0244 (8) | 0.0462 (10) | 0.0054 (7) | 0.0098 (7) | −0.0023 (7) |
| C2S | 0.0294 (10) | 0.0409 (12) | 0.0210 (9) | 0.0130 (9) | 0.0028 (7) | 0.0028 (8) |
| N2S | 0.0340 (9) | 0.0379 (9) | 0.0244 (8) | 0.0084 (7) | 0.0039 (7) | 0.0050 (7) |
| C3S | 0.0414 (12) | 0.0311 (11) | 0.0445 (13) | 0.0124 (9) | 0.0032 (10) | −0.0025 (9) |
| C4S | 0.0696 (17) | 0.0385 (12) | 0.0354 (12) | 0.0118 (12) | 0.0131 (11) | 0.0060 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.9128 (13) | C1S—H1S2 | 0.97 |
| Cu1—O2 | 1.9163 (13) | N1S—C3S | 1.485 (3) |
| Cu1—O2A | 1.9184 (13) | N1S—H2S1 | 0.90 |
| Cu1—O1A | 1.9572 (13) | N1S—H2S2 | 0.90 |
| O1—C1 | 1.282 (2) | C2S—N2S | 1.473 (3) |
| O2—C2 | 1.284 (2) | C2S—C2S[ii] | 1.511 (4) |
| O3—C2 | 1.218 (2) | C2S—H3S1 | 0.97 |
| O4—C1 | 1.218 (2) | C2S—H3S2 | 0.97 |
| O1A—C1A | 1.295 (2) | N2S—C4S | 1.474 (3) |
| O2A—C2A | 1.275 (2) | N2S—H4S1 | 0.90 |
| O3A—C2A | 1.220 (2) | N2S—H4S2 | 0.90 |
| O4A—C1A | 1.209 (2) | C3S—H1S3 | 0.96 |
| C1—C2 | 1.564 (3) | C3S—H1S4 | 0.96 |
| C1A—C2A | 1.558 (2) | C3S—H1S5 | 0.96 |
| C1S—N1S | 1.486 (3) | C4S—H2S3 | 0.96 |
| C1S—C1S[i] | 1.513 (4) | C4S—H2S4 | 0.96 |
| C1S—H1S1 | 0.97 | C4S—H2S5 | 0.96 |
| | | | |
| O1—Cu1—O2 | 85.90 (5) | C3S—N1S—H2S1 | 109.2 |
| O1—Cu1—O2A | 179.52 (5) | C1S—N1S—H2S1 | 109.2 |
| O2—Cu1—O2A | 93.63 (6) | C3S—N1S—H2S2 | 109.2 |
| O1—Cu1—O1A | 95.12 (5) | C1S—N1S—H2S2 | 109.2 |
| O2—Cu1—O1A | 178.10 (5) | H2S1—N1S—H2S2 | 107.9 |

