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# *catena*-Poly[[tetrakis(3,5-dimethyl-1*H*-pyrazole-$\kappa N^2$)copper(II)]-$\mu_2$-sulfato-$\kappa^2 O$:$O'$]: crystal structure and Hirshfeld surface analysis of a Cu$^{II}$ coordination polymer

Oleksandr S. Vynohradov,[a] Artur Dovzhik,[a] Vadim A. Pavlenko,[a] Dina D. Naumova,[a] Irina A. Golenya[a]* and Sergiu Shova[b]

[a]Department of Chemistry, Taras Shevchenko National University of Kyiv, Volodymyrska str. 64/13, 01601 Kyiv, Ukraine, and [b]"Poni Petru" Institute of Macromolecular Chemistry, Aleea Gr. Ghica, Voda 41A, 700487 Iasi, Romania. *Correspondence e-mail: igolenya@ua.fm

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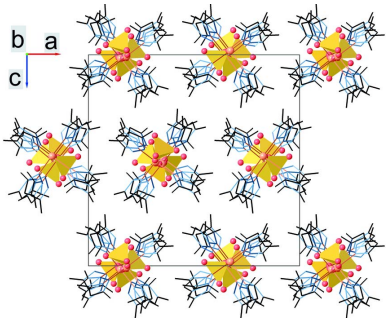
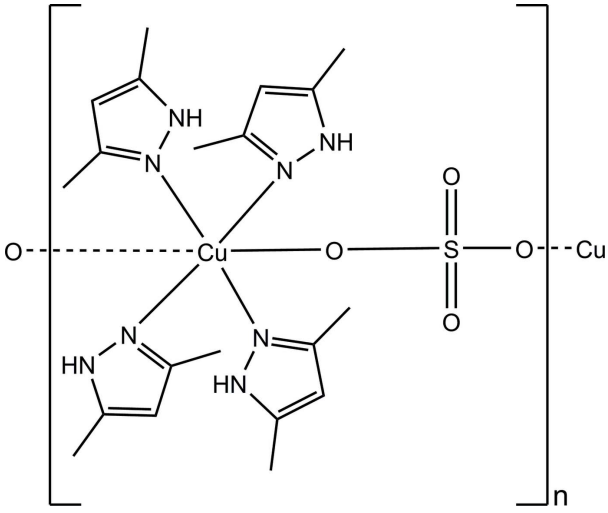
The title coordination polymer, $[Cu(SO_4)(C_5H_8N_2)_4]_n$, was synthesized using a one-pot reaction of copper powder, anhydrous copper(II) sulfate and 3,5-dimethyl-1*H*-pyrazole (Hdmpz) in acetonitrile under ambient conditions. The asymmetric unit can be described as a chain consisting of four $[Cu(SO_4)(Hdmpz)_4]$ formula units that are connected to each other by a $\mu_2$-sulfato-bridged ligand. The octahedral coordination geometry ($O_2N_4$) of all copper atoms is realized by coordination of four pyrazole ligands and two sulfate ligands. Four pyridine-like N atoms of the pyrazole ligands occupy the equatorial positions, while two oxygen atoms of two sulfate ligands are in axial positions. As a result of the sulfate ligand rotation, there is a pairwise alternation of terminal O atoms (which are not involved in coordination to the copper atom) of the $SO_4$ tetrahedra. The Cu···Cu distances within one asymmetric unit are in the range 7.0842 (12)–7.1554 (12) Å. The crystal structure is built up from polymeric chains packed in a parallel manner along the *b*-axis direction. Hirshfeld surface analysis suggests that the most important contributions to the surface contacts are from H···H (74.7%), H···O/O···H (14.8%) and H···C/C···H (8.2%) interactions.

## 1. Chemical context

The synthesis, structure and properties of metal complexes, including coordination polymers, is an important area of chemical research. The nature of the anion, which is part of a coordination compound, is one of several factors that has a great influence on the final structural topology of the complexes (Mondal *et al.*, 2009; Mahmoudi *et al.*, 2007; Kwak *et al.*, 2008; Balić *et al.*, 2018). A large number of coordination compounds have been synthesized and studied due to the development of supramolecular chemistry and the study of self-assembly of metal complexes with organic molecules, such as pyrazoles. These molecules have long been recognized as useful ligands for studying transition-metal coordination chemistry (Mihailov *et al.*, 1974; Nicholls *et al.*, 1971; Reedijk, 1971, 1970*a*,*b*; Reedijk & Smit, 1971; Reedijk *et al.*, 1971; Singh *et al.*, 1973; ten Hoedt *et al.*, 1982). Pyrazole-based ligands are used to construct supramolecular architectures due to the presence of a pyrrole NH group in the pyrazole ring, which is not necessarily coordinated by a metal atom, but may act as a donor of hydrogen bonds. In addition, substituents on the



pyrazole ring can also be involved in hydrogen-bond interactions. These facts are very important because there is a noticeable influence of hydrogen bonding on coordination compound assembly (Di Nicola *et al.*, 2007; Brewer *et al.*, 2020; Burrows *et al.*, 2011). The crystal packing of coordination polymers also depends on the different solvents employed, although not necessarily incorporating the solvents as crystallization molecules (Di Nicola *et al.*, 2014). Reaction of a metal salt with an organic ligand is a popular way for the synthesis of coordination compounds, including metal coordination polymers (Gogoi *et al.*, 2019; Shen *et al.*, 2004), but there are many types of coordination compounds and the methods of synthesis are varied (House *et al.*, 2016). In this article we report the preparation of the coordination polymer *catena*-poly[[tetrakis(3,5-dimethyl-1*H*-pyrazole-$\kappa N^2$)copper(II)]-$\mu_2$-sulfato-$\kappa^2 O{:}O'$] using the direct synthesis method, which is based on oxidative dissolution of a powdered metal in the presence of an organic ligand (Kokozay *et al.*, 2018; Li *et al.*, 2021).




## 2. Structural commentary

The title coordination polymer crystallizes in the orthorhombic *Pna*2$_1$ space group. The asymmetric unit is a chain consisting of four [Cu(Hdmpz)$_4$SO$_4$] formula units (Fig. 1) that are connected to each other by a $\mu_2$-sulfato-bridged ligand along the *b*-axis direction (Fig. 2). Each mononuclear unit [Cu(Hdmpz)$_4$SO$_4$] consists of four 3,5-dimethyl-1*H*-pyrazole molecules, which are coordinated in a monodentate way, and one sulfate ligand that is connected by one oxygen atom to the copper ion. The octahedral coordination environment of each copper atom consists of four pyridine-like nitrogen atoms of Hdmpz ligands, which occupy the equatorial positions, and two oxygen atoms of two SO$_4$ ligands, which are in axial positions. The difference in lengths of the axial Cu—O and equatorial Cu—N bonds is at least 0.235 Å. Bond lengths between the central atom and the nitrogen atoms in the equatorial position are approximately the same [in the range 2.028 (6) to 2.054 (6) Å]. The N1, N3, N5 and N7 nitrogen atoms slightly deviate from of the equatorial plane [by

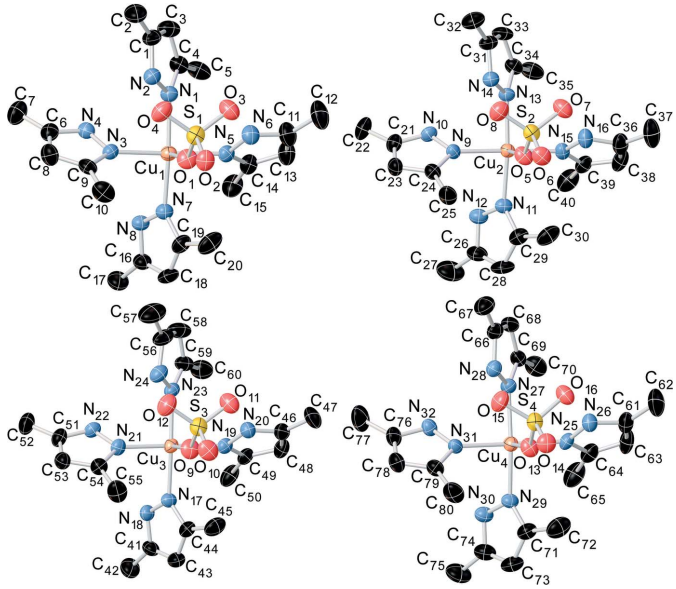



**Figure 1**
Representation of four [Cu(SO$_4$)(Hdmpz)$_4$] formula units in the structure of the title coordination polymer, with displacement ellipsoids at the 50% probability level.

−0.088 (3) Å for N1, 0.069 (3) Å for N3, 0.067 (3) Å for N5 and −0.086 (3) Å for N7]. The Cu1 atom is out of the equatorial plane, formed by four nitrogen atoms, by 0.038 (3) Å. The N—Cu—N angles are practically right angles, in the range of 88.0 (2)–91.2 (2)°. The intermetallic Cu···Cu distances between two neighboring [Cu(Hdmpz)$_4$SO$_4$] fragments within one asymmetric unit are in the range 7.0842 (12)–7.1554 (12) Å while the interchalcogenic S···S distances are in the range 7.166 (2)–7.223 (2) Å. Bridging oxygen atoms of sulfate ligands, which bind [Cu(Hdmpz)$_4$SO$_4$] formula units, are arranged in a spiral along the *b* axis (Fig. 3).

The molecular structure of the complex is stabilized by weak intramolecular hydrogen bonds in which hydrogen donors are carbon atoms (–CH$_3$ groups at the 3 and 5 positions of the pyrazole ring) and pyrrole-like nitrogen atoms of NH groups, while hydrogen acceptors are pyridine-like nitrogen atoms of the neighboring pyrazole ligands and O and S atoms of the sulfate ligands. Significant contributions to the hydrogen-bond network are made by N—H···O hydrogen bonds with lengths in the range of 2.022 (5) to 2.437 (4) Å.

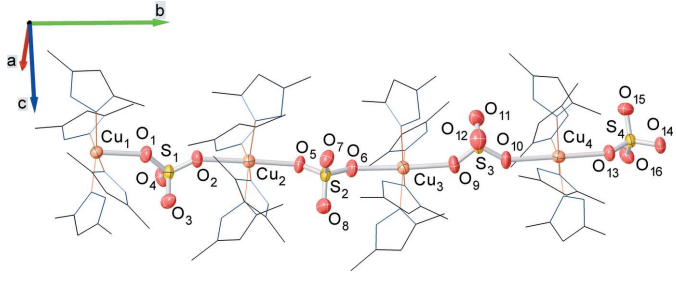



**Figure 2**
The asymmetric unit of the title compound. Selected pyrazole ring atoms are represented as wireframes. H atoms and hydrogen bonds are omitted for clarity.

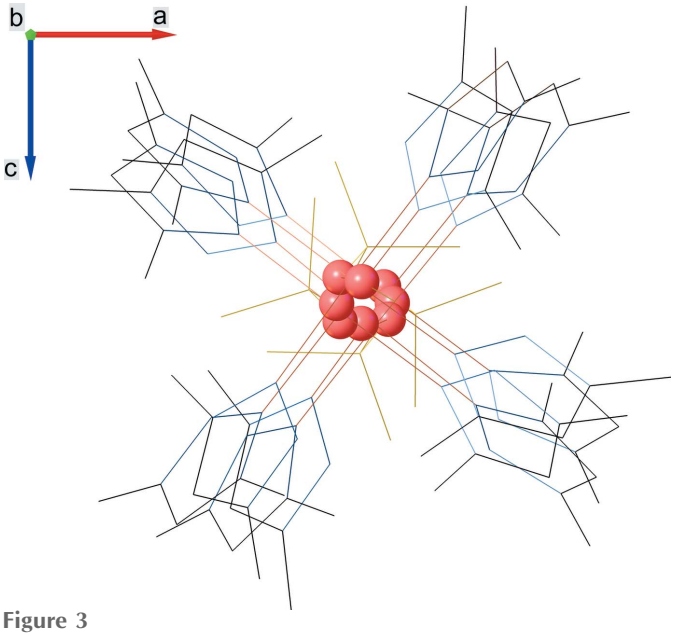



**Figure 3**
The spiral arrangement of the bridging oxygen atoms of the sulfate ligands, which bind $[Cu(SO_4)(Hdmpz)_4]$ formula units along the *b*-axis direction. Bridging oxygen atoms of sulfate ligands are represented as red spheres, while all other atoms are depicted as wireframes. Hydrogen atoms are omitted for clarity.

