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# Crystal structure of a copper–mefenamate complex solvated with diglyme and water

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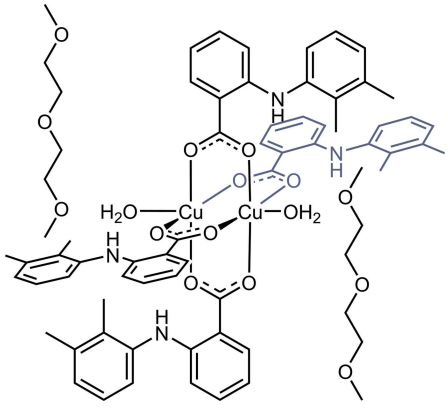
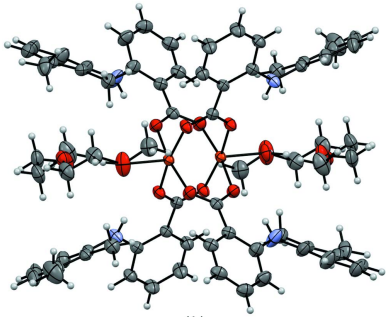
In the copper–mefenamate complex tetrakis[$\mu$-2-(2,3-dimethylanilino)benzoato-$\kappa^2O$:$O'$]bis[aquacopper(II)]–1-methoxy-2-(2-methoxyethoxy)ethane (1/2), $[Cu_2(C_{15}H_{14}NO_2)_4(H_2O)_2]\cdot 2C_6H_{14}O_3$, the asymmetric unit comprises a $Cu^{II}$ cation coordinated to two mefenamate ligands solvated with a water molecule and a diglyme molecule. The complex adopts a paddlewheel motif and is compared to structural analogues crystallized with dimethylformamide and dimethyl sulfoxide.

## 1. Chemical context

Mefenamic acid is a non-steroidal anti-inflammatory drug (NSAID) that is synthesized through reaction of 2-chlorobenzoic acid and 2,3-dimethylaniline in the presence of a copper catalyst (Trinus *et al.*, 1977). Subsequently, pharmacopoeia specifications for mefenamic acid specify a maximum limit of 10 ppm for the quantity of copper present in the final drug product (British Pharmacopoeia, 2017). In exploring strategies to ensure removal of copper from the crude reaction mixture, a new copper–mefenamate complex was isolated. The crystal structure of a copper–mefenamate complex solvated with water and diglyme is reported.



## 2. Structural commentary

The complex $[Cu_2(\text{mefenamate})_4(H_2O)_2]$.2(diglyme) crystallizes in the space group $P2_1/n$, with a $\{Cu_2(RCO_2)_4(H_2O)_2\}$

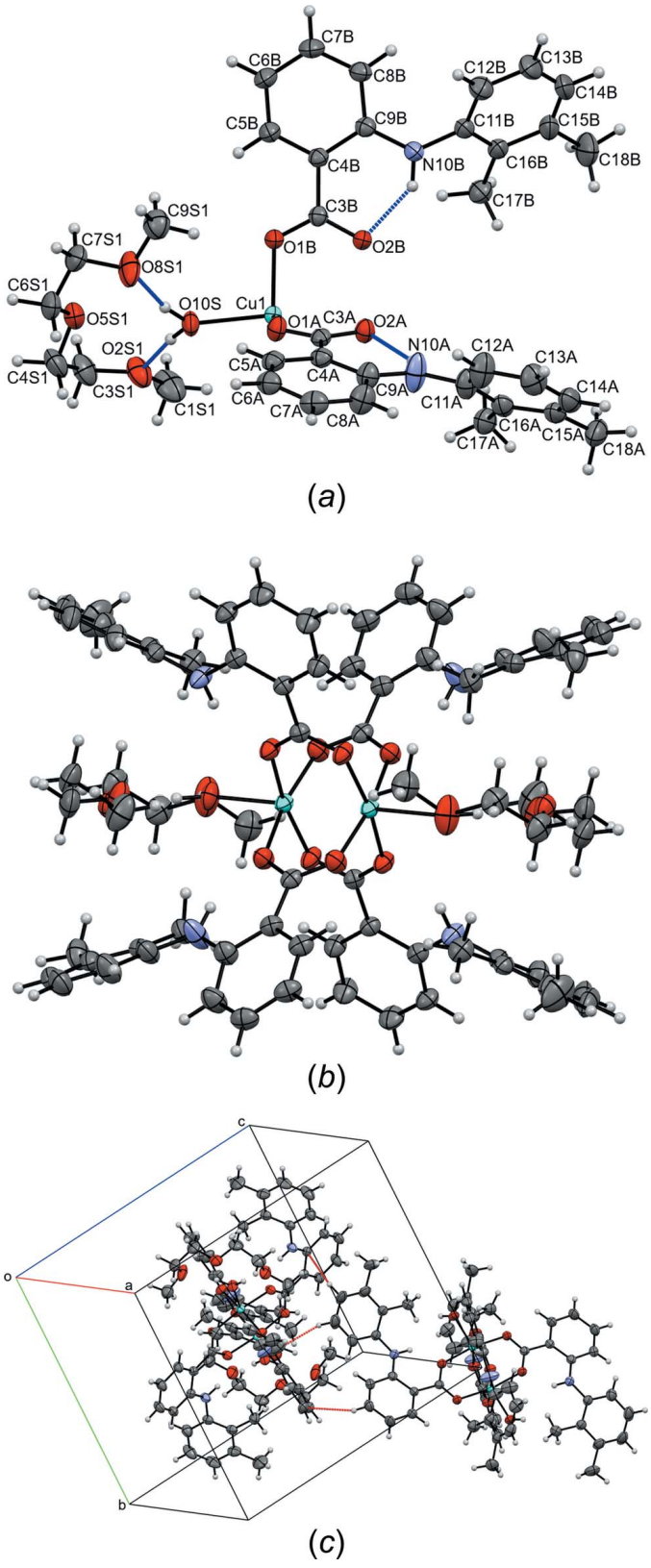



**Figure 1**
Views of $[Cu_2(mefenamate)_4(H_2O)_2]\cdot 2(diglyme)$ as an *ORTEP* representation with ellipsoids set to 50% probability: (*a*) asymmetric unit with hydrogen bonds highlighted (dashed blue lines), (*b*) a single paddlewheel unit of the complex, and (*c*) neighbouring units with edge-to-face interactions highlighted (dashed red lines).

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N10*A*—H10*D*···O2*A* | 0.86 (3) | 1.86 (3) | 2.604 (2) | 143 (2) |
| N10*B*—H10*C*···O2*B* | 0.89 (2) | 1.87 (2) | 2.6065 (18) | 139 (2) |

paddlewheel motif that is typical for coordination of four carboxylate groups to two $Cu^{II}$ cations (Chong *et al.*, 2022). Within the asymmetric unit (Fig. 1*a*), the planes of the 2,3-dimethylphenyls from the two mefenamate molecules are 42.61 (1)° apart. A water molecule occupies each of the apical positions of the paddlewheel motif, which is hydrogen bonded to a diglyme molecule (Fig. 1*a*). The diglyme molecule is oriented such that it fits between the 2,3-dimethyphenyl units of the two mefenamate molecules in the asymmetric unit and is hydrogen bonded to the coordinated water *via* the diglyme outer oxygen positions (Fig. 1*a*). A distorted square-pyramidal geometry is adopted by each $Cu^{II}$ cation in the paddlewheel motif (Fig. 1*b*), with equatorial Cu—O distances of 1.968 (1), 1.961 (1), 1.954 (1), and 1.969 (1) Å between $Cu^{II}$ and the carboxylate moieties. The axial Cu—O distance, between the copper(II) cation and water molecule, is 2.108 (1) Å. The distance between the two $Cu^{II}$ cations is 2.6126 (4) Å. There is an intramolecular bond between the amine and carboxylate groups of the mefenamate, with O···H distances of 1.86 (3) and 1.87 (2) Å for mefenamate units *A* and *B*, respectively (Table 1).