| | | | |
|---|---|---|---|
| O2A—Cu1—O1A | 85.36 (5) | N2S—C2S—C2S^ii | 110.15 (19) |
| C1—O1—Cu1 | 113.02 (11) | N2S—C2S—H3S1 | 109.6 |
| C2—O2—Cu1 | 112.98 (12) | C2S^ii—C2S—H3S1 | 109.6 |
| C1A—O1A—Cu1 | 111.82 (11) | N2S—C2S—H3S2 | 109.6 |
| C2A—O2A—Cu1 | 113.52 (11) | C2S^ii—C2S—H3S2 | 109.6 |
| O4—C1—O1 | 125.29 (18) | H3S1—C2S—H3S2 | 108.1 |
| O4—C1—C2 | 120.57 (17) | C2S—N2S—C4S | 112.34 (17) |
| O1—C1—C2 | 114.14 (15) | C2S—N2S—H4S1 | 109.1 |
| O3—C2—O2 | 125.64 (18) | C4S—N2S—H4S1 | 109.1 |
| O3—C2—C1 | 120.45 (17) | C2S—N2S—H4S2 | 109.1 |
| O2—C2—C1 | 113.90 (15) | C4S—N2S—H4S2 | 109.1 |
| O4A—C1A—O1A | 125.21 (17) | H4S1—N2S—H4S2 | 107.9 |
| O4A—C1A—C2A | 120.46 (16) | N1S—C3S—H1S3 | 109.5 |
| O1A—C1A—C2A | 114.33 (15) | N1S—C3S—H1S4 | 109.5 |
| O3A—C2A—O2A | 125.78 (17) | H1S3—C3S—H1S4 | 109.5 |
| O3A—C2A—C1A | 119.40 (17) | N1S—C3S—H1S5 | 109.5 |
| O2A—C2A—C1A | 114.82 (15) | H1S3—C3S—H1S5 | 109.5 |
| N1S—C1S—C1S^i | 110.2 (2) | H1S4—C3S—H1S5 | 109.5 |
| N1S—C1S—H1S1 | 109.6 | N2S—C4S—H2S3 | 109.5 |
| C1S^i—C1S—H1S1 | 109.6 | N2S—C4S—H2S4 | 109.5 |
| N1S—C1S—H1S2 | 109.6 | H2S3—C4S—H2S4 | 109.5 |
| C1S^i—C1S—H1S2 | 109.6 | N2S—C4S—H2S5 | 109.5 |
| H1S1—C1S—H1S2 | 108.1 | H2S3—C4S—H2S5 | 109.5 |
| C3S—N1S—C1S | 112.06 (16) | H2S4—C4S—H2S5 | 109.5 |
| | | | |
| O2—Cu1—O1—C1 | 0.30 (12) | O1—C1—C2—O3 | 176.97 (17) |
| O1A—Cu1—O1—C1 | 178.68 (12) | O4—C1—C2—O2 | 177.15 (17) |
| O1—Cu1—O2—C2 | −1.77 (13) | O1—C1—C2—O2 | −2.5 (2) |
| O2A—Cu1—O2—C2 | 178.14 (13) | Cu1—O1A—C1A—O4A | 179.71 (14) |
| O1—Cu1—O1A—C1A | 178.09 (11) | Cu1—O1A—C1A—C2A | 0.11 (17) |
| O2A—Cu1—O1A—C1A | −1.83 (12) | Cu1—O2A—C2A—O3A | 175.09 (15) |
| O2—Cu1—O2A—C2A | −178.11 (13) | Cu1—O2A—C2A—C1A | −4.23 (19) |
| O1A—Cu1—O2A—C2A | 3.51 (13) | O4A—C1A—C2A—O3A | 3.8 (3) |
| Cu1—O1—C1—O4 | −178.63 (15) | O1A—C1A—C2A—O3A | −176.58 (16) |
| Cu1—O1—C1—C2 | 0.99 (18) | O4A—C1A—C2A—O2A | −176.83 (16) |
| Cu1—O2—C2—O3 | −176.78 (17) | O1A—C1A—C2A—O2A | 2.8 (2) |
| Cu1—O2—C2—C1 | 2.64 (19) | C1S^i—C1S—N1S—C3S | 178.0 (2) |
| O4—C1—C2—O3 | −3.4 (3) | C2S^ii—C2S—N2S—C4S | −175.9 (2) |

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

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| N1S—H2S1···O3A^i | 0.90 | 2.22 | 2.939 (2) | 137 |
| N1S—H2S2···O1A^iii | 0.90 | 2.13 | 3.018 (2) | 169 |
| N2S—H4S1···O4A^iii | 0.90 | 2.15 | 2.939 (2) | 145 |
| N2S—H4S1···O3A^iii | 0.90 | 2.31 | 3.004 (2) | 134 |

| N2*S*—H4*S*2···O4[iv] | 0.90 | 2.11 | 2.861 (2) | 140 |
| N2*S*—H4*S*2···O3[ii] | 0.90 | 2.58 | 3.131 (2) | 120 |

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