Selected intramolecular geometric parameters of hydrogen bonds are given in Table 1. The hydrogen-bond network in the asymmetric unit of the title compound is shown in Fig. 4. The torsion angle Cu1—Cu2—Cu3—Cu4 is −80.2 (2)° and S1—S2—S3–S4 is −97.8 (2)° and O1—O2— O5—O6, O5—O6—O9—O10 and O9—O10—O13—O14 are 36 (4), 25 (7) and 51 (3)°, respectively.

All pyrazole rings are oriented unsymmetrically in the mononuclear fragment. Thus, the planes of pyrazole rings N1/N2/C1/C3/C4 (pyrazole ligand near the Cu1 atom) and N9/N10/C21/C23/C24 (pyrazole ligand near the Cu2 atom) are oriented almost parallel to each other with a small deviation [plane normal to plane normal angle = 12.8 (3)°]. The plane-to-plane twist angle is 4.2 (4)°, the plane-to-plane fold angle is 13.4 (4)° and the plane-to-plane shift = 4.879 (18) Å. Within one $[Cu(Hdmpz)_4SO_4]$ unit, pairs of pyrazole ring planes, for example N1/N2/C1/C3/C4, N7/N8/C16/C18/C19 and N3/N4/C6/C8/C9, N5/N6/C11/C13/C14, are placed in a non-parallel manner. The torsion angles N2—N1—N7—N8 and N4—N3—N5—N6 are 109.0 (6) and 111.3 (6)°, respectively.

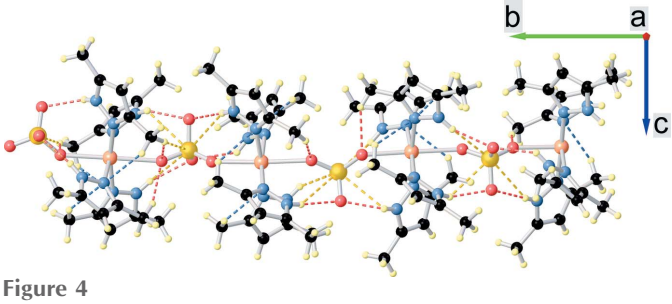



**Figure 4**
Intramolecular hydrogen-bond network in the asymmetric unit of the title compound. Hydrogen bonds with the participation of oxygen atoms are indicated in red, blue for nitrogen atoms and yellow for sulfur atoms. Hydrogen donors are carbon atoms of methyl groups and nitrogen atoms of NH groups, while hydrogen acceptors are sulfur and oxygen atoms, and pyridine-like nitrogen atoms of the pyrazole ring.

**Table 1**
Geometry of intramolecular hydrogen bonds (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O4 | 0.86 | 2.08 | 2.792 (7) | 139 |
| N6—H6···O3 | 0.86 | 2.04 | 2.889 (7) | 168 |
| N10—H10···O3 | 0.86 | 2.11 | 2.869 (7) | 146 |
| N12—H12···O4 | 0.86 | 2.12 | 2.951 (8) | 163 |
| N14—H14···O8 | 0.86 | 2.10 | 2.835 (7) | 143 |
| N16—H16···O5 | 0.86 | 2.44 | 2.889 (7) | 114 |
| N16—H16···O7 | 0.86 | 2.04 | 2.894 (8) | 173 |
| N18—H18···O6 | 0.86 | 2.39 | 2.866 (8) | 116 |
| N18—H18···O8 | 0.86 | 2.14 | 2.988 (7) | 169 |
| N20—H20···O9 | 0.86 | 2.41 | 2.885 (9) | 115 |
| N20—H20···O11 | 0.86 | 2.08 | 2.933 (7) | 171 |
| N22—H22···O7 | 0.86 | 2.05 | 2.828 (7) | 150 |
| N24—H24···O12 | 0.86 | 2.16 | 2.840 (8) | 135 |
| N26—H26···O16 | 0.86 | 2.02 | 2.875 (7) | 171 |
| N28—H28···O15 | 0.86 | 2.07 | 2.803 (7) | 143 |
| N30—H30···O10 | 0.86 | 2.31 | 2.817 (8) | 118 |
| N30—H30···O12 | 0.86 | 2.24 | 3.083 (8) | 165 |
| N32—H32···O11 | 0.86 | 2.12 | 2.857 (7) | 144 |
| C30—H30*C*···O5 | 0.96 | 2.39 | 3.213 (11) | 144 |
| C50—H50*A*···O6 | 0.96 | 2.23 | 3.124 (9) | 155 |
| C65—H65*B*···O10 | 0.96 | 2.27 | 3.192 (11) | 160 |
| C70—H70*B*···O10 | 0.96 | 2.35 | 3.116 (10) | 137 |

## 3. Supramolecular features

The crystal structure (Fig. 5) is built up from polymeric chains packed parallel along the *b*-axis direction. The unit-cell

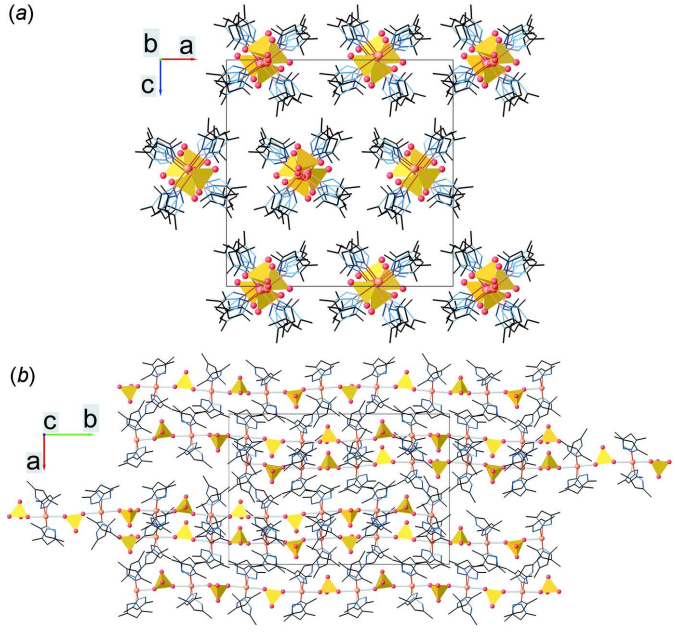



**Figure 5**
Crystal packing of the title compound viewed along the (*a*) *b*- and (*b*) *c*-axis directions: sulfate ligands are in a polyhedral representation with red spherical oxygen atoms, copper atoms are represented as orange spheres, while pyrazole rings atoms are depicted as wireframes. Hydrogen atoms are omitted for clarity.

**Table 2**
Geometric parameters of intermolecular hydrogen bonds (Å, °).

| | | | | |
|---|---|---|---|---|
| C2—H2*A*···N16$^{i}$ | 0.96 | 3.01 | 3.722 (10) | 132 |
| C2—H2*A*···O7$^{i}$ | 0.96 | 28 | 3.806 (9) | 146 |
| C53—H53···N8$^{ii}$ | 0.93 | 3.07 | 3.66 (1) | 123 |
| C32—H32*B*···N32$^{iii}$ | 0.96 | 3.00 | 3.792 (10) | 140 |
| C32—H32*B*···N31$^{iii}$ | 0.96 | 3.17 | 3.984 (10) | 143 |
| C32—H32*B*···N28$^{iii}$ | 0.96 | 2.87 | 3.735 (11) | 150 |

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

dimensions can be explained because of the presence of four complex moieties in the asymmetric unit ($Z'$ = 4, $Z$ = 16). As a result of the sulfate ligand rotation, there is a pairwise alternation of the terminal oxygen atoms (which are not involved in coordinating the copper atom) of the $SO_4$ tetrahedra. Within one chain the intermetallic distance between two copper atoms, which are located at the edges of two neighboring asymmetric units, is 7.1625 (12) Å, while the interchalcogenic distance between the nearest sulfur atoms is 7.227 (2) Å. Polymeric chains, which are formed with the participation of bridging sulfate ligands, are stabilized by an extensive hydrogen-bond network. Neighboring chains are connected to each other by weak C—H···N and C—H···O hydrogen bonds. Geometric parameters for intermolecular hydrogen bonds are given in Table 2.

## 4. Hirshfeld surface analysis

The Hirshfeld surface analysis was performed and the associated two-dimensional fingerprint plots generated using *Crystal Explorer 17.5* software (Spackman *et al.*, 2021), with a standard resolution of the three-dimensional $d_{norm}$ surfaces plotted over a fixed color scale of −0.5511 (red) to 1.8416 (blue) a.u. The red spots in Fig. 6. represent short contacts and negative $d_{norm}$ values on the surface corresponding to the interactions described above. The Hirshfeld surfaces mapped over $d_{norm}$ are shown for the H···H, H···O/O···H, H···C/C···H, Cu···O/O···Cu and H···N/N···H contacts, the overall two-dimensional fingerprint plot and the decomposed two-dimensional fingerprint plots are given in Fig. 7. For the title coordination polymer, the most significant contributions to the overall crystal packing are from H···H (74.7%), H···O/O···H (14.8%) and H···C/C···H (8.2%) contacts. Small contributions of weak Cu···O/O···Cu (1.1%), H···N/N···H (0.9%) and N···O/O···N (0.2%) contacts have a negligible effect on the packing. The total contribution of contacts involving hydrogen atoms is 85.9%, for O atoms is 8.4%, C atoms 4.4%, N atoms 0.7% and Cu atoms 0.5%. These values were calculated using the *Crystal Explorer 17.5* software (Spackman *et al.*, 2021). A special filter 'by elements' was chosen during the calculation of the contributions of selected individual interactions to the total Hirshfeld surface. Quantitative physical properties of Hirshfeld surface for the title compound were also obtained, such as the molecular volume (650.80 Å$^3$), surface area (512.94 Å$^2$), globularity (0.708), as well as sphericity (0.034). These properties provide significant information on the shape of the molecules and may serve in the future to identify and establish correlations with other properties.

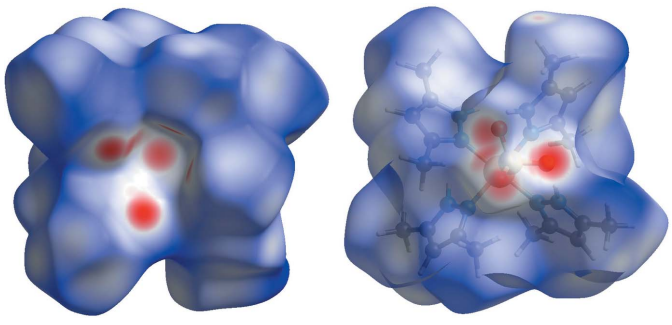


**Figure 6**
Two projections of Hirshfeld surfaces mapped over $d_{norm}$ showing the intermolecular interactions.

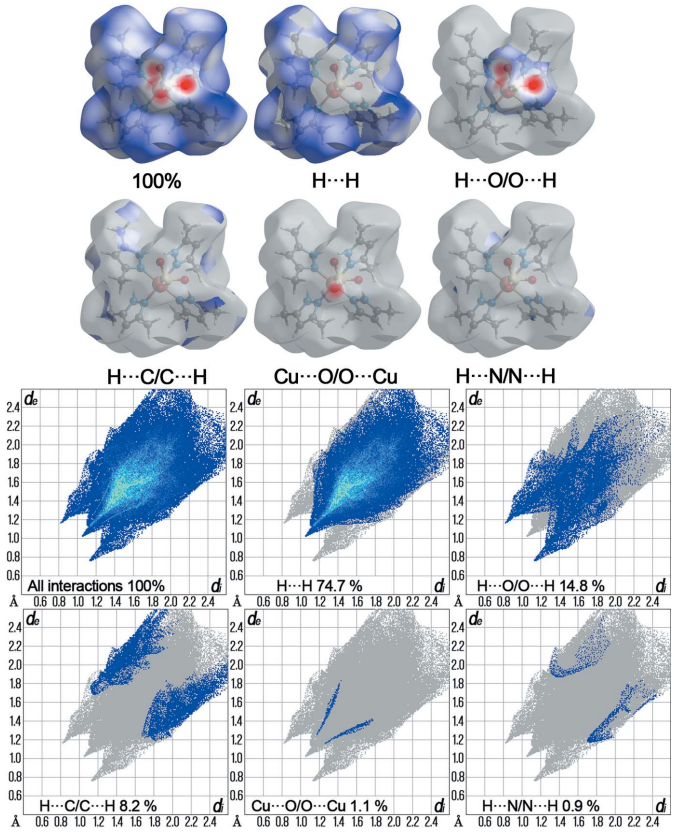



**Figure 7**
The overall two-dimensional fingerprint plot and those delineated into specified interactions. Hirshfeld surface representations with the function $d_{norm}$ plotted onto the surface for the different interactions.