## 3. Supramolecular features

There are no obvious interactions, such as $\pi$–$\pi$ stacking, between neighbouring paddlewheel units within the packed structure. The paddlewheel units interact through edge-to-face interactions of the phenyl groups of the mefanamate ligands (Fig. 1*c*). In the global packing of the structure, the paddlewheel units are arranged as 2D sheets along the crystallographic *ab* plane, with symmetry-equivalent sheets repeating throughout the crystallographic *c* axis at a distance corresponding to *c*. A second 2D arrangement is intercalated halfway between the symmetry-equivalent sheets.

## 4. Database survey

There are three other similar copper–mefenamate paddlewheel structures in the CSD (version 5.43, November 2021; Groom *et al.*, 2016), with different solvents occupying the apical positions. Two entries, MPANCU10 (Yatsimirskii *et al.*, 1979) and MPANCU20 (Mys'kiv *et al.*, 1982), are with *N*,*N*-dimethylformamide (DMF) and one entry, SUTPIG (Facchin *et al.*, 1998), has dimethyl sulfoxide (DMSO) occupying the apical position. The DMF analogue also crystallizes in a monoclinic space group (Table 2). The cell volume of $[Cu_2(mefenamate)_4(H_2O)_2]\cdot 2(diglyme)$ [3538.64 (12) Å$^3$] is larger than the DMF analogue (3026.535 Å$^3$), to accommodate the larger diglyme molecule. The axial Cu—O distance in $[Cu_2(mefenamate)_4(H_2O)_2]\cdot 2(diglyme)$ is shorter than those

**Table 2**
Comparison of selected geometries (Å, °).

Coordinates are unavailable for entry MPANCU10. There are two values per structure, corresponding to the two mefenamate units in the asymmetric unit as denoted *A* and *B* in our atom-numbering scheme.

| | This work | | MPANCU20 | | SUTPIG | |
|---|---|---|---|---|---|---|
| Space group | *P*21/*n* | | *P*21/*c* | | $P\overline{1}$ | |
| O1—C3—C4—C9 | 171.1 (2) | 179.7 (1) | 170.98 | 179.70 | 153 (1) | 180 (1) |
| C4—C9—N10—C11 | 174.3 (2) | 171.2 (2) | −166.40 | 171.56 | 171 (1) | 172 (1) |
| C9—N10—C11—C16 | 144.7 (2) | −124.9 (2) | −155.25 | −109.34 | −107 (2) | 135 (2) |
| Cu—$O_{mefenamate}$ | 1.961 (1) | 1.954 (1) | 1.9737 | 1.9605 | 1.972 (7) | 1.949 (7) |
| Cu—$O_{solvent}$ | 2.108 (1) | | 2.1561 | | 2.17 (1) | |
| Cu···Cu | 2.6126 (4) | | 2.6120 | | 2.627 (3) | |

in structures MPANCU20 and SUTPIG (Table 2). This may be attributed to the higher polarity of water (1.000) compared to DMF and DMSO (0.386 and 0.444, respectively; Reichardt & Welton, 2011). In the DMSO analogue, the 2,3-dimethylphenyls from the two mefenamate molecules within the asymmetric unit are almost coplanar, the planes are 9.06° apart, and the methyl groups of the DMSO point away from the 2,3-dimethylphenyls. For the DMF analogue, the two 2,3-dimethylphenyls are oriented such that they can accommodate one of the methyl groups from the DMF, therefore the planes are 70.22° apart.

Three polymorphic forms are known for mefenamic acid, with significant differences between the forms in the C9—N10—C11—C16 torsion angle $\tau_3$ (Fig. 1*a*; SeethaLekshmi & Guru Row, 2012). The larger torsion angle $\tau_3$ observed with the copper complex (Table 2) is more consistent with those of the form I polymorph of −119.99 ° (XYANAC; McConnell & Company, 1976) and −120.1 (1) ° (XYANAC06; Mague & Ouzidan, 2017). The increased torsional angle can be explained by the location of the dimethylphenyl group with respect to the diglyme group. The phenyl group needs to rotate to ensure a more planar packing arrangement with the diglyme molecule. In comparison to other polymorphs, the metastable form II suffers from significant disorder around the dimethylphenyl ring system, however the torsion angle $\tau_3$ is 68 (2)° for XYANAC04 (SeethaLekshmi & Guru Row, 2012), 74.5 (3)° for XYANAC05 (Yang *et al.*, 2012) and −90 (2)° for XYANAC07 (Abbas *et al.*, 2017). The latter of these data collections is at high pressure and the disorder is not modelled, possibly because of the lack of data present due to the diamond anvil cell. The thermal parameters indicate that some disorder may still be present even at these higher pressures. For metastable form III, the reported torsion angle $\tau_3$ is −80.8 (2)° (XYANAC03; SeethaLekshmi & Guru Row, 2012).

## 5. Synthesis and crystallization

Chemicals were purchased from commercial suppliers and used as received without further purification. Deionized water was obtained from an in-house Milli-Q (Millipore) purification system. A solution was prepared comprising mefenamic acid (25.0 g), diglyme (281.6 g), water (74.7 g) and copper (II) acetate (7.3 g). An aliquot (4 mL) of this solution was removed and mefenamic acid (0.4 g) added to generate a slurry. The mixture was filtered and the filtrate stored in the dark at room temperature for two weeks, after which large green block-shaped crystals of the complex had formed.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The diglyme moiety was found to be disordered over two positions. Initial isotropic refinement of the diglyme allowed the residual electron density to be observed. Using the functionality in *OLEX2*, the atoms were moved to ensure that they overlapped the electron density in a

**Table 3**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Cu_2(C_{15}H_{14}NO_2)_4(H_2O)_2]\cdot 2C_6H_{14}O_3$ |
| $M_r$ | 1392.54 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 105 |
| *a*, *b*, *c* (Å) | 15.5420 (3), 14.0010 (3), 16.3217 (3) |
| $\beta$ (°) | 94.791 (1) |
| $V$ (Å$^3$) | 3539.25 (12) |
| $Z$ | 2 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.30 |
| Crystal size (mm) | 0.2 × 0.15 × 0.1 |
| Data collection | |
| Diffractometer | Bruker Photon100 CMOS |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2016) |
| $T_{min}$, $T_{max}$ | 0.781, 0.881 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 209288, 6424, 5989 |
| $R_{int}$ | 0.039 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.603 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.033, 0.089, 1.06 |
| No. of reflections | 6424 |
| No. of parameters | 477 |
| No. of restraints | 410 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.28, −0.40 |

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

zigzag bonding pattern usually observed for alkyl chains. Distance restraints were applied to ensure the molecular integrity. Using the SPLIT function, the alkyl chain was duplicated and rotated to align with the remaining electron density. This model was refined isotropically before applying EADP restraints to the atoms and refining anisotropically. This provided a stable refined structure. The water hydrogen atoms were added from the difference map and refined with ideal DFIX restraints in place. C-bound hydrogen atoms were placed geometrically and a riding model applied [C—H = 0.95–0.99 Å; $U_{iso}$(H) = 1.2–1.5$U_{eq}$(C)]. All data underpinning this publication are openly available from the University of Strathclyde KnowledgeBase at https://doi.org/10.15129/39f97ad1-8173-4999-b0b6-41c6ae923fe6.

