Crystal structure of catena-poly[[bis(1-benzylimidazole-κN)copper(II)]-μ-sulfato-κ2O′-[tetra-kis(1-benzylimidazole-κN)copper(II)]-μ-sulfato-κ2O′] N,N-dimethylformamide disolvate dihydrate

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The title one-dimensional copper(II) coordination polymer, [[Cu(SO₄)₂-(C₁₀H₁₀N₂)₃][C₃H₇NO·H₂O]]ₙ or [[Cu(bzi)₃(μ-O₂S)]·H₂O·DMF]ₙ (bzi = 1-benzylimidazole, C₁₀H₁₀N₂; DMF = N,N-dimethylformamide, C₃H₇NO), is constructed by monodentate bzi ligands and bridging sulfate anions, leading to chains propagating parallel to the c axis. Within a chain, there are two crystallographic independent CuII ions, each with site symmetry 1, which form [CuN₂O₂] and [CuN₄O₂] polyhedra alternating along the chain direction. The crystal structure is consolidated by weak hydrogen-bonding, C—H⋯C and C—H⋯C interactions, leading to the formation of a three-dimensional supramolecular network.

1. Chemical context

The exploration of new transition-metal coordination polymers (CPs) is still an ongoing process since this class of molecular materials presents interesting properties and potential applications in adsorption, catalysis, storage, and photoluminescent sensing (Engel & Scott, 2020; Liu et al., 2021; Baruah, 2022; Ma & Horike, 2022). For the design and synthesis of new CPs, metal ions and bridging ligands play an important role, because they influence structural topologies, dimensionalities, and possible functions (Du et al., 2013). In this context, we focused on the copper(II) ion and O-donor sulfate (SO₄²⁻) and N-donor heterocyclic aromatic ligands for the current study. Copper(II) compounds show interesting electronic and magnetic properties, accompanied by various structural topologies, physical properties and applications (Das & Pal, 2001; Gao & Liu, 2022). The sulfate anion can act as a bridging ligand due to its versatile coordination modes supporting the increase of structural dimensionalities of the CPs (Yotnoi et al., 2014). The presence of mono- and/or bidentate N-donor heterocyclic aromatic imidazole derivatives as ligands in CPs is generally found to increase the extended structures and the stability of the crystal structures through supramolecular interactions such as π–π stacking and C—H⋯π bonding (Krinchampa et al., 2016; Assavajamroon et al., 2019). As previous studies suggest, there is limited research reported for CuII CPs constructed from mixed sulfate.

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and N-donor imidazole derivatives, for example \([\text{Cu}(L)_2(\mu-\text{O}_2\text{SO}_2)]_n\), where \(L = \text{imidazole}\) (Fransson & Lundberg, 1972; Kumar et al., 2014) and \(L = \text{N-methylimidazole}\) (Liu et al., 2003). During the current study, we used the imidazole derivative, 1-benzylimidazole (bzi), to investigate its influence on supramolecular interactions in the resulting network.

In the present communication, we report the crystal structure, spectroscopic characteristics and some physical properties of \([\text{Cu}(\text{bzi})_3(\mu-\text{O}_2\text{SO}_2)]\cdot\text{H}_2\text{O}\cdot\text{DMF}\)\(n\) (bzi = 1-benzylimidazole; DMF = \(N,N\)-dimethylformamide).

2. Structural commentary

The asymmetric unit of the solvated coordination polymer \([\text{Cu}(\text{bzi})_3(\mu-\text{O}_2\text{SO}_2)]\cdot\text{H}_2\text{O}\cdot\text{DMF}\)\(n\) comprises two Cu\textsuperscript{II} ions with site symmetry \(\overline{1}\) (Wyckoff letters \(b\) and \(d\)), three bzi molecules (see Fig. S1 in the supporting information), a coordinating sulfate anion, one water and one DMF solvent molecule (Fig. 1). The environments of the two Cu\textsuperscript{II} cations are different. Cu1 is surrounded by two nitrogen donor atoms from two monodentate bzi ligands and two oxygen donor atoms of two different sulfate bridging ligands, resulting in an [N\textsubscript{4}O\textsubscript{2}] coordination set with a typically Jahn–Teller-distorted octahedral shape with bond lengths of \(\text{Cu}1—\text{N}1 = 2.0210 (15), \text{Cu}1—\text{O}1 = 1.9951 (14)\) Å, respectively; the bite angles around Cu1 are in the range 89.25 (6)–90.75 (6)°. Cu2 is coordinated by four nitrogen donor atoms from four monodentate bzi ligands and two oxygen donor atoms of two different sulfate bridging ligands, resulting in an [N\textsubscript{2}O\textsubscript{2}] coordination set with a square-planar shape and Cu1—N1 and Cu1—O1 bond lengths of 1.9951 (14) and 1.9564 (12) Å, respectively; the bite angles around Cu1 are in the range 89.25 (6)–90.75 (6)°.

3. Supramolecular features

The crystal structure of the title compound is consolidated by weak interactions such as hydrogen-bonding, C—H⋅⋅⋅π and π–π interactions. Non-classical C—H⋅⋅⋅O hydrogen-bonding interactions are found between the C—H donor groups of the atoms of two different sulfate bridging ligands, resulting in an [N\textsubscript{2}O\textsubscript{2}] coordination set with a typically Jahn–Teller-distorted octahedral shape with bond lengths of Cu2—N3 = 2.0210 (15), Cu2—N5 = 2.013 (15) Å, and Cu2—O2 = 2.4912 (12) Å. Both Cu\textsuperscript{II} sites are alternatively connected by bis-monodentately binding and bridging sulfate ligands, \(\mu-\kappa^2\text{O},\text{O'}\), leading to a chain-like structure extending parallel to the c axis, as shown in Fig. 2. The Cu1⋅⋅⋅Cu2 distance within a chain is 6.1119 (4) Å.