## 5. Database survey

A search of the Cambridge Structural Database (CSD version 5.42, update February 2021; Groom *et al.*, 2016) for the $Cu_2(\mu_2\text{-}SO_4)(Hpz)_4$ moiety [two $Cu(Hpz)_2$ fragments connected through a bidentate-bridged $SO_4$ ligand] revealed two hits: QITCAZ, a coordination compound based on

**Table 3**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Cu(SO_4)(C_5H_8N_2)_4]$ |
| $M_r$ | 544.13 |
| Crystal system, space group | Orthorhombic, $Pna2_1$ |
| Temperature (K) | 293 |
| $a, b, c$ (Å) | 19.3656 (6), 28.4032 (6), 19.3456 (5) |
| $V$ (Å$^3$) | 10641.0 (5) |
| $Z$ | 16 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.94 |
| Crystal size (mm) | 0.35 × 0.25 × 0.25 |
| Data collection | |
| Diffractometer | Rigaku Oxford Diffraction Xcalibur, Eos |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021) |
| $T_{min}$, $T_{max}$ | 0.907, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 119732, 22862, 14389 |
| $R_{int}$ | 0.062 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.690 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.054, 0.133, 1.03 |
| No. of reflections | 22862 |
| No. of parameters | 1234 |
| No. of restraints | 1 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.19, −0.30 |
| Absolute structure | Refined as an inversion twin |
| Absolute structure parameter | 0.479 (15) |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

4-iodo-1*H*-pyrazole (Song *et al.*, 2013) and XACTUR, a 1*H*-pyrazole-containing complex (Shen *et al.*, 2004). These structures are similar to the title compound. Moreover there are 23 hits for the $Cu(C_3N_2)_2SO_4$ moiety, where $C_3N_2$ is the backbone of the pyrazole ring. Most similar to the title compound are two *catena*-[($\mu_2$-sulfato)bis(3,5-dimethyl-1*H*-pyrazole)aquacopper(II)dihydrate] complexes: EHOMEU (Wang *et al.*, 2010) and EHOMEU01 (Gogoi *et al.*, 2019); FITCUI, a complex based on 2-thienyl-1*H*-pyrazole (Pettinari *et al.*, 2014); ZZZALD01 a tetrakis(pyrazole)(sulfato-*O*)copper(II) monohydrate (Shen *et al.*, 2004); two monohydrated tetrapyrazole sulfato copper(II) complexes: LUNDAB (Kumar *et al.*, 2014) and LUNDAB01 (Zerguini *et al.*, 2019).

## 6. Synthesis and crystallization

The synthesis of $[Cu(SO_4)(Hdmpz)_4]_n$ was conducted at room temperature by the oxidative dissolution method as a result of the addition of a copper powder (1.56 mmol, 0.1 g) and anhydrous copper(II) sulfate (3.1 mmol, 0.5 g) mixture to an acetonitrile (9 ml) solution of 3,5-dimethyl-1*H*-pyrazole (4.68 mmol, 0.45g). The mixture was stirred without heating for three h with free air access until dissolution of the copper powder and a gray–blue precipitate of the product was obtained (the precipitate weight was 0.86 g). The precipitate was filtered off and the obtained green–blue solution was analyzed. Clear, intense blue crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of the solvent at room temperature in an open vessel. The relative yield of the single-crystal portion of the product with respect to the ligand was approximately 7%. The obtained blue crystals were studied by elemental analysis (calculated for $C_{20}H_{32}CuN_8O_4S$: C 44.1%, H 5.9%, N 20.6%, found: C 44.5%, H 6.3%, N 21%). The elemental analysis data of the obtained grey–blue precipitate was: found C 36.8%, H 5.5%, N 17.2%. IR spectra of the starting 3,5-dimethyl-1*H*-pyrazole, grey–blue precipitate and clear, intense blue crystals of the title coordination polymer are given in the supporting information for this article.

## 7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Refinement of the N—H bond lengths was attempted, but this provided unrealistic values. Thus, hydrogens were placed at calculated positions and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(N, C) or 1.5$U_{eq}$(C-methyl). The crystal studied was refined as a two-component inversion twin.

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# supporting information

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# *catena*-Poly[[tetrakis(3,5-dimethyl-1*H*-pyrazole-$\kappa N^2$)copper(II)]-$\mu_2$-sulfato-$\kappa^2 O{:}O'$]: crystal structure and Hirshfeld surface analysis of a $Cu^{II}$ coordination polymer

**Oleksandr S. Vynohradov, Artur Dovzhik, Vadim A. Pavlenko, Dina D. Naumova, Irina A. Golenya and Sergiu Shova**

## Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

### *catena*-Poly[[tetrakis(3,5-dimethyl-1*H*-pyrazole-$\kappa N^2$)copper(II)]-$\mu_2$-sulfato-$\kappa^2 O{:}O'$]

*Crystal data*

$[Cu(SO_4)(C_5H_8N_2)_4]$
$M_r$ = 544.13
Orthorhombic, $Pna2_1$
$a$ = 19.3656 (6) Å
$b$ = 28.4032 (6) Å
$c$ = 19.3456 (5) Å
$V$ = 10641.0 (5) Å$^3$
$Z$ = 16
$F(000)$ = 4560
$D_x$ = 1.359 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 24752 reflections
$\theta$ = 2.1–24.0°
$\mu$ = 0.94 mm$^{-1}$
$T$ = 293 K
Prism, clear intense blue
0.35 × 0.25 × 0.25 mm

*Data collection*

Rigaku Oxford Diffraction Xcalibur, Eos diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1593 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
$T_{min}$ = 0.907, $T_{max}$ = 1.000
119732 measured reflections
22862 independent reflections
14389 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.062
$\theta_{max}$ = 29.4°, $\theta_{min}$ = 1.7°
$h$ = −26→26
$k$ = −39→36
$l$ = −22→26

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.133
$S$ = 1.03
22862 reflections
1234 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 4.6894P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.19$ e Å$^{-3}$
$\Delta\rho_{min} = -0.30$ e Å$^{-3}$
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.479 (15)

*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.

**Refinement**. Refined as a 2-component inversion twin.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.32732 (4) | 0.08172 (3) | 0.47991 (5) | 0.0381 (2) |
| Cu2 | 0.35680 (4) | 0.33019 (3) | 0.49183 (4) | 0.0366 (2) |
| Cu3 | 0.34772 (4) | 0.57922 (3) | 0.51712 (5) | 0.0386 (2) |
| Cu4 | 0.31888 (4) | 0.83027 (3) | 0.50659 (4) | 0.0383 (2) |
| S1 | 0.38041 (9) | 0.20005 (5) | 0.50836 (11) | 0.0453 (4) |
| S2 | 0.33477 (9) | 0.45147 (5) | 0.54082 (11) | 0.0425 (5) |
| S3 | 0.29310 (9) | 0.69962 (5) | 0.48845 (12) | 0.0482 (5) |
| S4 | 0.34086 (9) | 0.94986 (5) | 0.45316 (11) | 0.0415 (4) |
| O1 | 0.3364 (2) | 0.16205 (14) | 0.4818 (3) | 0.0518 (14) |
| O2 | 0.3542 (2) | 0.24597 (13) | 0.4860 (3) | 0.0507 (13) |
| O3 | 0.3800 (3) | 0.19749 (17) | 0.5846 (3) | 0.0574 (15) |
| O4 | 0.4509 (2) | 0.19497 (15) | 0.4824 (3) | 0.0612 (15) |
| O5 | 0.3613 (2) | 0.41241 (13) | 0.4991 (3) | 0.0495 (14) |
| O6 | 0.3581 (2) | 0.49625 (14) | 0.5126 (3) | 0.0526 (14) |
| O7 | 0.2586 (2) | 0.44992 (15) | 0.5392 (3) | 0.0572 (14) |
| O8 | 0.3598 (3) | 0.44762 (16) | 0.6120 (3) | 0.0603 (16) |
| O9 | 0.3357 (2) | 0.66123 (14) | 0.5160 (4) | 0.0570 (15) |
| O10 | 0.3188 (3) | 0.74469 (14) | 0.5145 (3) | 0.0603 (15) |
| O11 | 0.2977 (3) | 0.69918 (17) | 0.4129 (3) | 0.0629 (16) |
| O12 | 0.2213 (3) | 0.69417 (17) | 0.5107 (4) | 0.0710 (16) |
| O13 | 0.3157 (2) | 0.91247 (13) | 0.4997 (3) | 0.0486 (14) |
| O14 | 0.3186 (2) | 0.99611 (14) | 0.4783 (3) | 0.0516 (14) |
| O15 | 0.3144 (3) | 0.94324 (18) | 0.3832 (3) | 0.0599 (16) |
| O16 | 0.4168 (2) | 0.94793 (16) | 0.4532 (3) | 0.0537 (14) |
| N1 | 0.4125 (3) | 0.07577 (18) | 0.5413 (3) | 0.0406 (14) |
| N2 | 0.4699 (3) | 0.10224 (17) | 0.5263 (3) | 0.0421 (13) |
| H2 | 0.471469 | 0.123444 | 0.494624 | 0.050* |
| N3 | 0.3918 (3) | 0.07707 (17) | 0.3958 (3) | 0.0371 (13) |
| N4 | 0.4314 (3) | 0.03765 (18) | 0.3906 (3) | 0.0406 (14) |
| H4 | 0.431493 | 0.015166 | 0.420404 | 0.049* |
| N5 | 0.2660 (3) | 0.08838 (18) | 0.5646 (3) | 0.0402 (14) |
| N6 | 0.2834 (3) | 0.12205 (18) | 0.6108 (3) | 0.0492 (15) |
| H6 | 0.316691 | 0.141689 | 0.604779 | 0.059* |
| N7 | 0.2437 (3) | 0.07873 (18) | 0.4170 (3) | 0.0404 (15) |

| | | | | |
|---|---|---|---|---|
| N8 | 0.2337 (3) | 0.03829 (18) | 0.3801 (3) | 0.0404 (14) |
| H8 | 0.261953 | 0.014945 | 0.380052 | 0.048* |
| N9 | 0.4407 (3) | 0.32578 (17) | 0.5546 (3) | 0.0363 (13) |
| N10 | 0.4483 (3) | 0.28685 (18) | 0.5947 (3) | 0.0412 (14) |
| H10 | 0.415730 | 0.266851 | 0.601978 | 0.049* |
| N11 | 0.4228 (3) | 0.32439 (18) | 0.4100 (3) | 0.0401 (14) |
| N12 | 0.4621 (3) | 0.28530 (19) | 0.4079 (3) | 0.0473 (15) |
| H12 | 0.459640 | 0.262546 | 0.437135 | 0.057* |
| N13 | 0.2952 (3) | 0.32716 (17) | 0.5767 (3) | 0.0374 (14) |
| N14 | 0.3102 (3) | 0.35464 (17) | 0.6314 (3) | 0.0401 (14) |
| H14 | 0.342157 | 0.375686 | 0.630656 | 0.048* |
| N15 | 0.2751 (3) | 0.33851 (18) | 0.4275 (3) | 0.0410 (15) |
| N16 | 0.2360 (3) | 0.37800 (19) | 0.4357 (3) | 0.0507 (16) |
| H16 | 0.241034 | 0.397862 | 0.468889 | 0.061* |
| N17 | 0.4299 (3) | 0.57622 (18) | 0.5830 (3) | 0.0408 (14) |
| N18 | 0.4410 (3) | 0.53691 (18) | 0.6198 (3) | 0.0425 (14) |
| H18 | 0.413143 | 0.513345 | 0.620048 | 0.051* |
| N19 | 0.4139 (3) | 0.58823 (18) | 0.4359 (3) | 0.0400 (14) |
| N20 | 0.4009 (3) | 0.62485 (18) | 0.3930 (3) | 0.0431 (14) |
| H20 | 0.367047 | 0.644127 | 0.398058 | 0.052* |
| N21 | 0.2827 (3) | 0.57547 (17) | 0.5999 (3) | 0.0407 (14) |
| N22 | 0.2421 (3) | 0.53702 (18) | 0.6081 (3) | 0.0416 (15) |
| H22 | 0.236905 | 0.515774 | 0.576872 | 0.050* |
| N23 | 0.2662 (3) | 0.57376 (18) | 0.4494 (3) | 0.0414 (14) |
| N24 | 0.2100 (3) | 0.60092 (19) | 0.4590 (4) | 0.0542 (16) |
| H24 | 0.204744 | 0.619756 | 0.493354 | 0.065* |
| N25 | 0.4015 (3) | 0.84053 (18) | 0.5680 (3) | 0.0398 (14) |
| N26 | 0.4448 (3) | 0.87635 (17) | 0.5545 (3) | 0.0435 (14) |
| H26 | 0.438945 | 0.895919 | 0.521062 | 0.052* |
| N27 | 0.3831 (3) | 0.82429 (18) | 0.4231 (3) | 0.0389 (14) |
| N28 | 0.3720 (3) | 0.85335 (18) | 0.3675 (3) | 0.0409 (14) |
| H28 | 0.338936 | 0.873473 | 0.365124 | 0.049* |
| N29 | 0.2546 (3) | 0.82565 (18) | 0.5892 (3) | 0.0409 (14) |
| N30 | 0.2132 (3) | 0.78693 (19) | 0.5931 (3) | 0.0476 (15) |
| H30 | 0.213789 | 0.764259 | 0.563671 | 0.057* |
| N31 | 0.2358 (3) | 0.82528 (17) | 0.4430 (3) | 0.0362 (13) |
| N32 | 0.2305 (3) | 0.78826 (18) | 0.3996 (3) | 0.0433 (15) |
| H32 | 0.263325 | 0.768555 | 0.392030 | 0.052* |
| C1 | 0.5230 (4) | 0.0909 (3) | 0.5672 (4) | 0.055 (2) |
| C2 | 0.5895 (4) | 0.1169 (3) | 0.5600 (5) | 0.076 (3) |
| H2A | 0.621893 | 0.097751 | 0.535050 | 0.114* |
| H2B | 0.581603 | 0.145661 | 0.535100 | 0.114* |
| H2C | 0.607663 | 0.123991 | 0.604930 | 0.114* |
| C3 | 0.5007 (4) | 0.0559 (3) | 0.6100 (5) | 0.064 (2) |
| H3 | 0.526299 | 0.040852 | 0.644164 | 0.077* |
| C4 | 0.4319 (4) | 0.0468 (2) | 0.5924 (4) | 0.0472 (19) |
| C5 | 0.3846 (4) | 0.0124 (3) | 0.6251 (5) | 0.067 (2) |
| H5A | 0.356433 | 0.028130 | 0.658716 | 0.100* |