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# supporting information

*Acta Cryst.* (2022). E**78** [https://doi.org/10.1107/S2056989022010647]

## Crystal structure of a copper–mefenamate complex solvated with diglyme and water

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### Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

**Tetrakis[$\mu$-2-(2,3-dimethylanilino)benzoato-$\kappa^2O$:$O'$]bis[aquacopper(II)]–1-methoxy-2-(2-methoxyethoxy)ethane (1/2)**

*Crystal data*

$[Cu_2(C_{15}H_{14}NO_2)_4(H_2O)_2]\cdot 2C_6H_{14}O_3$
$M_r$ = 1392.54
Monoclinic, $P2_1/n$
$a$ = 15.5420 (3) Å
$b$ = 14.0010 (3) Å
$c$ = 16.3217 (3) Å
$\beta$ = 94.791 (1)°
$V$ = 3539.25 (12) Å$^3$
$Z$ = 2
$F(000)$ = 1468
$D_x$ = 1.307 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å
Cell parameters from 9398 reflections
$\theta$ = 4.9–68.2°
$\mu$ = 1.30 mm$^{-1}$
$T$ = 105 K
Block, clear green
0.2 × 0.15 × 0.1 mm

*Data collection*

Bruker Photon100 CMOS diffractometer
Radiation source: Incoatec microfocus Cu source
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
$T_{min}$ = 0.781, $T_{max}$ = 0.881
209288 measured reflections
6424 independent reflections
5989 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039
$\theta_{max}$ = 68.3°, $\theta_{min}$ = 4.9°
$h$ = −18→18
$k$ = −16→16
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.089
$S$ = 1.06
6424 reflections
477 parameters
410 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 2.0003P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.40 e Å$^{-3}$

*Special details*

**Experimental**. The X-ray intensities were collected on a Bruker D8 Venture diffractometer using a Photon 100 Detector. The data were reduced using APEX3 and absorption correction applied using SADABS (Bruker, 2016). The crystal structure was solved and refined using SHELXT and SHELXL via the Olex2 refinement package (Dolomanov *et al.*, 2009). Non-hydrogen atom positions were refined anisotropically.

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. RIGU restarint applied. Diglyme disorder modelled using DFIX and SADI restraints. The ADPs for both diglyme parts were constrained using EADP constraint.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Cu1 | 0.54253 (2) | 0.42405 (2) | 0.48032 (2) | 0.02442 (8) | |
| O1B | 0.51049 (8) | 0.45091 (8) | 0.36430 (7) | 0.0329 (3) | |
| O2B | 0.43845 (8) | 0.58088 (8) | 0.39902 (7) | 0.0326 (3) | |
| O1A | 0.43605 (8) | 0.35049 (8) | 0.48736 (7) | 0.0351 (3) | |
| O2A | 0.36511 (7) | 0.48032 (8) | 0.52427 (7) | 0.0331 (3) | |
| O10S | 0.62229 (8) | 0.30515 (9) | 0.46326 (8) | 0.0376 (3) | |
| N10B | 0.37240 (10) | 0.69540 (10) | 0.28457 (9) | 0.0362 (3) | |
| O2S1 | 0.7835 (9) | 0.2813 (9) | 0.5321 (12) | 0.0540 (12) | 0.666 (3) |
| C3B | 0.46922 (10) | 0.52671 (11) | 0.34617 (9) | 0.0265 (3) | |
| C9B | 0.41162 (10) | 0.63824 (11) | 0.22997 (9) | 0.0285 (3) | |
| C3A | 0.37072 (10) | 0.39031 (11) | 0.51303 (9) | 0.0284 (3) | |
| C4A | 0.29745 (11) | 0.32888 (12) | 0.53288 (10) | 0.0308 (3) | |
| C4B | 0.45728 (10) | 0.55460 (11) | 0.25802 (9) | 0.0269 (3) | |
| O5S1 | 0.73581 (16) | 0.15001 (18) | 0.40989 (17) | 0.0438 (6) | 0.666 (3) |
| C11B | 0.33426 (11) | 0.78619 (12) | 0.27016 (10) | 0.0312 (3) | |
| C8B | 0.40932 (11) | 0.65984 (13) | 0.14555 (10) | 0.0345 (4) | |
| H8B | 0.3794 | 0.7152 | 0.1250 | 0.041* | |
| C5B | 0.49629 (11) | 0.49735 (13) | 0.20199 (10) | 0.0348 (4) | |
| H5B | 0.5262 | 0.4414 | 0.2212 | 0.042* | |
| C5A | 0.30263 (12) | 0.23152 (12) | 0.51507 (10) | 0.0349 (4) | |
| H5A | 0.3501 | 0.2088 | 0.4875 | 0.042* | |
| N10A | 0.21962 (12) | 0.45875 (13) | 0.59054 (14) | 0.0588 (5) | |
| C16A | 0.17474 (12) | 0.58519 (13) | 0.67658 (11) | 0.0367 (4) | |
| O8S1 | 0.5611 (3) | 0.1715 (4) | 0.3438 (5) | 0.0604 (14) | 0.666 (3) |
| C16B | 0.36286 (11) | 0.86224 (12) | 0.32109 (10) | 0.0322 (3) | |
| C15A | 0.10932 (12) | 0.64349 (13) | 0.70386 (11) | 0.0388 (4) | |
| C6B | 0.49276 (13) | 0.51950 (15) | 0.11960 (11) | 0.0447 (4) | |
| H6B | 0.5192 | 0.4792 | 0.0821 | 0.054* | |
| C7B | 0.44963 (13) | 0.60229 (15) | 0.09242 (11) | 0.0429 (4) | |
| H7B | 0.4481 | 0.6193 | 0.0360 | 0.052* | |
| C17A | 0.26827 (12) | 0.60465 (15) | 0.70369 (12) | 0.0441 (4) | |