| D—H⋅⋅⋅A | D—H | H⋅⋅⋅A | D⋅⋅⋅A | D—H⋅⋅⋅A |
|---------|------|-------|-------|---------|
| O5—H5A⋅⋅⋅O4 | 0.85 | 1.96 | 2.772 (3) | 159 |
| O5—H5B⋅⋅⋅O6 | 0.85 | 2.29 | 3.106 (5) | 160 |
| C1—H1⋅⋅⋅O2 | 0.93 | 2.23 | 3.131 (2) | 164 |
| C2—H2⋅⋅⋅O3\textsuperscript{b} | 0.93 | 2.34 | 3.227 (2) | 159 |
| C4—H4A⋅⋅⋅O3\textsuperscript{a} | 0.97 | 2.55 | 3.445 (3) | 153 |
| C10—H10⋅⋅⋅N2 | 0.93 | 2.54 | 2.866 (3) | 101 |
| C11—H11⋅⋅⋅O2 | 0.93 | 2.40 | 2.990 (2) | 121 |
| C12—H12⋅⋅⋅O3\textsuperscript{ii} | 0.93 | 2.48 | 3.378 (2) | 162 |
| C14—H14A⋅⋅⋅O5 | 0.97 | 2.50 | 3.425 (4) | 159 |
| C21—H21⋅⋅⋅O2\textsuperscript{ii} | 0.93 | 2.57 | 3.038 (2) | 112 |
| C21—H21⋅⋅⋅O3\textsuperscript{ii} | 0.93 | 2.36 | 3.274 (2) | 170 |
| C24—H24B⋅⋅⋅O4\textsuperscript{ii} | 0.97 | 2.40 | 3.346 (3) | 164 |
| C32—H32A⋅⋅⋅O6 | 0.96 | 2.29 | 2.705 (7) | 105 |
| C13—H13⋅⋅O4\textsuperscript{iv} | 0.93 | 2.87 | 3.759 (3) | 161 |
| C14—H14B⋅⋅O4\textsuperscript{iv} | 0.97 | 2.99 | 3.711 (3) | 132 |

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

**Figure 1**
Asymmetric unit of the title compound with displacement ellipsoids drawn at the 30% probability level.

**Figure 2**
Side (a) and top (b) views of the chain-like structure of the title compound extending parallel to the c axis. Hydrogen atoms bound to carbon atoms as well as solvent water and DMF molecules were omitted for clarity.
bzi imidazole rings to three different oxygen acceptor atoms (O1, O2 and O3) of a sulfate bridging ligand, together with a weak hydrogen bond within a bzi molecule, C10—H10/C1/C1/N2 (Table 1; Fig. S2 in the supporting information). Moreover, O—H/C1/C1/C1O hydrogen-bonding interactions between the bridging sulfate ion in the chain and the solvate water and DMF molecules are found (Table 1; Fig. S3 in the supporting information). Intermolecular interactions between adjacent chains (Fig. 3a) exist through hydrogen-bonding interactions between a methylene group and a sulfate ligand, C4—H4/C1/C1/C1O3ii and C24—H24/B/C1/C1/O4ii (Table 1; Fig. 3b) and by C—H/C1/C1/C1/C1 interactions, C13—H13/C1/C1/C1/C4iv and C14—H14/B/C1/C1/C1/C4iv (Table 1; Fig. 3c), leading to a two-dimensional supramolecular network extending parallel to the bc plane, as shown in Figs. S3 and S4 in the supporting information. Furthermore, π–π stacking interactions are present between the phenyl rings of bzi ligands (Fig. 4) with a centroid-to-centroid distance Cg5—Cg5’ of 3.7099 (18) Å along the a-axis direction [Cg5 is the centroid of the C15–C20 phenyl ring; symmetry code: (v) −x, −y + 1, −z + 1], eventually leading to a three-dimensional supramolecular framework of the title compound, as shown in Fig. 5.

4. Spectroscopic characterization

The FT–IR spectrum of the title compound (Fig. S5 in the supporting information) exhibits the characteristic broad bands (centered at 3454 cm\(^{-1}\)) assigned to the O—H stretching vibration of the solvent water molecule hydrogen-bonded to the DMF solvent molecule. Characteristic bands of the bzi ligand are observed at 3142 cm\(^{-1}\) for the aromatic C—H stretching, at 1523 and 1454 cm\(^{-1}\) and in the range of 700–500 cm\(^{-1}\) for the C—C, C—N stretching and C—H bending, respectively (Assavajamroon et al., 2019). The strong bands at 1675, 1116 and 713 cm\(^{-1}\) are due to the asymmetric stretching of the bridging sulfate ligand (Wang et al., 2014).

The solid-state diffuse reflectance spectrum of the title compound (Fig. S6 in the supporting information) shows a broad asymmetric band with \(\lambda_{\text{max}}\) at 602 nm (1660 kK) and a shoulder at about 756 nm (1324 kK). These bands might be assigned to electronic \(d\rightarrow d\) transitions, \((d_{xz}, d_{yz}, d_{x^2-y^2}) \rightarrow d_{z^2}, d_{x^2-y^2} \rightarrow d_{z^2}, d_{x^2-y^2}, d_{z^2} \rightarrow d_{x^2-y^2},\) corresponding to a distorted octahedral conformation.
Table 2
Experimental details.

| Crystal data       | Chemical formula                                      | [Cu(SO₄)(C₁₀H₁₀N₂)₃]·C₃H₇NO·H₂O |
|--------------------|--------------------------------------------------------|----------------------------------|
| M₀                 |                                                        | 725.31                           |
| Crystal system, space group | Monoclinic, P2₁/c                                          |                                  |
| Temperature (K)    |                                                        | 296                              |
| a, b, c (Å)        |                                                        | 15.8896 (10), 18.1195 (11), 12.2238 (7) |
| β (°)              |                                                        | 94.239 (2)                       |
| V (Å³)             |                                                        | 3509.7 (4)                       |
| Z                  |                                                        | 4                                |
| Radiation type     |                                                        | Mo K                             |
| μ (mm⁻¹)           |                                                        | 0.74                             |
| Crystal size (mm)  |                                                        | 0.38 × 0.35 × 0.32               |

Data collection
Diffractometer          | Bruker D8 QUEST CMOS(
Absorption correction   | Multi-scan (SADABS; Krause et al., 2015).