| | | | | |
|---|---|---|---|---|
| H5B | 0.355543 | −0.001530 | 0.590356 | 0.100* |
| H5C | 0.411053 | −0.011900 | 0.647336 | 0.100* |
| C6 | 0.4698 (4) | 0.0382 (2) | 0.3339 (4) | 0.0493 (19) |
| C7 | 0.5150 (4) | −0.0028 (3) | 0.3150 (5) | 0.074 (3) |
| H7A | 0.541754 | −0.012111 | 0.354541 | 0.110* |
| H7B | 0.486784 | −0.028761 | 0.300331 | 0.110* |
| H7C | 0.545514 | 0.006079 | 0.278111 | 0.110* |
| C8 | 0.4558 (4) | 0.0797 (2) | 0.3010 (4) | 0.057 (2) |
| H8A | 0.475469 | 0.090205 | 0.259971 | 0.069* |
| C9 | 0.4068 (4) | 0.1032 (2) | 0.3403 (4) | 0.0433 (17) |
| C10 | 0.3741 (5) | 0.1494 (2) | 0.3269 (4) | 0.064 (2) |
| H10A | 0.370788 | 0.154240 | 0.277892 | 0.095* |
| H10B | 0.328688 | 0.150070 | 0.346832 | 0.095* |
| H10C | 0.401648 | 0.173990 | 0.346972 | 0.095* |
| C11 | 0.2429 (5) | 0.1213 (3) | 0.6671 (5) | 0.064 (2) |
| C12 | 0.2525 (5) | 0.1557 (3) | 0.7255 (5) | 0.091 (3) |
| H12A | 0.228809 | 0.144454 | 0.765843 | 0.137* |
| H12B | 0.300869 | 0.158834 | 0.735583 | 0.137* |
| H12C | 0.234159 | 0.185804 | 0.712433 | 0.137* |
| C13 | 0.1985 (5) | 0.0846 (3) | 0.6565 (5) | 0.065 (2) |
| H13 | 0.163781 | 0.074778 | 0.686407 | 0.078* |
| C14 | 0.2144 (4) | 0.0648 (2) | 0.5933 (4) | 0.0498 (19) |
| C15 | 0.1806 (4) | 0.0235 (2) | 0.5586 (5) | 0.065 (2) |
| H15A | 0.164851 | 0.032739 | 0.513512 | 0.098* |
| H15B | 0.213211 | −0.001791 | 0.554232 | 0.098* |
| H15C | 0.141941 | 0.013189 | 0.585722 | 0.098* |
| C16 | 0.1745 (4) | 0.0393 (2) | 0.3441 (4) | 0.0472 (18) |
| C17 | 0.1537 (4) | −0.0010 (3) | 0.2990 (6) | 0.069 (3) |
| H17A | 0.183502 | −0.002395 | 0.259473 | 0.104* |
| H17B | 0.106820 | 0.003300 | 0.284058 | 0.104* |
| H17C | 0.157235 | −0.029876 | 0.324644 | 0.104* |
| C18 | 0.1448 (4) | 0.0824 (3) | 0.3581 (5) | 0.058 (2) |
| H18A | 0.103391 | 0.093839 | 0.340651 | 0.069* |
| C19 | 0.1889 (4) | 0.1050 (2) | 0.4032 (4) | 0.0492 (19) |
| C20 | 0.1813 (4) | 0.1533 (2) | 0.4351 (5) | 0.074 (3) |
| H20A | 0.150287 | 0.151529 | 0.473782 | 0.111* |
| H20B | 0.225577 | 0.164219 | 0.450522 | 0.111* |
| H20C | 0.163077 | 0.174749 | 0.401402 | 0.111* |
| C21 | 0.5111 (4) | 0.2829 (2) | 0.6214 (4) | 0.0485 (18) |
| C22 | 0.5304 (5) | 0.2404 (3) | 0.6634 (4) | 0.069 (2) |
| H22A | 0.559190 | 0.249827 | 0.701352 | 0.104* |
| H22B | 0.554996 | 0.218450 | 0.634818 | 0.104* |
| H22C | 0.489284 | 0.225722 | 0.680924 | 0.104* |
| C23 | 0.5467 (4) | 0.3217 (3) | 0.6007 (4) | 0.0514 (19) |
| H23 | 0.591877 | 0.329426 | 0.612165 | 0.062* |
| C24 | 0.5018 (4) | 0.3476 (2) | 0.5585 (4) | 0.0426 (16) |
| C25 | 0.5174 (4) | 0.3928 (2) | 0.5231 (5) | 0.060 (2) |
| H25A | 0.566328 | 0.398168 | 0.523457 | 0.090* |

| | | | | |
|---|---|---|---|---|
| H25B | 0.494508 | 0.418130 | 0.546674 | 0.090* |
| H25C | 0.501375 | 0.391373 | 0.476133 | 0.090* |
| C26 | 0.5061 (4) | 0.2867 (3) | 0.3537 (4) | 0.056 (2) |
| C27 | 0.5556 (6) | 0.2466 (3) | 0.3427 (6) | 0.104 (4) |
| H27A | 0.588553 | 0.254903 | 0.307665 | 0.156* |
| H27B | 0.579403 | 0.239943 | 0.385145 | 0.156* |
| H27C | 0.530273 | 0.219273 | 0.328355 | 0.156* |
| C28 | 0.4935 (5) | 0.3277 (3) | 0.3192 (4) | 0.064 (2) |
| H28A | 0.515504 | 0.338284 | 0.279364 | 0.077* |
| C29 | 0.4408 (4) | 0.3507 (2) | 0.3557 (4) | 0.0505 (19) |
| C30 | 0.4076 (5) | 0.3971 (3) | 0.3412 (4) | 0.071 (3) |
| H30A | 0.362296 | 0.392072 | 0.322493 | 0.107* |
| H30B | 0.435085 | 0.414249 | 0.308444 | 0.107* |
| H30C | 0.404123 | 0.414809 | 0.383313 | 0.107* |
| C31 | 0.2715 (4) | 0.3463 (2) | 0.6863 (4) | 0.0489 (18) |
| C32 | 0.2785 (5) | 0.3752 (3) | 0.7511 (4) | 0.071 (2) |
| H32A | 0.260913 | 0.406319 | 0.742753 | 0.106* |
| H32B | 0.252743 | 0.360759 | 0.787763 | 0.106* |
| H32C | 0.326293 | 0.377149 | 0.763903 | 0.106* |
| C33 | 0.2287 (4) | 0.3101 (3) | 0.6676 (4) | 0.059 (2) |
| H33 | 0.195432 | 0.295838 | 0.695224 | 0.070* |
| C34 | 0.2444 (4) | 0.2987 (2) | 0.5991 (4) | 0.0462 (19) |
| C35 | 0.2102 (4) | 0.2627 (3) | 0.5545 (5) | 0.067 (2) |
| H35A | 0.227412 | 0.232031 | 0.566120 | 0.101* |
| H35B | 0.161182 | 0.263641 | 0.562070 | 0.101* |
| H35C | 0.219822 | 0.269301 | 0.506840 | 0.101* |
| C36 | 0.1892 (4) | 0.3819 (3) | 0.3860 (5) | 0.062 (2) |
| C37 | 0.1406 (5) | 0.4231 (3) | 0.3818 (6) | 0.099 (4) |
| H37A | 0.093811 | 0.411965 | 0.382856 | 0.148* |
| H37B | 0.148371 | 0.443765 | 0.420305 | 0.148* |
| H37C | 0.148481 | 0.439946 | 0.339455 | 0.148* |
| C38 | 0.1967 (5) | 0.3428 (3) | 0.3447 (5) | 0.065 (2) |
| H38 | 0.170690 | 0.335538 | 0.305757 | 0.078* |
| C39 | 0.2504 (4) | 0.3164 (2) | 0.3720 (4) | 0.0490 (19) |
| C40 | 0.2795 (5) | 0.2713 (3) | 0.3473 (5) | 0.073 (3) |
| H40A | 0.256185 | 0.261897 | 0.305781 | 0.110* |
| H40B | 0.327845 | 0.275217 | 0.338011 | 0.110* |
| H40C | 0.273345 | 0.247627 | 0.382141 | 0.110* |
| C41 | 0.4994 (4) | 0.5381 (3) | 0.6556 (4) | 0.0498 (19) |
| C42 | 0.5231 (4) | 0.4972 (3) | 0.6985 (5) | 0.077 (3) |
| H42A | 0.516980 | 0.504359 | 0.746621 | 0.116* |
| H42B | 0.571074 | 0.491173 | 0.689528 | 0.116* |
| H42C | 0.496494 | 0.469786 | 0.686875 | 0.116* |
| C43 | 0.5285 (4) | 0.5809 (3) | 0.6422 (4) | 0.056 (2) |
| H43 | 0.569799 | 0.592359 | 0.659965 | 0.067* |
| C44 | 0.4843 (4) | 0.6040 (2) | 0.5965 (4) | 0.0471 (18) |
| C45 | 0.4919 (4) | 0.6522 (2) | 0.5650 (5) | 0.070 (2) |
| H45A | 0.539299 | 0.661929 | 0.568093 | 0.104* |