| | | | | | |
|---|---|---|---|---|---|
| H17A | 0.2948 | 0.6400 | 0.6605 | 0.066* | |
| H17B | 0.2987 | 0.5440 | 0.7139 | 0.066* | |
| H17C | 0.2720 | 0.6426 | 0.7543 | 0.066* | |
| C6A | 0.24089 (12) | 0.16743 (13) | 0.53636 (11) | 0.0400 (4) | |
| H6A | 0.2446 | 0.1018 | 0.5222 | 0.048* | |
| C9A | 0.22586 (11) | 0.36315 (13) | 0.57261 (12) | 0.0395 (4) | |
| C17B | 0.43678 (13) | 0.85116 (14) | 0.38602 (11) | 0.0418 (4) | |
| H17D | 0.4145 | 0.8498 | 0.4404 | 0.063* | |
| H17E | 0.4766 | 0.9051 | 0.3830 | 0.063* | |
| H17F | 0.4674 | 0.7914 | 0.3770 | 0.063* | |
| C11A | 0.15206 (12) | 0.50948 (14) | 0.62317 (13) | 0.0453 (4) | |
| C12B | 0.26720 (12) | 0.79882 (15) | 0.20959 (12) | 0.0439 (4) | |
| H12B | 0.2476 | 0.7465 | 0.1760 | 0.053* | |
| C14A | 0.02351 (12) | 0.62150 (15) | 0.68039 (12) | 0.0447 (4) | |
| H14A | −0.0210 | 0.6595 | 0.7002 | 0.054* | |
| C18A | 0.13044 (14) | 0.72995 (17) | 0.75676 (13) | 0.0536 (5) | |
| H18A | 0.1576 | 0.7096 | 0.8103 | 0.080* | |
| H18B | 0.0773 | 0.7651 | 0.7647 | 0.080* | |
| H18C | 0.1703 | 0.7714 | 0.7297 | 0.080* | |
| C15B | 0.32210 (14) | 0.95162 (14) | 0.30921 (12) | 0.0453 (4) | |
| C14B | 0.25653 (16) | 0.96269 (16) | 0.24775 (13) | 0.0561 (6) | |
| H14B | 0.2299 | 1.0234 | 0.2395 | 0.067* | |
| C7A | 0.17319 (12) | 0.20059 (14) | 0.57892 (11) | 0.0422 (4) | |
| H7A | 0.1319 | 0.1567 | 0.5964 | 0.051* | |
| C8A | 0.16519 (13) | 0.29586 (15) | 0.59604 (13) | 0.0473 (5) | |
| H8A | 0.1177 | 0.3170 | 0.6243 | 0.057* | |
| C13B | 0.22881 (14) | 0.88734 (18) | 0.19800 (13) | 0.0561 (6) | |
| H13B | 0.1835 | 0.8962 | 0.1559 | 0.067* | |
| C6S1 | 0.6846 (5) | 0.0737 (6) | 0.3762 (5) | 0.0517 (16) | 0.666 (3) |
| H6SA | 0.6530 | 0.0435 | 0.4196 | 0.062* | 0.666 (3) |
| H6SB | 0.7220 | 0.0247 | 0.3535 | 0.062* | 0.666 (3) |
| C13A | 0.00184 (13) | 0.54565 (16) | 0.62903 (15) | 0.0534 (5) | |
| H13A | −0.0572 | 0.5313 | 0.6143 | 0.064* | |
| C12A | 0.06577 (13) | 0.49027 (16) | 0.59881 (16) | 0.0569 (6) | |
| H12A | 0.0509 | 0.4395 | 0.5617 | 0.068* | |
| C3S1 | 0.8407 (4) | 0.2105 (3) | 0.5096 (3) | 0.0564 (12) | 0.666 (3) |
| H3SA | 0.8808 | 0.1936 | 0.5577 | 0.068* | 0.666 (3) |
| H3SB | 0.8753 | 0.2356 | 0.4661 | 0.068* | 0.666 (3) |
| C7S1 | 0.6224 (2) | 0.1110 (2) | 0.3099 (2) | 0.0487 (8) | 0.666 (3) |
| H7SA | 0.6538 | 0.1472 | 0.2697 | 0.058* | 0.666 (3) |
| H7SB | 0.5922 | 0.0570 | 0.2808 | 0.058* | 0.666 (3) |
| C18B | 0.3508 (2) | 1.03494 (17) | 0.36428 (18) | 0.0787 (8) | |
| H18D | 0.3400 | 1.0200 | 0.4212 | 0.118* | |
| H18E | 0.3182 | 1.0922 | 0.3463 | 0.118* | |
| H18F | 0.4126 | 1.0464 | 0.3609 | 0.118* | |
| C1S1 | 0.8212 (6) | 0.3611 (4) | 0.5730 (4) | 0.0698 (15) | 0.666 (3) |
| H1SA | 0.8572 | 0.3952 | 0.5361 | 0.105* | 0.666 (3) |
| H1SB | 0.8571 | 0.3400 | 0.6219 | 0.105* | 0.666 (3) |