T₀min - T₀max           | 0.640, 0.746
No. of measured, independent and observed | 50998, 10697, 7310
I reflections          | 0.054
θ/λ (max) (Å⁻¹)        | 0.714
Refinement
R[F² > 2σ(F²)], wR(F²), S | 0.044, 0.117, 1.02
No. of reflections     | 10697
No. of parameters      | 441
H-atom treatment       | H-atom parameters constrained
Δρmax, Δρmin (e Å⁻³)   | 0.39, −0.35

Computer programs: APEX3 and SAINT (Bruker, 2016), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), OLEX2 (Dolomanov et al., 2009) and publCIF (Westrip, 2010).

5. PXRD and thermal analysis

The plots of the experimental and simulated powder X-ray diffraction (PXRD) patterns of the title compound (Fig. S7 in the supporting information) show a good match, confirming reproducibility and phase purity.

The thermal stability of the title compound has been investigated by means of thermogravimetric analysis with the temperature in the range 303–1073 K under a nitrogen atmosphere. Based on the results (Fig. S8 in the supporting information), the title compound is stable to about 371 K. Above this temperature, the compound starts to decompose by a mass loss of 13%, which corresponds to the loss of solvent water and DMF molecules. The second step of mass loss (65%) corresponds to the release of the remaining coordinating bzi and sulfate ligands. Further increasing the temperature leads to another mass loss (22%) until CuO forms as the final product.

6. Database survey

According to a search of the Cambridge Structural Database (CSD; version 5.41, November 2019 update; Groom et al., 2016), there are some one-dimensional Cuᴵ⁺ coordination polymers containing the sulfate anion as a bridging ligand together with N-donor imidazole-based ligands. The ones most closely related to the title compound are [Cu(imida-

dote)SO₄] (TIMZCU02; Kumar et al., 2014) and [Cu(N-methylimidazole)₃(SO₄)] (IJEBII; Liu et al., 2003). These two Cuᴵ⁺ coordination polymers have the same octahedral [N₂O₂] coordination set around the Cuᴵ⁺ ion, while those of the title compound contain alternatively two different Cuᴵ⁺ polyhedra, as discussed in the Structural commentary.

7. Synthesis and crystallization

A methanolic solution (5 ml) of bzi (0.6329 g, 4.0 mmol) was dropped slowly into a methanolic solution (5 ml) of CuSO₄·5H₂O (0.2491 g, 1.0 mmol) under continuous stirring at 333 K over a period of 10 min, resulting in a blue solution. The solution was then filtered and allowed to evaporate slowly under atmospheric conditions at room temperature. After seven days, the solution became viscous, and 10 ml of DMF were added to the solution under continuous stirring at 333 K over a period of 5 min. Stirring was continued until the solution became clear. Finally, the solution was filtered and allowed to evaporate slowly in air at room temperature. Blue crystals of the title compound were obtained within a day (yield 38%, 93.4 mg, based on the Cuᴵ⁺ salt).

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All C-bound H atoms were calculated and refined using a riding model, with C—H = 0.93 Å for aromatic H atoms (0.97 Å for methyl H atoms), and Uiso(H) = 1.2Ueq(C) [Uiso(H) = 1.5Ueq(C)]. The O-bound H atoms of the water molecule were located in a difference-Fourier map, and were refined with an O—H bond length of 0.85 Å, and with Uiso(O) = 1.5Ueq(C).

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Crystal structure of catena-poly[[[bis(1-benzylimidazole-κN)copper(II)]-μ-sulfato-κ²O:O’-[tetrakis(1-benzylimidazole-κN)copper(II)]-μ-sulfato-κ²O:O’] N,N-dimethylformamide disolvate dihydrate]

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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: publCIF (Westrip, 2010).

catena-Poly[[[bis(1-benzylimidazole-κN)copper(II)]-μ-sulfato-κ²O:O’-[tetrakis(1-benzylimidazole-κN)copper(II)]-μ-sulfato-κ²O:O’] N,N-dimethylformamide disolvate dihydrate]

Crystal data

[Cu(SO4)(C10H10N2)3]·C3H7NO·H2O  
Mr = 725.31  
Monoclinic, P21/c  
a = 15.8896 (10) Å  
b = 18.1195 (11) Å  
c = 12.2238 (7) Å  
β = 94.239 (2)°  
V = 3509.7 (4) Å³  
Z = 4

F(000) = 1516  
Dc = 1.373 Mg m⁻³  
Mo Kα radiation, λ = 0.71073 Å  
Cell parameters from 9903 reflections  
θ = 2.3–29.9°  
μ = 0.74 mm⁻¹  
T = 296 K  
Block, dark blue  
0.38 × 0.35 × 0.32 mm

Data collection

BRUKER D8 QUEST CMOS PHOTON II diffractometer  
50998 measured reflections  
10697 independent reflections  
7310 reflections with I > 2σ(I)  
Rint = 0.054  
θmax = 30.5°, θmin = 2.3°  
h = −22→22  
k = −25→21  
l = −14→17

Refinement

Refinement on F²  
Least-squares matrix: full  
R[F² > 2σ(F²)] = 0.044  
wR(F²) = 0.117  
S = 1.02  
10697 reflections  
441 parameters  
0 restraints
### Supporting Information