| | | | | |
|---|---|---|---|---|
| H45B | 0.478179 | 0.651109 | 0.517373 | 0.104* |
| H45C | 0.463279 | 0.674139 | 0.589483 | 0.104* |
| C46 | 0.4464 (4) | 0.6273 (3) | 0.3424 (4) | 0.0526 (19) |
| C47 | 0.4456 (5) | 0.6662 (3) | 0.2898 (4) | 0.078 (3) |
| H47A | 0.452922 | 0.653232 | 0.244593 | 0.117* |
| H47B | 0.401622 | 0.681892 | 0.291063 | 0.117* |
| H47C | 0.481512 | 0.688432 | 0.300053 | 0.117* |
| C48 | 0.4908 (4) | 0.5902 (3) | 0.3515 (4) | 0.056 (2) |
| H48 | 0.528511 | 0.582495 | 0.324045 | 0.068* |
| C49 | 0.4680 (4) | 0.5665 (2) | 0.4099 (4) | 0.0431 (18) |
| C50 | 0.4983 (4) | 0.5240 (2) | 0.4440 (5) | 0.066 (2) |
| H50A | 0.462492 | 0.506713 | 0.466947 | 0.098* |
| H50B | 0.532356 | 0.533715 | 0.477141 | 0.098* |
| H50C | 0.519666 | 0.504384 | 0.409681 | 0.098* |
| C51 | 0.2114 (4) | 0.5354 (2) | 0.6688 (4) | 0.0495 (19) |
| C52 | 0.1679 (4) | 0.4945 (3) | 0.6911 (6) | 0.072 (3) |
| H52A | 0.183295 | 0.466551 | 0.667829 | 0.108* |
| H52B | 0.172145 | 0.490291 | 0.740129 | 0.108* |
| H52C | 0.120465 | 0.500471 | 0.679529 | 0.108* |
| C53 | 0.2305 (4) | 0.5758 (3) | 0.7027 (4) | 0.0517 (19) |
| H53 | 0.216045 | 0.585499 | 0.746269 | 0.062* |
| C54 | 0.2752 (4) | 0.5990 (2) | 0.6595 (4) | 0.0454 (17) |
| C55 | 0.3139 (5) | 0.6447 (3) | 0.6737 (5) | 0.072 (3) |
| H55A | 0.293584 | 0.669771 | 0.647370 | 0.109* |
| H55B | 0.361446 | 0.641088 | 0.660726 | 0.109* |
| H55C | 0.311095 | 0.652069 | 0.722096 | 0.109* |
| C56 | 0.1634 (4) | 0.5951 (3) | 0.4085 (5) | 0.069 (3) |
| C57 | 0.0974 (5) | 0.6235 (3) | 0.4060 (6) | 0.105 (4) |
| H57A | 0.060225 | 0.605184 | 0.424750 | 0.157* |
| H57B | 0.103045 | 0.651724 | 0.432740 | 0.157* |
| H57C | 0.087055 | 0.631684 | 0.358930 | 0.157* |
| C58 | 0.1910 (5) | 0.5612 (3) | 0.3649 (5) | 0.078 (3) |
| H58 | 0.170809 | 0.548858 | 0.325256 | 0.094* |
| C59 | 0.2541 (4) | 0.5495 (3) | 0.3921 (5) | 0.053 (2) |
| C60 | 0.3040 (5) | 0.5152 (3) | 0.3616 (5) | 0.076 (3) |
| H60A | 0.292885 | 0.510294 | 0.313798 | 0.114* |
| H60B | 0.350055 | 0.527494 | 0.365318 | 0.114* |
| H60C | 0.301045 | 0.485884 | 0.386008 | 0.114* |
| C61 | 0.4981 (4) | 0.8783 (3) | 0.5986 (4) | 0.059 (2) |
| C62 | 0.5536 (5) | 0.9155 (3) | 0.5916 (6) | 0.096 (4) |
| H62A | 0.549922 | 0.937439 | 0.629168 | 0.143* |
| H62B | 0.547886 | 0.931859 | 0.548573 | 0.143* |
| H62C | 0.598204 | 0.900764 | 0.592679 | 0.143* |
| C63 | 0.4896 (4) | 0.8416 (3) | 0.6425 (5) | 0.062 (2) |
| H63 | 0.518563 | 0.833641 | 0.679017 | 0.075* |
| C64 | 0.4295 (4) | 0.8180 (2) | 0.6230 (4) | 0.050 (2) |
| C65 | 0.3958 (5) | 0.7755 (3) | 0.6532 (5) | 0.077 (3) |
| H65A | 0.366272 | 0.784778 | 0.690652 | 0.115* |