| | | | | | |
|---|---|---|---|---|---|
| H1SC | 0.7758 | 0.4037 | 0.5896 | 0.105* | 0.666 (3) |
| C4S1 | 0.7934 (3) | 0.1233 (3) | 0.4788 (3) | 0.0558 (10) | 0.666 (3) |
| H4SA | 0.8347 | 0.0746 | 0.4623 | 0.067* | 0.666 (3) |
| H4SB | 0.7605 | 0.0959 | 0.5226 | 0.067* | 0.666 (3) |
| H10C | 0.3857 (14) | 0.6801 (16) | 0.3367 (15) | 0.049 (6)* | |
| H10D | 0.2643 (16) | 0.4898 (18) | 0.5786 (15) | 0.057 (7)* | |
| H10A | 0.6808 (5) | 0.2953 (16) | 0.4844 (13) | 0.064 (7)* | |
| H10B | 0.6103 (14) | 0.2545 (13) | 0.4247 (13) | 0.085 (9)* | |
| C9S2 | 0.4948 (9) | 0.2144 (16) | 0.3063 (12) | 0.0550 (15) | 0.31 (3) |
| H9SD | 0.4759 | 0.1747 | 0.2586 | 0.082* | 0.31 (3) |
| H9SE | 0.4922 | 0.2819 | 0.2903 | 0.082* | 0.31 (3) |
| H9SF | 0.4568 | 0.2033 | 0.3503 | 0.082* | 0.31 (3) |
| O2S2 | 0.795 (2) | 0.274 (2) | 0.536 (2) | 0.0540 (12) | 0.334 (3) |
| C3S2 | 0.8316 (8) | 0.1859 (8) | 0.5313 (7) | 0.0564 (12) | 0.334 (3) |
| H3SC | 0.8115 | 0.1445 | 0.5750 | 0.068* | 0.334 (3) |
| H3SD | 0.8951 | 0.1922 | 0.5410 | 0.068* | 0.334 (3) |
| C1S2 | 0.8244 (13) | 0.3376 (10) | 0.5961 (9) | 0.0698 (15) | 0.334 (3) |
| H1SD | 0.7960 | 0.3995 | 0.5862 | 0.105* | 0.334 (3) |
| H1SE | 0.8870 | 0.3454 | 0.5949 | 0.105* | 0.334 (3) |
| H1SF | 0.8116 | 0.3132 | 0.6500 | 0.105* | 0.334 (3) |
| C4S2 | 0.8103 (7) | 0.1404 (7) | 0.4509 (6) | 0.0558 (10) | 0.334 (3) |
| H4SC | 0.8281 | 0.1827 | 0.4068 | 0.067* | 0.334 (3) |
| H4SD | 0.8426 | 0.0796 | 0.4483 | 0.067* | 0.334 (3) |
| O5S2 | 0.7218 (4) | 0.1224 (4) | 0.4386 (3) | 0.0438 (6) | 0.334 (3) |
| C6S2 | 0.6944 (11) | 0.0843 (14) | 0.3610 (11) | 0.0517 (16) | 0.334 (3) |
| H6SC | 0.7120 | 0.0165 | 0.3589 | 0.062* | 0.334 (3) |
| H6SD | 0.7230 | 0.1193 | 0.3180 | 0.062* | 0.334 (3) |
| C7S2 | 0.6002 (5) | 0.0912 (5) | 0.3437 (5) | 0.0487 (8) | 0.334 (3) |
| H7SC | 0.5813 | 0.0560 | 0.2927 | 0.058* | 0.334 (3) |
| H7SD | 0.5705 | 0.0637 | 0.3896 | 0.058* | 0.334 (3) |
| O8S2 | 0.5806 (7) | 0.1903 (9) | 0.3344 (11) | 0.0604 (14) | 0.334 (3) |
| C9S1 | 0.5085 (5) | 0.2183 (6) | 0.2840 (7) | 0.0550 (15) | 0.69 (3) |
| H9SA | 0.5442 | 0.2550 | 0.2486 | 0.082* | 0.69 (3) |
| H9SB | 0.4697 | 0.2617 | 0.3103 | 0.082* | 0.69 (3) |
| H9SC | 0.4743 | 0.1713 | 0.2508 | 0.082* | 0.69 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.03002 (14) | 0.02114 (13) | 0.02236 (13) | 0.00405 (8) | 0.00367 (9) | −0.00087 (8) |
| O1B | 0.0443 (6) | 0.0296 (6) | 0.0245 (5) | 0.0110 (5) | 0.0006 (5) | −0.0010 (4) |
| O2B | 0.0447 (7) | 0.0288 (6) | 0.0245 (5) | 0.0108 (5) | 0.0040 (5) | 0.0000 (4) |
| O1A | 0.0371 (6) | 0.0271 (6) | 0.0420 (6) | 0.0001 (5) | 0.0089 (5) | −0.0062 (5) |
| O2A | 0.0346 (6) | 0.0259 (6) | 0.0394 (6) | −0.0001 (5) | 0.0078 (5) | −0.0027 (5) |
| O10S | 0.0403 (7) | 0.0311 (6) | 0.0403 (7) | 0.0141 (5) | −0.0020 (5) | −0.0086 (5) |
| N10B | 0.0532 (9) | 0.0289 (7) | 0.0262 (7) | 0.0110 (6) | 0.0012 (6) | 0.0013 (6) |
| O2S1 | 0.045 (4) | 0.046 (2) | 0.066 (2) | 0.0094 (16) | −0.020 (2) | −0.0047 (19) |
| C3B | 0.0281 (7) | 0.0246 (7) | 0.0268 (7) | −0.0014 (6) | 0.0016 (6) | −0.0018 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9B | 0.0307 (8) | 0.0270 (8) | 0.0273 (7) | −0.0023 (6) | −0.0005 (6) | −0.0005 (6) |
| C3A | 0.0351 (8) | 0.0281 (8) | 0.0213 (7) | 0.0004 (6) | −0.0015 (6) | −0.0016 (6) |
| C4A | 0.0350 (8) | 0.0298 (8) | 0.0272 (8) | −0.0032 (6) | 0.0004 (6) | −0.0011 (6) |
| C4B | 0.0295 (7) | 0.0265 (7) | 0.0243 (7) | −0.0008 (6) | 0.0000 (6) | −0.0008 (6) |
| O5S1 | 0.0477 (11) | 0.0355 (14) | 0.0483 (16) | 0.0125 (10) | 0.0050 (10) | −0.0008 (10) |
| C11B | 0.0338 (8) | 0.0309 (8) | 0.0296 (8) | 0.0056 (6) | 0.0063 (6) | 0.0038 (6) |
| C8B | 0.0415 (9) | 0.0342 (9) | 0.0269 (8) | 0.0021 (7) | −0.0024 (7) | 0.0022 (7) |
| C5B | 0.0409 (9) | 0.0349 (9) | 0.0281 (8) | 0.0064 (7) | 0.0003 (7) | −0.0022 (7) |
| C5A | 0.0436 (9) | 0.0321 (8) | 0.0284 (8) | −0.0026 (7) | 0.0001 (7) | −0.0021 (7) |
| N10A | 0.0418 (9) | 0.0365 (9) | 0.1029 (16) | −0.0080 (7) | 0.0353 (10) | −0.0175 (9) |
| C16A | 0.0372 (9) | 0.0356 (9) | 0.0390 (9) | 0.0052 (7) | 0.0128 (7) | 0.0097 (7) |
| O8S1 | 0.057 (2) | 0.045 (2) | 0.075 (2) | 0.0121 (18) | −0.018 (2) | −0.0332 (19) |
| C16B | 0.0368 (8) | 0.0312 (8) | 0.0297 (8) | 0.0053 (7) | 0.0099 (7) | 0.0026 (6) |
| C15A | 0.0424 (9) | 0.0416 (10) | 0.0337 (9) | 0.0107 (8) | 0.0103 (7) | 0.0103 (7) |
| C6B | 0.0567 (11) | 0.0521 (11) | 0.0254 (8) | 0.0160 (9) | 0.0036 (8) | −0.0046 (8) |
| C7B | 0.0528 (11) | 0.0512 (11) | 0.0243 (8) | 0.0080 (9) | 0.0001 (7) | 0.0024 (7) |
| C17A | 0.0387 (9) | 0.0484 (11) | 0.0462 (11) | 0.0061 (8) | 0.0093 (8) | −0.0007 (9) |
| C6A | 0.0521 (10) | 0.0306 (9) | 0.0364 (9) | −0.0079 (8) | −0.0010 (8) | −0.0018 (7) |
| C9A | 0.0370 (9) | 0.0341 (9) | 0.0478 (10) | −0.0039 (7) | 0.0062 (8) | −0.0050 (8) |
| C17B | 0.0481 (10) | 0.0396 (10) | 0.0371 (9) | 0.0009 (8) | −0.0005 (8) | −0.0044 (8) |
| C11A | 0.0384 (9) | 0.0359 (9) | 0.0645 (12) | −0.0005 (8) | 0.0205 (9) | −0.0007 (9) |
| C12B | 0.0419 (10) | 0.0491 (11) | 0.0396 (10) | 0.0082 (8) | −0.0038 (8) | −0.0009 (8) |
| C14A | 0.0396 (10) | 0.0490 (11) | 0.0474 (10) | 0.0120 (8) | 0.0141 (8) | 0.0103 (9) |
| C18A | 0.0523 (12) | 0.0632 (13) | 0.0456 (11) | 0.0199 (10) | 0.0059 (9) | −0.0103 (10) |
| C15B | 0.0596 (12) | 0.0338 (9) | 0.0444 (10) | 0.0148 (8) | 0.0160 (9) | 0.0014 (8) |
| C14B | 0.0713 (14) | 0.0515 (12) | 0.0467 (11) | 0.0362 (11) | 0.0115 (10) | 0.0074 (9) |
| C7A | 0.0441 (10) | 0.0414 (10) | 0.0403 (10) | −0.0143 (8) | −0.0004 (8) | 0.0007 (8) |
| C8A | 0.0400 (10) | 0.0432 (10) | 0.0604 (12) | −0.0096 (8) | 0.0142 (9) | −0.0069 (9) |
| C13B | 0.0518 (12) | 0.0723 (14) | 0.0433 (11) | 0.0313 (11) | −0.0020 (9) | 0.0054 (10) |
| C6S1 | 0.071 (2) | 0.033 (2) | 0.051 (3) | 0.0145 (16) | 0.006 (2) | −0.009 (2) |
| C13A | 0.0347 (10) | 0.0564 (13) | 0.0707 (14) | −0.0004 (9) | 0.0128 (9) | 0.0044 (11) |
| C12A | 0.0415 (10) | 0.0480 (12) | 0.0837 (16) | −0.0075 (9) | 0.0195 (10) | −0.0120 (11) |
| C3S1 | 0.0391 (17) | 0.053 (3) | 0.075 (3) | 0.0136 (18) | −0.0069 (19) | 0.0068 (19) |
| C7S1 | 0.067 (2) | 0.0370 (16) | 0.042 (2) | 0.0056 (13) | 0.0058 (14) | −0.0119 (14) |
| C18B | 0.123 (2) | 0.0385 (12) | 0.0743 (17) | 0.0224 (14) | 0.0046 (16) | −0.0143 (11) |
| C1S1 | 0.0702 (18) | 0.057 (3) | 0.076 (4) | 0.001 (3) | −0.032 (3) | −0.005 (2) |
| C4S1 | 0.058 (2) | 0.041 (2) | 0.067 (3) | 0.0176 (15) | −0.0042 (19) | 0.0105 (18) |
| C9S2 | 0.057 (2) | 0.0484 (16) | 0.059 (4) | 0.0007 (19) | −0.001 (2) | −0.009 (3) |
| O2S2 | 0.045 (4) | 0.046 (2) | 0.066 (2) | 0.0094 (16) | −0.020 (2) | −0.0047 (19) |
| C3S2 | 0.0391 (17) | 0.053 (3) | 0.075 (3) | 0.0136 (18) | −0.0069 (19) | 0.0068 (19) |
| C1S2 | 0.0702 (18) | 0.057 (3) | 0.076 (4) | 0.001 (3) | −0.032 (3) | −0.005 (2) |
| C4S2 | 0.058 (2) | 0.041 (2) | 0.067 (3) | 0.0176 (15) | −0.0042 (19) | 0.0105 (18) |
| O5S2 | 0.0477 (11) | 0.0355 (14) | 0.0483 (16) | 0.0125 (10) | 0.0050 (10) | −0.0008 (10) |
| C6S2 | 0.071 (2) | 0.033 (2) | 0.051 (3) | 0.0145 (16) | 0.006 (2) | −0.009 (2) |
| C7S2 | 0.067 (2) | 0.0370 (16) | 0.042 (2) | 0.0056 (13) | 0.0058 (14) | −0.0119 (14) |
| O8S2 | 0.057 (2) | 0.045 (2) | 0.075 (2) | 0.0121 (18) | −0.018 (2) | −0.0332 (19) |
| C9S1 | 0.057 (2) | 0.0484 (16) | 0.059 (4) | 0.0007 (19) | −0.001 (2) | −0.009 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—Cu1$^{i}$ | 2.6126 (4) | C11A—C12A | 1.393 (3) |
| Cu1—O1B | 1.9539 (11) | C12B—H12B | 0.9500 |
| Cu1—O2B$^{i}$ | 1.9682 (11) | C12B—C13B | 1.382 (3) |
| Cu1—O1A | 1.9608 (12) | C14A—H14A | 0.9500 |
| Cu1—O2A$^{i}$ | 1.9689 (11) | C14A—C13A | 1.377 (3) |
| Cu1—O10S | 2.1078 (11) | C18A—H18A | 0.9800 |
| O1B—C3B | 1.2624 (19) | C18A—H18B | 0.9800 |
| O2B—Cu1$^{i}$ | 1.9682 (11) | C18A—H18C | 0.9800 |
| O2B—C3B | 1.2715 (19) | C15B—C14B | 1.378 (3) |
| O1A—C3A | 1.260 (2) | C15B—C18B | 1.517 (3) |
| O2A—Cu1$^{i}$ | 1.9690 (11) | C14B—H14B | 0.9500 |
| O2A—C3A | 1.278 (2) | C14B—C13B | 1.378 (3) |
| O10S—H10A | 0.956 (3) | C7A—H7A | 0.9500 |
| O10S—H10B | 0.956 (3) | C7A—C8A | 1.371 (3) |
| N10B—C9B | 1.377 (2) | C8A—H8A | 0.9500 |
| N10B—C11B | 1.414 (2) | C13B—H13B | 0.9500 |
| N10B—H10C | 0.88 (2) | C6S1—H6SA | 0.9900 |
| O2S1—C3S1 | 1.401 (10) | C6S1—H6SB | 0.9900 |
| O2S1—C1S1 | 1.404 (10) | C6S1—C7S1 | 1.484 (8) |
| C3B—C4B | 1.487 (2) | C13A—H13A | 0.9500 |
| C9B—C4B | 1.425 (2) | C13A—C12A | 1.383 (3) |
| C9B—C8B | 1.408 (2) | C12A—H12A | 0.9500 |
| C3A—C4A | 1.484 (2) | C3S1—H3SA | 0.9900 |
| C4A—C5A | 1.397 (2) | C3S1—H3SB | 0.9900 |
| C4A—C9A | 1.418 (2) | C3S1—C4S1 | 1.490 (7) |
| C4B—C5B | 1.392 (2) | C7S1—H7SA | 0.9900 |
| O5S1—C6S1 | 1.416 (8) | C7S1—H7SB | 0.9900 |
| O5S1—C4S1 | 1.428 (5) | C18B—H18D | 0.9800 |
| C11B—C16B | 1.400 (2) | C18B—H18E | 0.9800 |
| C11B—C12B | 1.387 (2) | C18B—H18F | 0.9800 |
| C8B—H8B | 0.9500 | C1S1—H1SA | 0.9800 |
| C8B—C7B | 1.373 (3) | C1S1—H1SB | 0.9800 |
| C5B—H5B | 0.9500 | C1S1—H1SC | 0.9800 |
| C5B—C6B | 1.377 (2) | C4S1—H4SA | 0.9900 |
| C5A—H5A | 0.9500 | C4S1—H4SB | 0.9900 |
| C5A—C6A | 1.379 (3) | C9S2—H9SD | 0.9800 |
| N10A—C9A | 1.375 (2) | C9S2—H9SE | 0.9800 |
| N10A—C11A | 1.409 (2) | C9S2—H9SF | 0.9800 |
| N10A—H10D | 0.86 (2) | C9S2—O8S2 | 1.414 (14) |
| C16A—C15A | 1.405 (2) | O2S2—C3S2 | 1.369 (19) |
| C16A—C17A | 1.509 (3) | O2S2—C1S2 | 1.37 (2) |
| C16A—C11A | 1.399 (3) | C3S2—H3SC | 0.9900 |
| O8S1—C7S1 | 1.421 (7) | C3S2—H3SD | 0.9900 |
| O8S1—C9S1 | 1.383 (8) | C3S2—C4S2 | 1.471 (15) |
| C16B—C17B | 1.505 (2) | C1S2—H1SD | 0.9800 |
| C16B—C15B | 1.409 (2) | C1S2—H1SE | 0.9800 |