Primary atom site location: dual
Hydrogen site location: mixed
H-atom parameters constrained

\[ w = \frac{1}{\sigma^2(F_{o}^2) + (0.049P)^2 + 1.1168P} \]
where \( P = (F_{o}^2 + 2F_{c}^2)/3 \)

\[ (\Delta/\sigma)_{\text{max}} = 0.001 \]
\[ \Delta \rho_{\text{max}} = 0.39 \text{ e Å}^{-3} \]
\[ \Delta \rho_{\text{min}} = -0.35 \text{ e Å}^{-3} \]

### Special details

**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.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

|      | x    | y    | z    | Ueq  |
|------|------|------|------|------|
| Cu1  | 0.500000 | 0.500000 | 1.000000 | 0.02929 (8) |
| Cu2  | 0.500000 | 0.500000 | 0.500000 | 0.03313 (8) |
| S1   | 0.45600 (3) | 0.57757 (2) | 0.78307 (3) | 0.03415 (10) |
| O1   | 0.52363 (8) | 0.53965 (7) | 0.85659 (10) | 0.0390 (3) |
| O2   | 0.44811 (9) | 0.53635 (7) | 0.67969 (10) | 0.0422 (3) |
| O3   | 0.48237 (10) | 0.65349 (8) | 0.76450 (11) | 0.0478 (3) |
| N1   | 0.45657 (10) | 0.40654 (8) | 0.93045 (12) | 0.0348 (3) |
| N2   | 0.40670 (10) | 0.32616 (8) | 0.80834 (12) | 0.0371 (3) |
| N3   | 0.38640 (9) | 0.45109 (8) | 0.46926 (12) | 0.0360 (3) |
| N4   | 0.25298 (9) | 0.42410 (10) | 0.48218 (13) | 0.0421 (4) |
| N5   | 0.55242 (10) | 0.40576 (8) | 0.55904 (12) | 0.0360 (3) |
| N6   | 0.61544 (11) | 0.29797 (9) | 0.55906 (14) | 0.0452 (4) |
| C1   | 0.43083 (13) | 0.39607 (10) | 0.82595 (14) | 0.0386 (4) |
| H1   | 0.429704 | 0.432455 | 0.772195 | 0.046* |
| C2   | 0.44734 (13) | 0.33958 (10) | 0.98116 (16) | 0.0423 (4) |
| H2   | 0.460152 | 0.330123 | 1.055305 | 0.051* |
| C3   | 0.41682 (14) | 0.28984 (11) | 0.90649 (16) | 0.0461 (5) |
| H3   | 0.404953 | 0.240457 | 0.919213 | 0.055* |
| C4   | 0.37274 (13) | 0.29476 (12) | 0.70396 (15) | 0.0448 (5) |
| H4A  | 0.403354 | 0.249878 | 0.689678 | 0.054* |
| H4B  | 0.381868 | 0.329382 | 0.645483 | 0.054* |
| C5   | 0.28021 (14) | 0.27738 (11) | 0.70233 (16) | 0.0431 (4) |
| C6   | 0.24550 (18) | 0.22769 (15) | 0.6250 (2) | 0.0642 (7) |
| H6   | 0.279780 | 0.205532 | 0.575961 | 0.077* |
| C7   | 0.1604 (2) | 0.21093 (19) | 0.6203 (3) | 0.0835 (9) |
| H7   | 0.137660 | 0.178043 | 0.567717 | 0.100* |
| C8   | 0.1095 (2) | 0.24268 (19) | 0.6930 (3) | 0.0829 (9) |
| H8   | 0.052397 | 0.230936 | 0.690094 | 0.099* |
| C9   | 0.14248 (17) | 0.29133 (18) | 0.7694 (2) | 0.0735 (8) |
| H9   | 0.107963 | 0.312823 | 0.818691 | 0.088* |
| C10  | 0.22742 (15) | 0.30879 (13) | 0.77361 (19) | 0.0560 (6) |
| H10  | 0.249295 | 0.342443 | 0.825678 | 0.067* |
| C11  | 0.31994 (12) | 0.46172 (12) | 0.52597 (16) | 0.0418 (4) |
| Atom | x     | y     | z     | Ueq  |
|------|-------|-------|-------|------|
| H11  | 0.319568 | 0.491353 | 0.588053 | 0.050* |
| C12  | 0.35995 (12) | 0.40518 (11) | 0.38466 (17) | 0.0433 (4) |
| H12  | 0.393428 | 0.388213 | 0.330678 | 0.052* |
| C13  | 0.27752 (13) | 0.38826 (12) | 0.39170 (19) | 0.0497 (5) |
| H13  | 0.244297 | 0.358230 | 0.344333 | 0.060* |
| C14  | 0.16745 (13) | 0.42591 (15) | 0.52061 (19) | 0.0547 (6) |
| H14A | 0.169174 | 0.449836 | 0.591730 | 0.066* |
| H14B | 0.147524 | 0.375799 | 0.529264 | 0.066* |
| C15  | 0.10724 (13) | 0.46645 (15) | 0.44190 (18) | 0.0512 (5) |
| H16  | 0.054466 | 0.378218 | 0.366189 | 0.092* |
| C17  | -0.00141 (19) | 0.4666 (3) | 0.2943 (3) | 0.0967 (11) |
| H17  | -0.036817 | 0.440720 | 0.243896 | 0.116* |
| C18  | -0.0031 (2) | 0.5408 (3) | 0.2970 (3) | 0.0937 (11) |
| H18  | -0.040304 | 0.566072 | 0.248004 | 0.112* |
| C19  | 0.0481 (2) | 0.5794 (2) | 0.3696 (3) | 0.0999 (11) |
| H19  | 0.045884 | 0.630676 | 0.370829 | 0.120* |
| C20  | 0.1044 (2) | 0.54141 (18) | 0.4426 (2) | 0.0764 (8) |
| H20  | 0.140257 | 0.567632 | 0.492089 | 0.092* |
| C21  | 0.56890 (12) | 0.34753 (10) | 0.49988 (16) | 0.0398 (4) |
| H21  | 0.550585 | 0.341533 | 0.426391 | 0.048* |
| C22  | 0.59092 (14) | 0.39326 (13) | 0.66186 (16) | 0.0494 (5) |
| H22  | 0.590355 | 0.425125 | 0.721445 | 0.059* |
| C23  | 0.62978 (16) | 0.32677 (14) | 0.66178 (18) | 0.0596 (6) |
| H23  | 0.660522 | 0.304825 | 0.720784 | 0.072* |
| C24  | 0.64896 (16) | 0.22883 (12) | 0.5175 (2) | 0.0573 (6) |
| H24A | 0.615387 | 0.214479 | 0.451417 | 0.069* |
| H24B | 0.643667 | 0.190319 | 0.571681 | 0.069* |
| C25  | 0.73985 (16) | 0.23489 (12) | 0.4922 (2) | 0.0534 (5) |
| C26  | 0.7648 (2) | 0.28263 (17) | 0.4128 (2) | 0.0751 (8) |
| H26  | 0.725232 | 0.313005 | 0.375349 | 0.090* |
| C27  | 0.8488 (3) | 0.2855 (2) | 0.3887 (3) | 0.1061 (13) |
| H27  | 0.865192 | 0.317801 | 0.335160 | 0.127* |
| C28  | 0.9074 (3) | 0.2412 (3) | 0.4429 (5) | 0.1199 (16) |
| H28  | 0.963483 | 0.243075 | 0.425907 | 0.144* |
| C29  | 0.8836 (2) | 0.1941 (3) | 0.5221 (4) | 0.1134 (14) |
| H29  | 0.923590 | 0.164019 | 0.559236 | 0.136* |
| C30  | 0.80019 (19) | 0.19079 (17) | 0.5476 (3) | 0.0774 (8) |
| H30  | 0.784610 | 0.158837 | 0.602104 | 0.093* |
| O5   | 0.22185 (17) | 0.5284 (2) | 0.7504 (2) | 0.1226 (10) |
| H5A  | 0.267379 | 0.551864 | 0.766519 | 0.184* |
| H5B  | 0.206889 | 0.512904 | 0.811700 | 0.184* |
| O6   | 0.1289 (3) | 0.4550 (2) | 0.9369 (3) | 0.1648 (15) |
| N7   | 0.20211 (14) | 0.50470 (13) | 1.07952 (19) | 0.0669 (6) |
| C31  | 0.1313 (2) | 0.4916 (2) | 1.0252 (3) | 0.0986 (11) |
| H31  | 0.081506 | 0.509183 | 1.051085 | 0.118* |
| C32  | 0.2811 (3) | 0.4808 (3) | 1.0442 (4) | 0.1303 (17) |
| H32A | 0.271751 | 0.451665 | 0.978836 | 0.195* |
supporting information