| | | | | |
|---|---|---|---|---|
| H65B | 0.368892 | 0.760019 | 0.618272 | 0.115* |
| H65C | 0.430652 | 0.754378 | 0.670042 | 0.115* |
| C66 | 0.4183 (4) | 0.8468 (2) | 0.3178 (4) | 0.0473 (18) |
| C67 | 0.4217 (5) | 0.8754 (3) | 0.2557 (4) | 0.068 (2) |
| H67A | 0.468548 | 0.877074 | 0.239690 | 0.102* |
| H67B | 0.393268 | 0.861564 | 0.220500 | 0.102* |
| H67C | 0.405298 | 0.906574 | 0.265840 | 0.102* |
| C68 | 0.4596 (4) | 0.8108 (3) | 0.3422 (4) | 0.055 (2) |
| H68 | 0.496530 | 0.797369 | 0.318549 | 0.066* |
| C69 | 0.4375 (4) | 0.7979 (2) | 0.4067 (4) | 0.0422 (19) |
| C70 | 0.4662 (4) | 0.7622 (3) | 0.4553 (5) | 0.067 (2) |
| H70A | 0.483103 | 0.777673 | 0.496045 | 0.100* |
| H70B | 0.430573 | 0.740303 | 0.467885 | 0.100* |
| H70C | 0.503403 | 0.745543 | 0.433365 | 0.100* |
| C71 | 0.2370 (4) | 0.8513 (2) | 0.6433 (4) | 0.0496 (19) |
| C72 | 0.2728 (5) | 0.8978 (3) | 0.6572 (5) | 0.080 (3) |
| H72A | 0.244398 | 0.923201 | 0.640899 | 0.120* |
| H72B | 0.280248 | 0.901271 | 0.706029 | 0.120* |
| H72C | 0.316388 | 0.898421 | 0.633629 | 0.120* |
| C73 | 0.1851 (4) | 0.8299 (3) | 0.6812 (4) | 0.063 (2) |
| H73 | 0.163823 | 0.841381 | 0.720887 | 0.076* |
| C74 | 0.1716 (4) | 0.7884 (3) | 0.6479 (5) | 0.058 (2) |
| C75 | 0.1211 (5) | 0.7494 (3) | 0.6620 (6) | 0.086 (3) |
| H75A | 0.075626 | 0.762464 | 0.667102 | 0.129* |
| H75B | 0.121366 | 0.727504 | 0.624292 | 0.129* |
| H75C | 0.133946 | 0.733504 | 0.703852 | 0.129* |
| C76 | 0.1681 (4) | 0.7857 (2) | 0.3697 (4) | 0.052 (2) |
| C77 | 0.1515 (5) | 0.7477 (3) | 0.3181 (6) | 0.090 (3) |
| H77A | 0.158352 | 0.717433 | 0.339191 | 0.135* |
| H77B | 0.104222 | 0.750633 | 0.303761 | 0.135* |
| H77C | 0.181192 | 0.750673 | 0.278651 | 0.135* |
| C78 | 0.1310 (4) | 0.8229 (3) | 0.3945 (4) | 0.055 (2) |
| H78 | 0.085662 | 0.830445 | 0.383381 | 0.066* |
| C79 | 0.1740 (3) | 0.8474 (2) | 0.4397 (4) | 0.0445 (17) |
| C80 | 0.1588 (4) | 0.8913 (2) | 0.4792 (5) | 0.068 (2) |
| H80A | 0.115620 | 0.904245 | 0.463907 | 0.102* |
| H80B | 0.155950 | 0.884095 | 0.527647 | 0.102* |
| H80C | 0.195000 | 0.913715 | 0.471527 | 0.102* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0354 (4) | 0.0381 (4) | 0.0408 (6) | −0.0023 (3) | −0.0030 (4) | −0.0003 (4) |
| Cu2 | 0.0354 (4) | 0.0365 (4) | 0.0380 (5) | −0.0001 (3) | 0.0027 (4) | 0.0004 (4) |
| Cu3 | 0.0340 (4) | 0.0375 (4) | 0.0443 (6) | −0.0002 (3) | 0.0000 (4) | 0.0033 (4) |
| Cu4 | 0.0361 (4) | 0.0427 (4) | 0.0363 (5) | −0.0003 (3) | −0.0013 (4) | 0.0022 (4) |
| S1 | 0.0503 (10) | 0.0279 (7) | 0.0578 (13) | −0.0068 (7) | 0.0034 (10) | −0.0005 (8) |
| S2 | 0.0462 (10) | 0.0256 (8) | 0.0556 (13) | −0.0035 (7) | −0.0002 (9) | −0.0013 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| S3 | 0.0541 (11) | 0.0306 (8) | 0.0598 (14) | 0.0086 (7) | 0.0045 (10) | −0.0009 (9) |
| S4 | 0.0467 (10) | 0.0276 (8) | 0.0502 (12) | 0.0015 (7) | −0.0062 (9) | 0.0039 (8) |
| O1 | 0.059 (3) | 0.030 (2) | 0.066 (4) | −0.011 (2) | −0.001 (3) | −0.001 (3) |
| O2 | 0.063 (3) | 0.028 (2) | 0.061 (4) | −0.0023 (19) | 0.008 (3) | 0.004 (3) |
| O3 | 0.072 (4) | 0.052 (3) | 0.049 (4) | −0.020 (3) | −0.003 (3) | 0.001 (3) |
| O4 | 0.049 (3) | 0.048 (3) | 0.086 (4) | 0.004 (2) | 0.008 (3) | 0.009 (3) |
| O5 | 0.050 (3) | 0.030 (2) | 0.069 (4) | 0.0009 (18) | 0.003 (3) | −0.012 (2) |
| O6 | 0.057 (3) | 0.030 (2) | 0.071 (4) | −0.0073 (19) | 0.003 (3) | 0.001 (3) |
| O7 | 0.045 (3) | 0.048 (3) | 0.078 (4) | −0.005 (2) | 0.003 (3) | −0.014 (3) |
| O8 | 0.077 (4) | 0.048 (3) | 0.056 (4) | −0.010 (3) | −0.008 (3) | 0.004 (3) |
| O9 | 0.070 (3) | 0.029 (2) | 0.072 (4) | 0.008 (2) | 0.002 (3) | 0.004 (3) |
| O10 | 0.087 (4) | 0.025 (2) | 0.069 (4) | 0.007 (2) | −0.001 (3) | −0.003 (3) |
| O11 | 0.076 (4) | 0.057 (3) | 0.055 (4) | 0.020 (3) | 0.003 (3) | −0.004 (3) |
| O12 | 0.057 (3) | 0.062 (3) | 0.094 (5) | 0.002 (2) | 0.016 (3) | −0.001 (3) |
| O13 | 0.051 (3) | 0.029 (2) | 0.066 (4) | −0.0021 (18) | −0.001 (3) | 0.007 (2) |
| O14 | 0.061 (3) | 0.029 (2) | 0.064 (4) | 0.005 (2) | 0.000 (3) | 0.001 (3) |
| O15 | 0.073 (4) | 0.060 (3) | 0.046 (4) | 0.010 (3) | −0.017 (3) | −0.002 (3) |
| O16 | 0.043 (3) | 0.050 (3) | 0.069 (4) | −0.001 (2) | −0.003 (3) | 0.017 (3) |
| N1 | 0.039 (3) | 0.038 (3) | 0.044 (4) | −0.005 (2) | −0.002 (3) | 0.004 (3) |
| N2 | 0.040 (3) | 0.037 (3) | 0.049 (4) | −0.003 (2) | −0.002 (3) | −0.001 (3) |
| N3 | 0.035 (3) | 0.032 (3) | 0.044 (4) | 0.000 (2) | −0.001 (3) | −0.002 (3) |
| N4 | 0.041 (3) | 0.040 (3) | 0.041 (4) | −0.007 (3) | −0.001 (3) | 0.005 (3) |
| N5 | 0.041 (3) | 0.032 (3) | 0.047 (4) | 0.001 (2) | 0.001 (3) | −0.004 (3) |
| N6 | 0.055 (4) | 0.039 (3) | 0.054 (4) | −0.010 (3) | 0.003 (3) | −0.007 (3) |
| N7 | 0.040 (3) | 0.035 (3) | 0.047 (4) | −0.001 (3) | −0.003 (3) | 0.003 (3) |
| N8 | 0.039 (3) | 0.036 (3) | 0.045 (4) | −0.002 (2) | −0.007 (3) | 0.000 (3) |
| N9 | 0.036 (3) | 0.030 (3) | 0.042 (4) | 0.000 (2) | 0.000 (3) | 0.004 (2) |
| N10 | 0.052 (4) | 0.034 (3) | 0.038 (4) | −0.006 (3) | 0.000 (3) | 0.004 (2) |
| N11 | 0.047 (4) | 0.028 (3) | 0.046 (4) | −0.003 (2) | 0.007 (3) | −0.002 (3) |
| N12 | 0.051 (4) | 0.042 (3) | 0.049 (4) | −0.003 (3) | 0.011 (3) | −0.005 (3) |
| N13 | 0.039 (3) | 0.036 (3) | 0.037 (4) | −0.006 (2) | 0.005 (3) | −0.003 (3) |
| N14 | 0.045 (3) | 0.034 (3) | 0.041 (4) | −0.004 (2) | 0.003 (3) | −0.003 (3) |
| N15 | 0.039 (3) | 0.034 (3) | 0.050 (4) | −0.004 (3) | −0.004 (3) | 0.006 (3) |
| N16 | 0.048 (4) | 0.044 (3) | 0.060 (4) | 0.001 (3) | −0.013 (3) | 0.001 (3) |
| N17 | 0.044 (4) | 0.034 (3) | 0.044 (4) | −0.002 (3) | −0.006 (3) | 0.004 (3) |
| N18 | 0.045 (3) | 0.038 (3) | 0.044 (4) | −0.003 (2) | 0.001 (3) | 0.006 (3) |
| N19 | 0.040 (3) | 0.030 (3) | 0.050 (4) | −0.001 (2) | 0.000 (3) | 0.004 (3) |
| N20 | 0.046 (3) | 0.039 (3) | 0.044 (4) | 0.003 (3) | 0.002 (3) | 0.001 (3) |
| N21 | 0.044 (3) | 0.029 (3) | 0.049 (4) | −0.004 (2) | 0.004 (3) | −0.001 (3) |
| N22 | 0.037 (3) | 0.032 (3) | 0.056 (4) | −0.001 (2) | −0.001 (3) | −0.004 (3) |
| N23 | 0.031 (3) | 0.043 (3) | 0.050 (4) | 0.001 (2) | −0.002 (3) | 0.004 (3) |
| N24 | 0.039 (3) | 0.048 (3) | 0.076 (5) | −0.001 (3) | 0.002 (3) | 0.004 (3) |
| N25 | 0.050 (4) | 0.036 (3) | 0.033 (3) | 0.003 (3) | −0.009 (3) | −0.004 (3) |
| N26 | 0.044 (3) | 0.037 (3) | 0.049 (4) | −0.001 (3) | −0.008 (3) | 0.004 (3) |
| N27 | 0.038 (3) | 0.040 (3) | 0.039 (4) | 0.007 (3) | 0.001 (3) | 0.000 (3) |
| N28 | 0.045 (3) | 0.039 (3) | 0.039 (4) | 0.003 (3) | −0.005 (3) | 0.002 (3) |
| N29 | 0.043 (3) | 0.037 (3) | 0.043 (4) | −0.002 (3) | 0.009 (3) | 0.002 (3) |
| N30 | 0.050 (4) | 0.042 (3) | 0.050 (4) | −0.002 (3) | 0.010 (3) | 0.001 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N31 | 0.031 (3) | 0.037 (3) | 0.041 (4) | 0.000 (2) | 0.002 (3) | −0.005 (3) |
| N32 | 0.039 (3) | 0.036 (3) | 0.054 (4) | 0.000 (3) | −0.002 (3) | −0.003 (3) |
| C1 | 0.040 (4) | 0.064 (5) | 0.061 (5) | 0.005 (4) | −0.012 (4) | −0.017 (4) |
| C2 | 0.048 (5) | 0.103 (7) | 0.076 (7) | −0.012 (4) | −0.011 (5) | −0.011 (5) |
| C3 | 0.063 (5) | 0.063 (5) | 0.067 (6) | 0.008 (4) | −0.021 (5) | 0.002 (5) |
| C4 | 0.055 (5) | 0.037 (4) | 0.050 (5) | −0.004 (3) | −0.005 (4) | 0.001 (3) |
| C5 | 0.081 (6) | 0.062 (5) | 0.057 (6) | −0.009 (4) | −0.019 (5) | 0.009 (4) |
| C6 | 0.041 (4) | 0.051 (4) | 0.056 (5) | −0.007 (3) | 0.002 (4) | −0.005 (4) |
| C7 | 0.064 (6) | 0.063 (5) | 0.093 (8) | 0.004 (4) | 0.014 (5) | −0.016 (5) |
| C8 | 0.070 (5) | 0.056 (4) | 0.047 (5) | −0.008 (4) | 0.012 (4) | 0.008 (4) |
| C9 | 0.049 (4) | 0.043 (4) | 0.038 (4) | −0.014 (3) | −0.009 (3) | 0.001 (3) |
| C10 | 0.087 (6) | 0.043 (4) | 0.061 (6) | −0.007 (4) | −0.005 (5) | 0.016 (4) |
| C11 | 0.083 (6) | 0.055 (5) | 0.055 (6) | −0.011 (4) | 0.017 (5) | −0.010 (4) |
| C12 | 0.114 (8) | 0.092 (7) | 0.068 (7) | −0.018 (6) | 0.024 (6) | −0.033 (5) |
| C13 | 0.072 (6) | 0.062 (5) | 0.061 (6) | −0.011 (4) | 0.024 (5) | −0.005 (4) |
| C14 | 0.051 (5) | 0.039 (4) | 0.060 (5) | −0.003 (3) | 0.008 (4) | −0.002 (4) |
| C15 | 0.050 (5) | 0.057 (4) | 0.089 (7) | −0.022 (4) | 0.009 (5) | −0.013 (4) |
| C16 | 0.040 (4) | 0.054 (4) | 0.048 (5) | −0.007 (3) | −0.006 (4) | −0.003 (3) |
| C17 | 0.059 (6) | 0.082 (6) | 0.066 (7) | −0.014 (4) | −0.012 (5) | −0.018 (5) |
| C18 | 0.039 (4) | 0.066 (5) | 0.069 (6) | 0.011 (4) | −0.009 (4) | 0.008 (4) |
| C19 | 0.042 (4) | 0.037 (4) | 0.069 (6) | 0.004 (3) | 0.006 (4) | 0.007 (4) |
| C20 | 0.055 (5) | 0.041 (4) | 0.126 (9) | 0.011 (4) | 0.002 (5) | −0.004 (5) |
| C21 | 0.057 (5) | 0.047 (4) | 0.042 (4) | 0.003 (4) | −0.012 (4) | −0.004 (3) |
| C22 | 0.088 (6) | 0.062 (5) | 0.057 (6) | 0.004 (4) | −0.025 (5) | 0.014 (4) |
| C23 | 0.042 (4) | 0.061 (5) | 0.051 (5) | 0.000 (4) | −0.009 (4) | −0.002 (4) |
| C24 | 0.041 (4) | 0.039 (3) | 0.048 (4) | 0.000 (3) | 0.002 (3) | −0.005 (3) |
| C25 | 0.046 (4) | 0.059 (4) | 0.076 (6) | −0.018 (3) | −0.002 (4) | 0.016 (4) |
| C26 | 0.054 (5) | 0.063 (5) | 0.052 (5) | −0.005 (4) | 0.015 (4) | −0.016 (4) |
| C27 | 0.109 (9) | 0.095 (7) | 0.107 (10) | 0.024 (7) | 0.043 (8) | −0.019 (6) |
| C28 | 0.078 (6) | 0.071 (5) | 0.044 (5) | −0.014 (5) | 0.027 (5) | −0.009 (4) |
| C29 | 0.066 (5) | 0.045 (4) | 0.041 (5) | −0.018 (4) | 0.000 (4) | −0.004 (3) |
| C30 | 0.114 (8) | 0.050 (5) | 0.049 (5) | −0.005 (5) | 0.004 (5) | 0.010 (4) |
| C31 | 0.059 (5) | 0.045 (4) | 0.043 (5) | 0.006 (3) | 0.013 (4) | 0.004 (3) |
| C32 | 0.094 (7) | 0.073 (5) | 0.044 (5) | −0.006 (5) | 0.013 (5) | −0.007 (4) |
| C33 | 0.057 (5) | 0.060 (5) | 0.059 (6) | −0.003 (4) | 0.028 (4) | 0.008 (4) |
| C34 | 0.041 (4) | 0.038 (4) | 0.059 (6) | −0.008 (3) | 0.005 (4) | −0.003 (3) |
| C35 | 0.057 (5) | 0.062 (5) | 0.083 (7) | −0.020 (4) | 0.020 (5) | −0.013 (4) |
| C36 | 0.056 (5) | 0.052 (4) | 0.077 (6) | 0.000 (4) | −0.016 (5) | 0.017 (4) |
| C37 | 0.088 (7) | 0.077 (6) | 0.131 (10) | 0.029 (5) | −0.039 (7) | 0.015 (6) |
| C38 | 0.078 (6) | 0.065 (5) | 0.052 (5) | −0.013 (4) | −0.027 (5) | 0.007 (4) |
| C39 | 0.061 (5) | 0.043 (4) | 0.042 (5) | −0.009 (4) | −0.007 (4) | 0.007 (3) |
| C40 | 0.111 (8) | 0.050 (5) | 0.060 (6) | −0.010 (5) | −0.014 (6) | −0.010 (4) |
| C41 | 0.049 (5) | 0.060 (5) | 0.040 (5) | 0.008 (4) | −0.005 (4) | 0.004 (4) |
| C42 | 0.070 (6) | 0.090 (6) | 0.073 (7) | 0.012 (5) | −0.006 (5) | 0.030 (5) |
| C43 | 0.040 (4) | 0.072 (5) | 0.055 (5) | −0.001 (4) | −0.007 (4) | 0.001 (4) |
| C44 | 0.038 (4) | 0.047 (4) | 0.056 (5) | −0.005 (3) | 0.001 (4) | −0.001 (3) |
| C45 | 0.058 (5) | 0.051 (4) | 0.100 (7) | −0.012 (4) | −0.010 (5) | 0.004 (4) |
| C46 | 0.055 (5) | 0.054 (4) | 0.049 (5) | −0.009 (4) | −0.001 (4) | 0.007 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C47 | 0.098 (7) | 0.086 (6) | 0.050 (5) | −0.002 (5) | 0.001 (5) | 0.026 (5) |
| C48 | 0.044 (4) | 0.063 (5) | 0.062 (6) | −0.004 (4) | 0.017 (4) | −0.002 (4) |
| C49 | 0.038 (4) | 0.032 (3) | 0.060 (5) | −0.004 (3) | 0.004 (4) | −0.002 (3) |
| C50 | 0.043 (4) | 0.050 (4) | 0.104 (7) | 0.006 (4) | 0.017 (5) | 0.004 (4) |
| C51 | 0.040 (4) | 0.043 (4) | 0.065 (6) | 0.003 (3) | 0.010 (4) | 0.009 (4) |
| C52 | 0.059 (6) | 0.073 (6) | 0.084 (8) | −0.013 (4) | 0.016 (5) | 0.019 (5) |
| C53 | 0.046 (4) | 0.061 (5) | 0.048 (5) | 0.005 (4) | 0.005 (4) | 0.000 (4) |
| C54 | 0.049 (4) | 0.037 (4) | 0.050 (5) | 0.003 (3) | 0.001 (4) | −0.004 (3) |
| C55 | 0.102 (7) | 0.047 (5) | 0.068 (7) | −0.017 (4) | 0.009 (5) | −0.014 (4) |
| C56 | 0.047 (5) | 0.061 (5) | 0.099 (8) | −0.009 (4) | −0.026 (5) | 0.032 (5) |
| C57 | 0.065 (6) | 0.100 (7) | 0.149 (11) | 0.012 (6) | −0.035 (7) | 0.023 (7) |
| C58 | 0.085 (7) | 0.069 (6) | 0.081 (7) | −0.019 (5) | −0.038 (6) | 0.001 (5) |
| C59 | 0.058 (5) | 0.046 (4) | 0.055 (5) | −0.006 (4) | −0.017 (4) | 0.003 (4) |
| C60 | 0.082 (6) | 0.074 (6) | 0.072 (7) | −0.002 (5) | −0.010 (5) | −0.016 (5) |
| C61 | 0.057 (5) | 0.058 (5) | 0.060 (5) | −0.001 (4) | −0.016 (4) | −0.013 (4) |
| C62 | 0.081 (7) | 0.097 (7) | 0.109 (9) | −0.038 (6) | −0.028 (6) | −0.012 (6) |
| C63 | 0.066 (5) | 0.055 (5) | 0.065 (6) | 0.013 (4) | −0.037 (5) | −0.008 (4) |
| C64 | 0.066 (5) | 0.042 (4) | 0.042 (5) | 0.012 (4) | −0.011 (4) | 0.001 (3) |
| C65 | 0.122 (8) | 0.053 (5) | 0.055 (6) | 0.002 (5) | −0.022 (6) | 0.016 (4) |
| C66 | 0.055 (5) | 0.041 (4) | 0.046 (5) | −0.007 (3) | 0.004 (4) | −0.011 (3) |
| C67 | 0.080 (6) | 0.076 (5) | 0.047 (5) | −0.006 (4) | 0.003 (4) | 0.004 (4) |
| C68 | 0.044 (4) | 0.064 (5) | 0.056 (5) | 0.000 (4) | 0.011 (4) | −0.014 (4) |
| C69 | 0.041 (4) | 0.036 (4) | 0.050 (5) | 0.001 (3) | 0.001 (4) | −0.005 (3) |
| C70 | 0.057 (5) | 0.057 (5) | 0.086 (7) | 0.021 (4) | 0.001 (5) | 0.005 (4) |
| C71 | 0.063 (5) | 0.046 (4) | 0.040 (5) | 0.010 (4) | 0.004 (4) | 0.002 (3) |
| C72 | 0.119 (8) | 0.054 (5) | 0.066 (6) | −0.005 (5) | 0.012 (6) | −0.009 (5) |
| C73 | 0.078 (6) | 0.069 (5) | 0.043 (5) | 0.010 (4) | 0.017 (5) | 0.003 (4) |
| C74 | 0.057 (5) | 0.056 (5) | 0.061 (6) | 0.007 (4) | 0.016 (4) | 0.011 (4) |
| C75 | 0.078 (7) | 0.084 (6) | 0.096 (8) | −0.021 (5) | 0.030 (6) | 0.017 (5) |
| C76 | 0.050 (5) | 0.048 (4) | 0.059 (5) | −0.012 (4) | −0.007 (4) | −0.004 (4) |
| C77 | 0.073 (7) | 0.072 (6) | 0.126 (9) | −0.020 (5) | −0.015 (6) | −0.033 (6) |
| C78 | 0.040 (4) | 0.059 (5) | 0.065 (6) | 0.002 (4) | −0.012 (4) | 0.003 (4) |
| C79 | 0.038 (4) | 0.041 (4) | 0.055 (5) | 0.005 (3) | 0.002 (4) | 0.005 (3) |
| C80 | 0.051 (5) | 0.058 (4) | 0.095 (7) | 0.018 (3) | 0.003 (5) | −0.012 (5) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| Cu1—O1 | 2.289 (4) | C17—H17B | 0.9600 |
| Cu1—O14$^{i}$ | 2.438 (4) | C17—H17C | 0.9600 |
| Cu1—N1 | 2.039 (6) | C18—H18A | 0.9300 |
| Cu1—N3 | 2.054 (6) | C18—C19 | 1.379 (11) |
| Cu1—N5 | 2.033 (6) | C19—C20 | 1.510 (10) |
| Cu1—N7 | 2.028 (6) | C20—H20A | 0.9600 |
| Cu2—O2 | 2.395 (4) | C20—H20B | 0.9602 |
| Cu2—O5 | 2.341 (4) | C20—H20C | 0.9599 |
| Cu2—N9 | 2.033 (6) | C21—C22 | 1.504 (10) |
| Cu2—N11 | 2.042 (6) | C21—C23 | 1.358 (10) |
| Cu2—N13 | 2.031 (6) | C22—H22A | 0.9600 |