| | | | |
|---|---|---|---|
| C15A—C14A | 1.391 (3) | C1S2—H1SF | 0.9800 |
| C15A—C18A | 1.507 (3) | C4S2—H4SC | 0.9900 |
| C6B—H6B | 0.9500 | C4S2—H4SD | 0.9900 |
| C6B—C7B | 1.393 (3) | C4S2—O5S2 | 1.397 (12) |
| C7B—H7B | 0.9500 | O5S2—C6S2 | 1.407 (17) |
| C17A—H17A | 0.9800 | C6S2—H6SC | 0.9900 |
| C17A—H17B | 0.9800 | C6S2—H6SD | 0.9900 |
| C17A—H17C | 0.9800 | C6S2—C7S2 | 1.471 (17) |
| C6A—H6A | 0.9500 | C7S2—H7SC | 0.9900 |
| C6A—C7A | 1.388 (3) | C7S2—H7SD | 0.9900 |
| C9A—C8A | 1.408 (3) | C7S2—O8S2 | 1.426 (14) |
| C17B—H17D | 0.9800 | C9S1—H9SA | 0.9800 |
| C17B—H17E | 0.9800 | C9S1—H9SB | 0.9800 |
| C17B—H17F | 0.9800 | C9S1—H9SC | 0.9800 |