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Atomic displacement parameters (Å²)

| Atom | U¹¹ | U¹² | U¹³ | U¹² | U¹³ | U¹³ |
|------|-----|-----|-----|-----|-----|-----|
| Cu1  | 0.03603 (16) | 0.02569 (14) | 0.02567 (14) | −0.00356 (12) | −0.00096 (10) | −0.00254 (10) |
| Cu2  | 0.02823 (15) | 0.02747 (15) | 0.04268 (17) | −0.00080 (12) | −0.00426 (12) | 0.00424 (12) |
| S1   | 0.0459 (3) | 0.0306 (2) | 0.02570 (19) | −0.00432 (19) | 0.00091 (16) | −0.00219 (16) |
| O1   | 0.0489 (8) | 0.0388 (7) | 0.0286 (6) | −0.0049 (6) | 0.0004 (5) | −0.0020 (5) |
| O2   | 0.0630 (9) | 0.0373 (7) | 0.0259 (6) | −0.0068 (6) | 0.0003 (6) | −0.0048 (5) |
| O3   | 0.0747 (10) | 0.0305 (7) | 0.0370 (7) | −0.0090 (7) | −0.0045 (6) | 0.0008 (5) |
| O4   | 0.0518 (9) | 0.0589 (10) | 0.0553 (9) | −0.0014 (8) | 0.0141 (7) | −0.0097 (7) |
| N1   | 0.0442 (9) | 0.0290 (7) | 0.0308 (7) | −0.0054 (6) | 0.0001 (6) | −0.0032 (6) |
| N2   | 0.0465 (9) | 0.0310 (8) | 0.0330 (8) | −0.0052 (7) | −0.0022 (6) | −0.0068 (6) |
| N3   | 0.0316 (8) | 0.0333 (8) | 0.0425 (8) | −0.0007 (6) | −0.0027 (6) | 0.0010 (6) |
| N4   | 0.0295 (8) | 0.0479 (9) | 0.0482 (9) | −0.0023 (7) | −0.0026 (6) | 0.0014 (7) |
| N5   | 0.0375 (8) | 0.0316 (8) | 0.0379 (8) | 0.0116 (6) | −0.0037 (6) | 0.0031 (6) |
| N6   | 0.0533 (10) | 0.0346 (8) | 0.0474 (9) | 0.0085 (8) | 0.0022 (7) | 0.0087 (7) |
| C1   | 0.0544 (11) | 0.0304 (9) | 0.0307 (9) | −0.0062 (8) | 0.0018 (8) | −0.0022 (7) |
| C2   | 0.0549 (12) | 0.0320 (9) | 0.0383 (10) | −0.0076 (9) | −0.0090 (8) | 0.0025 (7) |
| C3   | 0.0626 (13) | 0.0283 (9) | 0.0452 (11) | −0.0068 (9) | −0.0114 (9) | 0.0005 (8) |
| C4   | 0.0595 (13) | 0.0415 (10) | 0.0325 (9) | −0.0064 (9) | −0.0021 (8) | −0.0120 (8) |
| C5   | 0.0552 (12) | 0.0354 (10) | 0.0370 (10) | −0.0037 (9) | −0.0086 (8) | 0.0009 (8) |
| C6   | 0.0745 (17) | 0.0397 (14) | 0.0563 (14) | −0.0149 (13) | −0.0090 (12) | −0.0150 (12) |
| C7   | 0.080 (2) | 0.083 (2) | 0.038 (2) | −0.0319 (18) | −0.0231 (16) | −0.0080 (17) |
| C8   | 0.0575 (16) | 0.094 (2) | 0.094 (2) | −0.0167 (16) | −0.0151 (16) | 0.0204 (18) |
| C9   | 0.0572 (16) | 0.086 (2) | 0.0769 (18) | 0.0080 (15) | −0.0006 (13) | 0.0101 (15) |
| C10  | 0.0585 (14) | 0.0544 (13) | 0.0533 (13) | 0.0036 (11) | −0.0082 (10) | −0.0055 (10) |
| C11  | 0.0338 (9) | 0.0503 (12) | 0.0404 (10) | −0.0012 (9) | −0.0030 (7) | −0.0024 (8) |
| C12  | 0.0384 (10) | 0.0371 (10) | 0.0542 (12) | 0.0016 (8) | 0.0018 (8) | −0.0109 (8) |
| C13  | 0.0376 (10) | 0.0459 (12) | 0.0644 (13) | −0.0046 (9) | −0.0037 (9) | −0.0163 (10) |
| C14  | 0.0331 (10) | 0.0757 (16) | 0.0555 (13) | −0.0050 (11) | 0.0040 (9) | 0.0079 (11) |
| C15  | 0.0326 (10) | 0.0720 (16) | 0.0493 (12) | 0.0029 (10) | 0.0054 (8) | −0.0023 (11) |
| C16  | 0.0492 (14) | 0.094 (2) | 0.0830 (19) | −0.0083 (14) | −0.0131 (13) | −0.0027 (16) |
| C17  | 0.0540 (17) | 0.150 (4) | 0.082 (2) | 0.000 (2) | −0.0196 (14) | −0.007 (2) |
| C18  | 0.071 (2) | 0.137 (4) | 0.074 (2) | 0.039 (2) | 0.0059 (16) | 0.010 (2) |
| C19  | 0.107 (3) | 0.086 (2) | 0.108 (3) | 0.039 (2) | 0.017 (2) | 0.001 (2) |
| C20  | 0.0769 (19) | 0.079 (2) | 0.0731 (18) | 0.0134 (16) | 0.0012 (14) | −0.0134 (15) |
| C21  | 0.0464 (11) | 0.0326 (9) | 0.0390 (10) | 0.0001 (8) | −0.0055 (8) | 0.0051 (7) |
| C22  | 0.0575 (13) | 0.0541 (13) | 0.0356 (10) | 0.0108 (10) | −0.0028 (9) | 0.0034 (9) |
| C23  | 0.0733 (16) | 0.0623 (15) | 0.0419 (12) | 0.0227 (12) | −0.0052 (10) | 0.0143 (10) |
| C24  | 0.0644 (15) | 0.0319 (10) | 0.0764 (16) | 0.0059 (10) | 0.0105 (12) | 0.0048 (10) |
| C25  | 0.0597 (14) | 0.0374 (11) | 0.0635 (14) | 0.0041 (10) | 0.0076 (11) | −0.0038 (10) |
| C26 | 0.082 (2) | 0.0669 (18) | 0.0775 (19) | −0.0057 (15) | 0.0153 (15) | 0.0040 (15) |
| C27 | 0.105 (3) | 0.107 (3) | 0.112 (3) | −0.034 (3) | 0.047 (2) | −0.012 (2) |
| C28 | 0.070 (2) | 0.127 (4) | 0.167 (5) | −0.008 (2) | 0.031 (3) | −0.035 (3) |
| C29 | 0.062 (2) | 0.112 (3) | 0.163 (4) | 0.018 (2) | −0.016 (2) | −0.018 (3) |
| C30 | 0.0710 (19) | 0.0675 (18) | 0.092 (2) | 0.0128 (15) | −0.0051 (15) | 0.0025 (15) |
| O5 | 0.0773 (16) | 0.200 (3) | 0.0881 (17) | −0.0242 (18) | −0.0116 (13) | −0.028 (2) |
| O6 | 0.211 (4) | 0.168 (3) | 0.105 (2) | −0.027 (3) | −0.061 (2) | −0.021 (2) |
| N7 | 0.0562 (13) | 0.0857 (17) | 0.0590 (13) | 0.0047 (11) | 0.0061 (10) | 0.0064 (11) |
| C31 | 0.080 (2) | 0.117 (3) | 0.095 (3) | −0.005 (2) | −0.0134 (19) | 0.013 (2) |
| C32 | 0.089 (3) | 0.170 (4) | 0.135 (4) | 0.038 (3) | 0.036 (3) | 0.036 (3) |
| C33 | 0.133 (4) | 0.161 (4) | 0.088 (3) | −0.021 (3) | −0.004 (2) | −0.021 (3) |