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|---|---|---|---|
| Cu2—N15 | 2.028 (6) | C22—H22B | 0.9600 |
| Cu3—O6 | 2.367 (4) | C22—H22C | 0.9600 |
| Cu3—O9 | 2.341 (4) | C23—H23 | 0.9300 |
| Cu3—N17 | 2.041 (6) | C23—C24 | 1.401 (10) |
| Cu3—N19 | 2.044 (6) | C24—C25 | 1.487 (9) |
| Cu3—N21 | 2.040 (6) | C25—H25A | 0.9600 |
| Cu3—N23 | 2.058 (6) | C25—H25B | 0.9600 |
| Cu4—O10 | 2.435 (4) | C25—H25C | 0.9600 |
| Cu4—O13 | 2.339 (4) | C26—C27 | 1.504 (11) |
| Cu4—N25 | 2.014 (6) | C26—C28 | 1.364 (11) |
| Cu4—N27 | 2.045 (6) | C27—H27A | 0.9602 |
| Cu4—N29 | 2.031 (6) | C27—H27B | 0.9598 |
| Cu4—N31 | 2.030 (6) | C27—H27C | 0.9597 |
| S1—O1 | 1.468 (5) | C28—H28A | 0.9300 |
| S1—O2 | 1.465 (4) | C28—C29 | 1.403 (11) |
| S1—O3 | 1.477 (6) | C29—C30 | 1.493 (10) |
| S1—O4 | 1.462 (5) | C30—H30A | 0.9600 |
| S2—O5 | 1.465 (5) | C30—H30B | 0.9600 |
| S2—O6 | 1.456 (5) | C30—H30C | 0.9600 |
| S2—O7 | 1.475 (5) | C31—C32 | 1.504 (10) |
| S2—O8 | 1.463 (6) | C31—C33 | 1.369 (10) |
| S3—O9 | 1.468 (5) | C32—H32A | 0.9599 |
| S3—O10 | 1.463 (5) | C32—H32B | 0.9602 |
| S3—O11 | 1.465 (6) | C32—H32C | 0.9600 |
| S3—O12 | 1.465 (5) | C33—H33 | 0.9300 |
| S4—O13 | 1.475 (5) | C33—C34 | 1.398 (11) |
| S4—O14 | 1.466 (5) | C34—C35 | 1.492 (10) |
| S4—O15 | 1.459 (6) | C35—H35A | 0.9600 |
| S4—O16 | 1.473 (5) | C35—H35B | 0.9600 |
| N1—N2 | 1.373 (7) | C35—H35C | 0.9599 |
| N1—C4 | 1.339 (9) | C36—C37 | 1.506 (10) |
| N2—H2 | 0.8600 | C36—C38 | 1.374 (11) |
| N2—C1 | 1.338 (9) | C37—H37A | 0.9596 |
| N3—N4 | 1.361 (7) | C37—H37B | 0.9601 |
| N3—C9 | 1.338 (9) | C37—H37C | 0.9604 |
| N4—H4 | 0.8600 | C38—H38 | 0.9300 |
| N4—C6 | 1.325 (9) | C38—C39 | 1.387 (11) |
| N5—N6 | 1.351 (8) | C39—C40 | 1.477 (11) |
| N5—C14 | 1.325 (9) | C40—H40A | 0.9601 |
| N6—H6 | 0.8600 | C40—H40B | 0.9599 |
| N6—C11 | 1.343 (10) | C40—H40C | 0.9598 |
| N7—N8 | 1.365 (7) | C41—C42 | 1.500 (10) |
| N7—C19 | 1.325 (9) | C41—C43 | 1.364 (10) |
| N8—H8 | 0.8600 | C42—H42A | 0.9600 |
| N8—C16 | 1.341 (9) | C42—H42B | 0.9600 |
| N9—N10 | 1.358 (7) | C42—H42C | 0.9600 |
| N9—C24 | 1.337 (8) | C43—H43 | 0.9300 |
| N10—H10 | 0.8600 | C43—C44 | 1.395 (10) |

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|---|---|---|---|
| N10—C21 | 1.326 (9) | C44—C45 | 1.505 (10) |
| N11—N12 | 1.347 (7) | C45—H45A | 0.9601 |
| N11—C29 | 1.335 (9) | C45—H45B | 0.9600 |
| N12—H12 | 0.8600 | C45—H45C | 0.9601 |
| N12—C26 | 1.352 (9) | C46—C47 | 1.503 (10) |
| N13—N14 | 1.347 (7) | C46—C48 | 1.371 (10) |
| N13—C34 | 1.345 (8) | C47—H47A | 0.9598 |
| N14—H14 | 0.8600 | C47—H47B | 0.9607 |
| N14—C31 | 1.322 (9) | C47—H47C | 0.9599 |
| N15—N16 | 1.362 (7) | C48—H48 | 0.9300 |
| N15—C39 | 1.333 (9) | C48—C49 | 1.387 (11) |
| N16—H16 | 0.8600 | C49—C50 | 1.495 (10) |
| N16—C36 | 1.326 (9) | C50—H50A | 0.9600 |
| N17—N18 | 1.341 (7) | C50—H50B | 0.9600 |
| N17—C44 | 1.341 (8) | C50—H50C | 0.9600 |
| N18—H18 | 0.8600 | C51—C52 | 1.499 (10) |
| N18—C41 | 1.327 (9) | C51—C53 | 1.372 (10) |
| N19—N20 | 1.355 (7) | C52—H52A | 0.9600 |
| N19—C49 | 1.315 (9) | C52—H52B | 0.9599 |
| N20—H20 | 0.8600 | C52—H52C | 0.9609 |
| N20—C46 | 1.318 (9) | C53—H53 | 0.9300 |
| N21—N22 | 1.355 (7) | C53—C54 | 1.371 (10) |
| N21—C54 | 1.342 (9) | C54—C55 | 1.524 (10) |
| N22—H22 | 0.8600 | C55—H55A | 0.9600 |
| N22—C51 | 1.316 (9) | C55—H55B | 0.9600 |
| N23—N24 | 1.346 (7) | C55—H55C | 0.9600 |
| N23—C59 | 1.324 (10) | C56—C57 | 1.512 (11) |
| N24—H24 | 0.8600 | C56—C58 | 1.387 (13) |
| N24—C56 | 1.341 (10) | C57—H57A | 0.9605 |
| N25—N26 | 1.344 (7) | C57—H57B | 0.9602 |
| N25—C64 | 1.355 (9) | C57—H57C | 0.9599 |
| N26—H26 | 0.8600 | C58—H58 | 0.9300 |
| N26—C61 | 1.340 (9) | C58—C59 | 1.371 (11) |
| N27—N28 | 1.373 (7) | C59—C60 | 1.494 (11) |
| N27—C69 | 1.331 (8) | C60—H60A | 0.9599 |
| N28—H28 | 0.8600 | C60—H60B | 0.9604 |
| N28—C66 | 1.327 (9) | C60—H60C | 0.9597 |
| N29—N30 | 1.363 (7) | C61—C62 | 1.512 (11) |
| N29—C71 | 1.319 (9) | C61—C63 | 1.355 (11) |
| N30—H30 | 0.8600 | C62—H62A | 0.9600 |
| N30—C74 | 1.332 (10) | C62—H62B | 0.9600 |
| N31—N32 | 1.350 (7) | C62—H62C | 0.9600 |
| N31—C79 | 1.354 (8) | C63—H63 | 0.9300 |
| N32—H32 | 0.8600 | C63—C64 | 1.396 (10) |
| N32—C76 | 1.341 (9) | C64—C65 | 1.490 (11) |
| C1—C2 | 1.490 (10) | C65—H65A | 0.9599 |
| C1—C3 | 1.364 (11) | C65—H65B | 0.9603 |
| C2—H2A | 0.9605 | C65—H65C | 0.9604 |

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|---|---|---|---|
| C2—H2B | 0.9601 | C66—C67 | 1.453 (10) |
| C2—H2C | 0.9600 | C66—C68 | 1.382 (10) |
| C3—H3 | 0.9300 | C67—H67A | 0.9600 |
| C3—C4 | 1.400 (11) | C67—H67B | 0.9599 |
| C4—C5 | 1.482 (10) | C67—H67C | 0.9605 |
| C5—H5A | 0.9599 | C68—H68 | 0.9300 |
| C5—H5B | 0.9605 | C68—C69 | 1.369 (11) |
| C5—H5C | 0.9609 | C69—C70 | 1.492 (10) |
| C6—C7 | 1.504 (10) | C70—H70A | 0.9603 |
| C6—C8 | 1.366 (10) | C70—H70B | 0.9599 |
| C7—H7A | 0.9604 | C70—H70C | 0.9599 |
| C7—H7B | 0.9602 | C71—C72 | 1.516 (11) |
| C7—H7C | 0.9599 | C71—C73 | 1.385 (10) |
| C8—H8A | 0.9300 | C72—H72A | 0.9603 |
| C8—C9 | 1.386 (10) | C72—H72B | 0.9601 |
| C9—C10 | 1.482 (10) | C72—H72C | 0.9600 |
| C10—H10A | 0.9600 | C73—H73 | 0.9300 |
| C10—H10B | 0.9600 | C73—C74 | 1.369 (11) |
| C10—H10C | 0.9600 | C74—C75 | 1.501 (11) |
| C11—C12 | 1.505 (11) | C75—H75A | 0.9600 |
| C11—C13 | 1.368 (11) | C75—H75B | 0.9596 |
| C12—H12A | 0.9596 | C75—H75C | 0.9600 |
| C12—H12B | 0.9600 | C76—C77 | 1.505 (11) |
| C12—H12C | 0.9604 | C76—C78 | 1.365 (10) |
| C13—H13 | 0.9300 | C77—H77A | 0.9602 |
| C13—C14 | 1.381 (11) | C77—H77B | 0.9601 |
| C14—C15 | 1.502 (10) | C77—H77C | 0.9598 |
| C15—H15A | 0.9599 | C78—H78 | 0.9300 |
| C15—H15B | 0.9606 | C78—C79 | 1.393 (10) |
| C15—H15C | 0.9597 | C79—C80 | 1.490 (9) |
| C16—C17 | 1.495 (11) | C80—H80A | 0.9599 |
| C16—C18 | 1.378 (10) | C80—H80B | 0.9599 |
| C17—H17A | 0.9600 | C80—H80C | 0.9600 |