| | | | |
|---|---|---|---|
| O1B—Cu1—Cu1$^{i}$ | 89.34 (3) | H18A—C18A—H18C | 109.5 |
| O1B—Cu1—O2B$^{i}$ | 168.92 (5) | H18B—C18A—H18C | 109.5 |
| O1B—Cu1—O1A | 90.57 (5) | C16B—C15B—C18B | 119.69 (19) |
| O1B—Cu1—O2A$^{i}$ | 87.70 (5) | C14B—C15B—C16B | 119.80 (19) |
| O1B—Cu1—O10S | 97.42 (5) | C14B—C15B—C18B | 120.51 (19) |
| O2B$^{i}$—Cu1—Cu1$^{i}$ | 79.58 (3) | C15B—C14B—H14B | 119.4 |
| O2B$^{i}$—Cu1—O2A$^{i}$ | 90.74 (5) | C15B—C14B—C13B | 121.24 (18) |
| O2B$^{i}$—Cu1—O10S | 93.65 (5) | C13B—C14B—H14B | 119.4 |
| O1A—Cu1—Cu1$^{i}$ | 88.07 (3) | C6A—C7A—H7A | 119.6 |
| O1A—Cu1—O2B$^{i}$ | 88.85 (5) | C8A—C7A—C6A | 120.85 (17) |
| O1A—Cu1—O2A$^{i}$ | 168.82 (5) | C8A—C7A—H7A | 119.6 |
| O1A—Cu1—O10S | 95.82 (5) | C9A—C8A—H8A | 119.3 |
| O2A$^{i}$—Cu1—Cu1$^{i}$ | 80.87 (3) | C7A—C8A—C9A | 121.44 (18) |
| O2A$^{i}$—Cu1—O10S | 95.36 (5) | C7A—C8A—H8A | 119.3 |
| O10S—Cu1—Cu1$^{i}$ | 172.15 (4) | C12B—C13B—H13B | 120.1 |
| C3B—O1B—Cu1 | 118.18 (10) | C14B—C13B—C12B | 119.72 (19) |
| C3B—O2B—Cu1$^{i}$ | 128.64 (10) | C14B—C13B—H13B | 120.1 |
| C3A—O1A—Cu1 | 119.63 (10) | O5S1—C6S1—H6SA | 109.8 |
| C3A—O2A—Cu1$^{i}$ | 127.34 (10) | O5S1—C6S1—H6SB | 109.8 |
| Cu1—O10S—H10A | 128.2 (12) | O5S1—C6S1—C7S1 | 109.2 (6) |
| Cu1—O10S—H10B | 126.1 (13) | H6SA—C6S1—H6SB | 108.3 |
| H10A—O10S—H10B | 104.9 (7) | C7S1—C6S1—H6SA | 109.8 |
| C9B—N10B—C11B | 128.08 (14) | C7S1—C6S1—H6SB | 109.8 |
| C9B—N10B—H10C | 113.6 (14) | C14A—C13A—H13A | 119.9 |
| C11B—N10B—H10C | 116.1 (15) | C14A—C13A—C12A | 120.19 (19) |
| C3S1—O2S1—C1S1 | 116.0 (10) | C12A—C13A—H13A | 119.9 |
| O1B—C3B—O2B | 123.71 (14) | C11A—C12A—H12A | 120.2 |
| O1B—C3B—C4B | 117.85 (13) | C13A—C12A—C11A | 119.6 (2) |
| O2B—C3B—C4B | 118.43 (13) | C13A—C12A—H12A | 120.2 |
| N10B—C9B—C4B | 120.34 (14) | O2S1—C3S1—H3SA | 109.4 |
| N10B—C9B—C8B | 122.13 (15) | O2S1—C3S1—H3SB | 109.4 |
| C8B—C9B—C4B | 117.53 (15) | O2S1—C3S1—C4S1 | 111.3 (7) |
| O1A—C3A—O2A | 123.41 (15) | H3SA—C3S1—H3SB | 108.0 |

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| O1A—C3A—C4A | 118.05 (14) | C4S1—C3S1—H3SA | 109.4 |
| O2A—C3A—C4A | 118.53 (14) | C4S1—C3S1—H3SB | 109.4 |
| C5A—C4A—C3A | 117.47 (15) | O8S1—C7S1—C6S1 | 110.1 (5) |
| C5A—C4A—C9A | 119.10 (16) | O8S1—C7S1—H7SA | 109.6 |
| C9A—C4A—C3A | 123.33 (15) | O8S1—C7S1—H7SB | 109.6 |
| C9B—C4B—C3B | 123.03 (14) | C6S1—C7S1—H7SA | 109.6 |
| C5B—C4B—C3B | 117.28 (14) | C6S1—C7S1—H7SB | 109.6 |
| C5B—C4B—C9B | 119.64 (14) | H7SA—C7S1—H7SB | 108.1 |
| C6S1—O5S1—C4S1 | 113.8 (4) | C15B—C18B—H18D | 109.5 |
| C16B—C11B—N10B | 118.49 (15) | C15B—C18B—H18E | 109.5 |
| C12B—C11B—N10B | 120.86 (16) | C15B—C18B—H18F | 109.5 |
| C12B—C11B—C16B | 120.58 (16) | H18D—C18B—H18E | 109.5 |
| C9B—C8B—H8B | 119.5 | H18D—C18B—H18F | 109.5 |
| C7B—C8B—C9B | 121.08 (16) | H18E—C18B—H18F | 109.5 |
| C7B—C8B—H8B | 119.5 | O2S1—C1S1—H1SA | 109.5 |
| C4B—C5B—H5B | 119.1 | O2S1—C1S1—H1SB | 109.5 |
| C6B—C5B—C4B | 121.86 (16) | O2S1—C1S1—H1SC | 109.5 |
| C6B—C5B—H5B | 119.1 | H1SA—C1S1—H1SB | 109.5 |
| C4A—C5A—H5A | 119.0 | H1SA—C1S1—H1SC | 109.5 |
| C6A—C5A—C4A | 121.92 (17) | H1SB—C1S1—H1SC | 109.5 |
| C6A—C5A—H5A | 119.0 | O5S1—C4S1—C3S1 | 108.0 (4) |
| C9A—N10A—C11A | 129.73 (17) | O5S1—C4S1—H4SA | 110.1 |
| C9A—N10A—H10D | 111.9 (16) | O5S1—C4S1—H4SB | 110.1 |
| C11A—N10A—H10D | 118.3 (16) | C3S1—C4S1—H4SA | 110.1 |
| C15A—C16A—C17A | 120.49 (17) | C3S1—C4S1—H4SB | 110.1 |
| C11A—C16A—C15A | 119.10 (17) | H4SA—C4S1—H4SB | 108.4 |
| C11A—C16A—C17A | 120.41 (16) | H9SD—C9S2—H9SE | 109.5 |
| C9S1—O8S1—C7S1 | 112.6 (8) | H9SD—C9S2—H9SF | 109.5 |
| C11B—C16B—C17B | 121.71 (15) | H9SE—C9S2—H9SF | 109.5 |
| C11B—C16B—C15B | 118.49 (16) | O8S2—C9S2—H9SD | 109.5 |
| C15B—C16B—C17B | 119.78 (17) | O8S2—C9S2—H9SE | 109.5 |
| C16A—C15A—C18A | 121.28 (17) | O8S2—C9S2—H9SF | 109.5 |
| C14A—C15A—C16A | 119.14 (18) | C3S2—O2S2—C1S2 | 121 (2) |
| C14A—C15A—C18A | 119.57 (17) | O2S2—C3S2—H3SC | 109.1 |
| C5B—C6B—H6B | 120.7 | O2S2—C3S2—H3SD | 109.1 |
| C5B—C6B—C7B | 118.52 (17) | O2S2—C3S2—C4S2 | 112.4 (15) |
| C7B—C6B—H6B | 120.7 | H3SC—C3S2—H3SD | 107.9 |
| C8B—C7B—C6B | 121.35 (16) | C4S2—C3S2—H3SC | 109.1 |
| C8B—C7B—H7B | 119.3 | C4S2—C3S2—H3SD | 109.1 |
| C6B—C7B—H7B | 119.3 | O2S2—C1S2—H1SD | 109.5 |
| C16A—C17A—H17A | 109.5 | O2S2—C1S2—H1SE | 109.5 |
| C16A—C17A—H17B | 109.5 | O2S2—C1S2—H1SF | 109.5 |
| C16A—C17A—H17C | 109.5 | H1SD—C1S2—H1SE | 109.5 |
| H17A—C17A—H17B | 109.5 | H1SD—C1S2—H1SF | 109.5 |
| H17A—C17A—H17C | 109.5 | H1SE—C1S2—H1SF | 109.5 |
| H17B—C17A—H17C | 109.5 | C3S2—C4S2—H4SC | 109.5 |
| C5A—C6A—H6A | 120.6 | C3S2—C4S2—H4SD | 109.5 |
| C5A—C6A—C7A | 118.74 (17) | H4SC—C4S2—H4SD | 108.1 |