**Geometric parameters (Å, °)**

| C1—O1i | 1.9564 (12) | C12—C13 | 1.354 (3) |
| Cu1—O1 | 1.9564 (12) | C13—H13 | 0.9300 |
| Cu1—N1i | 1.9951 (14) | C14—H14A | 0.9700 |
| Cu1—N1 | 1.9951 (14) | C14—H14B | 0.9700 |
| Cu2—O2 | 2.4912 (12) | C14—C15 | 1.498 (3) |
| Cu2—N3ii | 2.0210 (15) | C15—C16 | 1.375 (3) |
| Cu2—N3 | 2.0210 (15) | C15—C20 | 1.359 (4) |
| Cu2—N5 | 2.0103 (15) | C16—H16 | 0.9300 |
| Cu2—N5ii | 2.0103 (15) | C16—C17 | 1.377 (4) |
| S1—O1 | 1.5139 (13) | C17—H17 | 0.9300 |
| S1—O2 | 1.4653 (13) | C17—C18 | 1.345 (6) |
| S1—O3 | 1.4608 (14) | C18—H18 | 0.9300 |
| S1—O4 | 1.4567 (15) | C18—C19 | 1.354 (5) |
| N1—C1 | 1.326 (2) | C19—H19 | 0.9300 |
| N1—C2 | 1.375 (2) | C19—C20 | 1.398 (4) |
| N2—C1 | 1.336 (2) | C20—H20 | 0.9300 |
| N2—C3 | 1.367 (2) | C21—H21 | 0.9300 |
| N2—C4 | 1.463 (2) | C22—H22 | 0.9300 |
| N3—C11 | 1.320 (2) | C22—C23 | 1.354 (3) |
| N3—C12 | 1.369 (2) | C23—H23 | 0.9300 |
| N4—C11 | 1.341 (2) | C24—H24A | 0.9700 |
| N4—C13 | 1.364 (3) | C24—H24B | 0.9700 |
| N4—C14 | 1.471 (3) | C24—C25 | 1.503 (3) |
| N5—C21 | 1.316 (2) | C25—C26 | 1.380 (4) |
| N5—C22 | 1.375 (2) | C25—C30 | 1.386 (4) |
| N6—C21 | 1.341 (2) | C26—H26 | 0.9300 |
| N6—C23 | 1.363 (3) | C26—C27 | 1.389 (4) |
| N6—C24 | 1.467 (3) | C27—H27 | 0.9300 |
| C1—H1 | 0.9300 | C27—C28 | 1.363 (6) |
| C2—H2 | 0.9300 | C28—H28 | 0.9300 |
| C2—C3 | 1.347 (3) | C28—C29 | 1.366 (6) |
| C3—H3 | 0.9300 | C29—H29 | 0.9300 |
| C4—H4A | 0.9700 | C29—C30 | 1.384 (5) |
| C4—H4B | 0.9700 | C30—H30 | 0.9300 |
| Bond          | Distance  | 2.000  | Bond          | Distance  | 2.000  |
|--------------|-----------|--------|--------------|-----------|--------|
| C4—C5        | 1.502 (3) | 0.8500 | O5—H5A       | 1.390 (3) | 0.8499 |
| C5—C6        | 1.377 (3) | 1.266 (5)| O6—C31      | 0.9300   | 1.285 (4)|
| C5—C10       | 1.382 (4) | 1.425 (4)| N7—C32      | 0.9300   | 1.451 (4)|
| C6—H6        | 0.9300   | 1.502 (3)| N7—C33      | 0.9300   | 1.502 (3)|
| C6—C7        | 1.372 (5) | 0.9300 | C31—H31      | 1.360 (4) | 0.9600 |
| C7—H7        | 0.9300   | 0.9400 | C32—H32A     | 1.383 (4) | 0.9600 |
| C7—C8        | 0.9300   | 0.9300 | C32—H32B     | 0.9300   | 0.9300 |
| C8—H8        | 1.380 (4) | 1.465 (4)| C33—H33A    | 1.360 (4) | 0.9600 |
| C8—C9        | 0.9300   | 0.9300 | C33—H33B     | 0.9300   | 0.9300 |
| C9—C10       | 0.9300   | 0.9300 | C33—H33C     | 0.9300   | 0.9300 |
| C11—H11      | 0.9300   | 0.9300 | C31—H31      |         |        |
| C12—H12      | 0.9300   | 0.9300 | C32—H32A     |         |        |
| O1i—Cu1—O1   | 180.0    | 125.2  | C13—C12—H12 |         |        |
| O1—Cu1—N1i   | 89.25 (6)| 126.9  | N4—C13—H13  |         |        |
| O1—Cu1—N1    | 90.75 (6)| 106.24 (17)| C12—C13—N4 |         |        |
| O1i—Cu1—N1i  | 90.75 (6)| 126.9  | C12—C13—H13 |         |        |
| O1i—Cu1—N1i  | 90.75 (6)| 126.9  | C12—C13—H13 |         |        |
| O1i—Cu1—N1i  | 90.75 (6)| 126.9  | C12—C13—N4  |         |        |
| N3—Cu2—O2    | 93.98 (5)| 108.0  | N4—C14—C15  |         |        |
| N3—Cu2—N3    | 180.0    | 109.3  | H14A—C14—H14B|         |        |