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| C7A—C6A—H6A | 120.6 | O5S2—C4S2—C3S2 | 110.6 (9) |
| N10A—C9A—C4A | 119.92 (16) | O5S2—C4S2—H4SC | 109.5 |
| N10A—C9A—C8A | 122.18 (17) | O5S2—C4S2—H4SD | 109.5 |
| C8A—C9A—C4A | 117.82 (17) | C4S2—O5S2—C6S2 | 114.8 (10) |
| C16B—C17B—H17D | 109.5 | O5S2—C6S2—H6SC | 109.3 |
| C16B—C17B—H17E | 109.5 | O5S2—C6S2—H6SD | 109.3 |
| C16B—C17B—H17F | 109.5 | O5S2—C6S2—C7S2 | 111.7 (14) |
| H17D—C17B—H17E | 109.5 | H6SC—C6S2—H6SD | 107.9 |
| H17D—C17B—H17F | 109.5 | C7S2—C6S2—H6SC | 109.3 |
| H17E—C17B—H17F | 109.5 | C7S2—C6S2—H6SD | 109.3 |
| C16A—C11A—N10A | 117.43 (17) | C6S2—C7S2—H7SC | 110.4 |
| C12A—C11A—N10A | 121.68 (19) | C6S2—C7S2—H7SD | 110.4 |
| C12A—C11A—C16A | 120.71 (18) | H7SC—C7S2—H7SD | 108.6 |
| C11B—C12B—H12B | 119.9 | O8S2—C7S2—C6S2 | 106.5 (10) |
| C13B—C12B—C11B | 120.15 (19) | O8S2—C7S2—H7SC | 110.4 |
| C13B—C12B—H12B | 119.9 | O8S2—C7S2—H7SD | 110.4 |
| C15A—C14A—H14A | 119.4 | C9S2—O8S2—C7S2 | 117.0 (13) |
| C13A—C14A—C15A | 121.22 (18) | O8S1—C9S1—H9SA | 109.5 |
| C13A—C14A—H14A | 119.4 | O8S1—C9S1—H9SB | 109.5 |
| C15A—C18A—H18A | 109.5 | O8S1—C9S1—H9SC | 109.5 |
| C15A—C18A—H18B | 109.5 | H9SA—C9S1—H9SB | 109.5 |
| C15A—C18A—H18C | 109.5 | H9SA—C9S1—H9SC | 109.5 |
| H18A—C18A—H18B | 109.5 | H9SB—C9S1—H9SC | 109.5 |

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| Cu1—O1B—C3B—O2B | −8.6 (2) | C5B—C6B—C7B—C8B | −1.7 (3) |
| Cu1—O1B—C3B—C4B | 170.41 (10) | C5A—C4A—C9A—N10A | −179.92 (18) |
| Cu1$^{i}$—O2B—C3B—O1B | 9.2 (2) | C5A—C4A—C9A—C8A | 3.2 (3) |
| Cu1$^{i}$—O2B—C3B—C4B | −169.80 (10) | C5A—C6A—C7A—C8A | 3.2 (3) |
| Cu1—O1A—C3A—O2A | 10.2 (2) | N10A—C9A—C8A—C7A | −178.9 (2) |
| Cu1—O1A—C3A—C4A | −168.37 (10) | N10A—C11A—C12A—C13A | −176.3 (2) |
| Cu1$^{i}$—O2A—C3A—O1A | −8.7 (2) | C16A—C15A—C14A—C13A | −2.0 (3) |
| Cu1$^{i}$—O2A—C3A—C4A | 169.93 (10) | C16A—C11A—C12A—C13A | −1.2 (3) |
| O1B—C3B—C4B—C9B | 179.72 (14) | C16B—C11B—C12B—C13B | 1.1 (3) |
| O1B—C3B—C4B—C5B | −3.1 (2) | C16B—C15B—C14B—C13B | 1.0 (3) |
| O2B—C3B—C4B—C9B | −1.2 (2) | C15A—C16A—C11A—N10A | 173.66 (18) |
| O2B—C3B—C4B—C5B | 176.01 (15) | C15A—C16A—C11A—C12A | −1.6 (3) |
| O1A—C3A—C4A—C5A | −5.4 (2) | C15A—C14A—C13A—C12A | −0.8 (3) |
| O1A—C3A—C4A—C9A | 171.06 (16) | C17A—C16A—C15A—C14A | −177.50 (17) |
| O2A—C3A—C4A—C5A | 175.93 (14) | C17A—C16A—C15A—C18A | 3.5 (3) |
| O2A—C3A—C4A—C9A | −7.6 (2) | C17A—C16A—C11A—N10A | −5.6 (3) |
| N10B—C9B—C4B—C3B | −3.1 (2) | C17A—C16A—C11A—C12A | 179.1 (2) |
| N10B—C9B—C4B—C5B | 179.74 (15) | C6A—C7A—C8A—C9A | −1.2 (3) |
| N10B—C9B—C8B—C7B | 179.34 (17) | C9A—C4A—C5A—C6A | −1.2 (3) |
| N10B—C11B—C16B—C17B | 4.4 (2) | C9A—N10A—C11A—C16A | 144.7 (2) |
| N10B—C11B—C16B—C15B | −177.08 (16) | C9A—N10A—C11A—C12A | −40.0 (4) |
| N10B—C11B—C12B—C13B | 177.97 (18) | C17B—C16B—C15B—C14B | 177.61 (19) |
| O2S1—C3S1—C4S1—O5S1 | 58.7 (11) | C17B—C16B—C15B—C18B | −2.4 (3) |
| C3B—C4B—C5B—C6B | −176.76 (17) | C11A—N10A—C9A—C4A | 174.3 (2) |

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| C9B—N10B—C11B—C16B | −124.92 (18) | C11A—N10A—C9A—C8A | −8.9 (4) |
| C9B—N10B—C11B—C12B | 58.1 (3) | C11A—C16A—C15A—C14A | 3.2 (3) |
| C9B—C4B—C5B—C6B | 0.5 (3) | C11A—C16A—C15A—C18A | −175.80 (18) |
| C9B—C8B—C7B—C6B | 1.3 (3) | C12B—C11B—C16B—C17B | −178.61 (17) |
| C3A—C4A—C5A—C6A | 175.39 (15) | C12B—C11B—C16B—C15B | −0.1 (3) |
| C3A—C4A—C9A—N10A | 3.7 (3) | C14A—C13A—C12A—C11A | 2.4 (4) |
| C3A—C4A—C9A—C8A | −173.24 (17) | C18A—C15A—C14A—C13A | 177.00 (19) |
| C4A—C5A—C6A—C7A | −2.0 (3) | C15B—C14B—C13B—C12B | 0.0 (4) |
| C4A—C9A—C8A—C7A | −2.0 (3) | C6S1—O5S1—C4S1—C3S1 | −178.1 (5) |
| C4B—C9B—C8B—C7B | 0.0 (3) | C18B—C15B—C14B—C13B | −179.0 (2) |
| C4B—C5B—C6B—C7B | 0.8 (3) | C1S1—O2S1—C3S1—C4S1 | 171.1 (12) |
| O5S1—C6S1—C7S1—O8S1 | −67.3 (7) | C4S1—O5S1—C6S1—C7S1 | 175.2 (4) |
| C11B—N10B—C9B—C4B | 171.23 (16) | O2S2—C3S2—C4S2—O5S2 | −64 (2) |
| C11B—N10B—C9B—C8B | −8.1 (3) | C3S2—C4S2—O5S2—C6S2 | 176.1 (11) |
| C11B—C16B—C15B—C14B | −0.9 (3) | C1S2—O2S2—C3S2—C4S2 | −163 (3) |
| C11B—C16B—C15B—C18B | 179.1 (2) | C4S2—O5S2—C6S2—C7S2 | −164.7 (10) |
| C11B—C12B—C13B—C14B | −1.0 (3) | O5S2—C6S2—C7S2—O8S2 | 68.1 (17) |
| C8B—C9B—C4B—C3B | 176.22 (15) | C6S2—C7S2—O8S2—C9S2 | 171.6 (16) |
| C8B—C9B—C4B—C5B | −0.9 (2) | C9S1—O8S1—C7S1—C6S1 | 172.0 (6) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N10*A*—H10*D*···O2*A* | 0.86 (3) | 1.86 (3) | 2.604 (2) | 143 (2) |
| N10*B*—H10*C*···O2*B* | 0.89 (2) | 1.87 (2) | 2.6065 (18) | 139 (2) |