| N5—Cu2—O2    | 93.63 (5)| 109.3  | C15—C14—H14B|         |        |
| N5—Cu2—N3    | 87.99 (6)| 118.1 (3)| C15—C14—C15|         |        |
| N5—Cu2—N5    | 92.00 (6)| 119.2  | C15—C14—H14B|         |        |
| O2—S1—O1     | 106.99 (8)| 120.5  | C16—C17—H17 |         |        |
| O3—S1—O1     | 108.69 (8)| 119.0 (3)| C18—C17—C16|         |        |
| O3—S1—O2     | 110.68 (8)| 120.5  | C18—C17—H17 |         |        |
| O4—S1—O1     | 106.63 (9)| 119.3  | C17—C18—H18 |         |        |
| O4—S1—O2     | 111.57 (9)| 121.3 (3)| C17—C18—C19|         |        |
| O4—S1—O3     | 112.02 (10)| 119.3  | C19—C18—H18 |         |        |
| S1—O1—Cu1    | 121.58 (8)| 120.3  | C18—C19—H19 |         |        |
| S1—O2—Cu2    | 151.93 (9)| 119.3 (4)| C18—C19—C20|         |        |
| C1—N1—Cu1    | 127.18 (13)| 120.3  | C20—C19—H19 |         |        |
| C1—N1—C2     | 105.82 (15)| 120.5 (3)| C15—C20—C19|         |        |
| C2—N1—Cu1    | 127.00 (12)| 119.7  | C15—C20—H20 |         |        |
| C1—N2—C3     | 107.53 (15)| 119.7  | C19—C20—H20 |         |        |
| C1—N2—C4     | 126.30 (16)| 111.39 (17)| N5—C21—N6 |         |        |
| C3—N2—C4     | 126.14 (16)| 124.3  | N5—C21—H21  |         |        |
| C11—N3—Cu2   | 125.23 (13)| 124.3  | N6—C21—H21  |         |        |
| C11—N3—C12   | 105.81 (16)| 125.7  | N5—C22—H22  |         |        |
| C12—N3—Cu2   | 128.84 (13)| 108.54 (19)||         |        |
| Bond                  | Angle (°) (deg) |
|----------------------|----------------|
| C11—N4—C13          | 107.44 (16)    |
| C11—N4—C14          | 125.85 (18)    |
| C13—N4—C14          | 126.58 (17)    |
| C21—N5—Cu2          | 125.28 (12)    |
| C21—N5—C22          | 106.07 (16)    |
| C22—N5—Cu2          | 127.77 (14)    |
| C21—N6—C23          | 106.77 (17)    |
| C21—N6—C24          | 125.82 (18)    |
| C23—N6—C24          | 127.27 (18)    |
| N1—C1—N2            | 110.80 (16)    |
| N1—C1—C2            | 124.6          |
| N2—C1—H1            | 124.6          |
| N1—C2—H2            | 125.4          |
| C3—C2—N1            | 109.25 (16)    |
| C3—C2—H2            | 126.7          |
| N2—C3—H3            | 106.60 (17)    |
| C2—C3—N2            | 126.7          |
| C2—C3—H3            | 109.0          |
| N2—C4—H4A           | 112.99 (16)    |
| H4A—C4—H4B          | 107.8          |
| C5—C4—H4A           | 109.0          |
| N3—C11—N4           | 110.99 (18)    |
| N3—C11—H11          | 124.5          |
| N4—C11—H11          | 124.5          |
| N3—C12—H12          | 125.2          |
| C13—C12—N3          | 109.52 (18)    |
Cu1—N1—C1—N2  179.36 (13)  C10—C5—C6—C7  0.2 (4)
Cu1—N1—C2—C3  −179.47 (15)  C11—N3—C12—C13  −0.3 (2)
Cu2—N3—C11—N4  177.06 (12)  C11—N4—C13—C12  0.6 (2)
Cu2—N3—C12—C13  −176.47 (14)  C11—N4—C14—C15  108.7 (2)
Cu2—N5—C21—N6  170.55 (13)  C12—N3—C11—N4  0.7 (2)
Cu2—N5—C22—C23  −169.85 (16)  C13—N4—C14—C15  −66.4 (3)
O1—S1—O2—Cu2  −74.37 (19)  C11—N4—C12—C13  −176.80 (18)
O2—S1—O1—Cu1  −121.26 (9)  C13—N4—C12—C13  176.5 (2)
O3—S1—O2—Cu2  −121.26 (9)  C14—N4—C13—C12  176.5 (2)
O4—S1—O1—Cu1  119.19 (9)  C14—C15—C16—C17  −0.2 (3)
Symmetry codes: (i) −x+1, −y+1, −z+2; (ii) −x+1, −y+1, −z+1.

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| O5—H5A···O4  | 0.85 | 1.96  | 2.772 (3) | 159 |
| O5—H5B···O6  | 0.85 | 2.29  | 3.106 (5) | 160 |
| C1—H1···O2  | 0.93 | 2.23  | 3.131 (2) | 164 |
| C2—H2···O1i  | 0.93 | 2.60  | 2.966 (2) | 104 |
| C2—H2···O3i  | 0.93 | 2.34  | 3.227 (2) | 159 |

Cg is the centroid of the C5—C10 ring.

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|          | d (Å) | D (Å) | d·D (Å²) | ϕ (°) |
|----------|-------|-------|----------|-------|
| C4—H4···O3^iii | 0.97  | 2.55  | 3.445 (3) | 153   |
| C10—H10···N2  | 0.93  | 2.54  | 2.866 (3) | 101   |
| C11—H11···O2  | 0.93  | 2.40  | 2.990 (2) | 121   |
| C12—H12···O3^ii| 0.93  | 2.48  | 3.378 (2) | 162   |
| C14—H14···O5  | 0.97  | 2.50  | 3.425 (4) | 159   |
| C21—H21···O2^ii| 0.93  | 2.57  | 3.038 (2) | 112   |
| C21—H21···O3^ii| 0.93  | 2.36  | 3.274 (2) | 170   |
| C24—H24···O4^iii| 0.97  | 2.40  | 3.346 (3) | 164   |
| C32—H32···O6  | 0.96  | 2.29  | 2.705 (7) | 105   |
| C13—H13···Cg4^iv| 0.93  | 2.87  | 3.759 (3) | 161   |
| C14—H14···Cg4^iv| 0.97  | 2.99  | 3.711 (3) | 132   |

Symmetry codes: (i) −x+1, −y+1, −z+2; (ii) −x+1, −y+1, −z+1; (iii) −x+1, −y+1/2, −z+3/2; (iv) x, −y+1/2, −z+1/2.