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| O1—Cu1—O14$^{i}$ | 179.5 (2) | C16—C18—C19 | 106.3 (6) |
| N1—Cu1—O1 | 90.64 (19) | C19—C18—H18A | 126.8 |
| N1—Cu1—O14$^{i}$ | 88.90 (19) | N7—C19—C18 | 111.0 (6) |
| N1—Cu1—N3 | 88.0 (2) | N7—C19—C20 | 120.5 (7) |
| N3—Cu1—O1 | 91.7 (2) | C18—C19—C20 | 128.5 (7) |
| N3—Cu1—O14$^{i}$ | 88.2 (2) | C19—C20—H20A | 109.4 |
| N5—Cu1—O1 | 86.5 (2) | C19—C20—H20B | 109.5 |
| N5—Cu1—O14$^{i}$ | 93.6 (2) | C19—C20—H20C | 109.5 |
| N5—Cu1—N1 | 90.6 (2) | H20A—C20—H20B | 109.5 |
| N5—Cu1—N3 | 177.7 (2) | H20A—C20—H20C | 109.5 |
| N7—Cu1—O1 | 96.5 (2) | H20B—C20—H20C | 109.5 |
| N7—Cu1—O14$^{i}$ | 83.98 (19) | N10—C21—C22 | 120.4 (7) |
| N7—Cu1—N1 | 172.8 (2) | N10—C21—C23 | 106.4 (6) |
| N7—Cu1—N3 | 90.4 (2) | C23—C21—C22 | 133.2 (7) |

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| N7—Cu1—N5 | 91.2 (2) | C21—C22—H22A | 109.5 |
| O5—Cu2—O2 | 178.8 (2) | C21—C22—H22B | 109.5 |
| N9—Cu2—O2 | 89.05 (19) | C21—C22—H22C | 109.5 |
| N9—Cu2—O5 | 89.76 (19) | H22A—C22—H22B | 109.5 |
| N9—Cu2—N11 | 87.6 (2) | H22A—C22—H22C | 109.5 |
| N11—Cu2—O2 | 84.0 (2) | H22B—C22—H22C | 109.5 |
| N11—Cu2—O5 | 96.0 (2) | C21—C23—H23 | 126.8 |
| N13—Cu2—O2 | 89.1 (2) | C21—C23—C24 | 106.4 (6) |
| N13—Cu2—O5 | 90.9 (2) | C24—C23—H23 | 126.8 |
| N13—Cu2—N9 | 89.1 (2) | N9—C24—C23 | 109.7 (6) |
| N13—Cu2—N11 | 172.4 (2) | N9—C24—C25 | 123.6 (6) |
| N15—Cu2—O2 | 94.08 (19) | C23—C24—C25 | 126.6 (7) |
| N15—Cu2—O5 | 87.11 (19) | C24—C25—H25A | 109.5 |
| N15—Cu2—N9 | 176.5 (2) | C24—C25—H25B | 109.5 |
| N15—Cu2—N11 | 91.2 (2) | C24—C25—H25C | 109.5 |
| N15—Cu2—N13 | 92.4 (2) | H25A—C25—H25B | 109.5 |
| O9—Cu3—O6 | 177.2 (3) | H25A—C25—H25C | 109.5 |
| N17—Cu3—O6 | 85.2 (2) | H25B—C25—H25C | 109.5 |
| N17—Cu3—O9 | 97.2 (2) | N12—C26—C27 | 119.2 (8) |
| N17—Cu3—N19 | 89.8 (2) | N12—C26—C28 | 107.0 (7) |
| N17—Cu3—N23 | 173.2 (2) | C28—C26—C27 | 133.8 (8) |
| N19—Cu3—O6 | 92.5 (2) | C26—C27—H27A | 109.7 |
| N19—Cu3—O9 | 86.0 (2) | C26—C27—H27B | 109.6 |
| N19—Cu3—N23 | 90.1 (2) | C26—C27—H27C | 109.1 |
| N21—Cu3—O6 | 91.7 (2) | H27A—C27—H27B | 109.5 |
| N21—Cu3—O9 | 89.9 (2) | H27A—C27—H27C | 109.5 |
| N21—Cu3—N17 | 89.4 (2) | H27B—C27—H27C | 109.5 |
| N21—Cu3—N19 | 175.7 (2) | C26—C28—H28A | 126.8 |
| N21—Cu3—N23 | 91.3 (2) | C26—C28—C29 | 106.3 (7) |
| N23—Cu3—O6 | 88.1 (2) | C29—C28—H28A | 126.8 |
| N23—Cu3—O9 | 89.6 (2) | N11—C29—C28 | 109.0 (7) |
| O13—Cu4—O10 | 178.39 (17) | N11—C29—C30 | 122.0 (7) |
| N25—Cu4—O10 | 96.2 (2) | C28—C29—C30 | 129.0 (7) |
| N25—Cu4—O13 | 84.87 (19) | C29—C30—H30A | 109.5 |
| N25—Cu4—N27 | 89.7 (2) | C29—C30—H30B | 109.5 |
| N25—Cu4—N29 | 91.8 (2) | C29—C30—H30C | 109.5 |
| N25—Cu4—N31 | 175.6 (2) | H30A—C30—H30B | 109.5 |
| N27—Cu4—O10 | 88.1 (2) | H30A—C30—H30C | 109.5 |
| N27—Cu4—O13 | 93.1 (2) | H30B—C30—H30C | 109.5 |
| N29—Cu4—O10 | 83.4 (2) | N14—C31—C32 | 121.3 (7) |
| N29—Cu4—O13 | 95.3 (2) | N14—C31—C33 | 105.4 (7) |
| N29—Cu4—N27 | 171.5 (2) | C33—C31—C32 | 133.2 (7) |
| N31—Cu4—O10 | 88.2 (2) | C31—C32—H32A | 109.3 |
| N31—Cu4—O13 | 90.79 (19) | C31—C32—H32B | 109.6 |
| N31—Cu4—N27 | 89.9 (2) | C31—C32—H32C | 109.5 |
| N31—Cu4—N29 | 89.2 (2) | H32A—C32—H32B | 109.5 |
| O1—S1—O3 | 108.0 (3) | H32A—C32—H32C | 109.5 |
| O2—S1—O1 | 110.5 (3) | H32B—C32—H32C | 109.5 |

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| O2—S1—O3 | 109.7 (4) | C31—C33—H33 | 126.5 |
| O4—S1—O1 | 110.5 (3) | C31—C33—C34 | 107.0 (7) |
| O4—S1—O2 | 108.0 (3) | C34—C33—H33 | 126.5 |
| O4—S1—O3 | 110.1 (4) | N13—C34—C33 | 109.0 (6) |
| O5—S2—O7 | 108.4 (3) | N13—C34—C35 | 123.4 (7) |
| O6—S2—O5 | 110.2 (3) | C33—C34—C35 | 127.6 (7) |
| O6—S2—O7 | 109.1 (3) | C34—C35—H35A | 109.4 |
| O6—S2—O8 | 108.4 (3) | C34—C35—H35B | 109.4 |
| O8—S2—O5 | 110.2 (3) | C34—C35—H35C | 109.6 |
| O8—S2—O7 | 110.4 (4) | H35A—C35—H35B | 109.5 |
| O10—S3—O9 | 109.5 (3) | H35A—C35—H35C | 109.5 |
| O10—S3—O11 | 109.3 (4) | H35B—C35—H35C | 109.5 |
| O10—S3—O12 | 108.3 (3) | N16—C36—C37 | 122.1 (8) |
| O11—S3—O9 | 108.7 (4) | N16—C36—C38 | 106.4 (7) |
| O11—S3—O12 | 110.5 (4) | C38—C36—C37 | 131.5 (9) |
| O12—S3—O9 | 110.4 (3) | C36—C37—H37A | 109.4 |
| O14—S4—O13 | 110.2 (3) | C36—C37—H37B | 109.6 |
| O14—S4—O16 | 109.1 (3) | C36—C37—H37C | 109.5 |
| O15—S4—O13 | 110.9 (3) | H37A—C37—H37B | 109.5 |
| O15—S4—O14 | 108.6 (3) | H37A—C37—H37C | 109.5 |
| O15—S4—O16 | 110.3 (4) | H37B—C37—H37C | 109.4 |
| O16—S4—O13 | 107.7 (3) | C36—C38—H38 | 126.4 |
| S1—O1—Cu1 | 141.5 (3) | C36—C38—C39 | 107.2 (7) |
| S1—O2—Cu2 | 150.2 (3) | C39—C38—H38 | 126.4 |
| S2—O5—Cu2 | 140.8 (3) | N15—C39—C38 | 108.7 (7) |
| S2—O6—Cu3 | 146.0 (3) | N15—C39—C40 | 122.1 (7) |
| S3—O9—Cu3 | 143.0 (3) | C38—C39—C40 | 129.2 (8) |
| S3—O10—Cu4 | 148.4 (4) | C39—C40—H40A | 109.4 |
| S4—O13—Cu4 | 138.1 (3) | C39—C40—H40B | 109.5 |
| Cu1$^{ii}$—O14—Cu1$^{i}$ | 175.78 (12) | C39—C40—H40C | 109.5 |
| S4—O14—Cu1$^{i}$ | 26.2 (2) | H40A—C40—H40B | 109.5 |
| S4—O14—Cu1$^{ii}$ | 151.4 (3) | H40A—C40—H40C | 109.5 |
| N2—N1—Cu1 | 119.1 (4) | H40B—C40—H40C | 109.5 |
| C4—N1—Cu1 | 135.0 (5) | N18—C41—C42 | 122.1 (7) |
| C4—N1—N2 | 105.4 (6) | N18—C41—C43 | 105.9 (6) |
| N1—N2—H2 | 124.3 | C43—C41—C42 | 132.0 (8) |
| C1—N2—N1 | 111.5 (6) | C41—C42—H42A | 109.5 |
| C1—N2—H2 | 124.3 | C41—C42—H42B | 109.5 |
| N4—N3—Cu1 | 117.0 (4) | C41—C42—H42C | 109.5 |
| C9—N3—Cu1 | 137.1 (5) | H42A—C42—H42B | 109.5 |
| C9—N3—N4 | 105.9 (6) | H42A—C42—H42C | 109.5 |
| N3—N4—H4 | 124.2 | H42B—C42—H42C | 109.5 |
| C6—N4—N3 | 111.6 (6) | C41—C43—H43 | 126.7 |
| C6—N4—H4 | 124.2 | C41—C43—C44 | 106.7 (7) |
| N6—N5—Cu1 | 116.9 (4) | C44—C43—H43 | 126.7 |
| C14—N5—Cu1 | 137.0 (5) | N17—C44—C43 | 109.1 (6) |
| C14—N5—N6 | 105.7 (6) | N17—C44—C45 | 122.3 (7) |
| N5—N6—H6 | 123.9 | C43—C44—C45 | 128.6 (7) |

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| C11—N6—N5 | 112.3 (6) | C44—C45—H45A | 109.4 |
| C11—N6—H6 | 123.9 | C44—C45—H45B | 109.5 |
| N8—N7—Cu1 | 117.5 (4) | C44—C45—H45C | 109.5 |
| C19—N7—Cu1 | 137.5 (5) | H45A—C45—H45B | 109.5 |
| C19—N7—N8 | 104.8 (6) | H45A—C45—H45C | 109.5 |
| N7—N8—H8 | 124.0 | H45B—C45—H45C | 109.5 |
| C16—N8—N7 | 112.0 (6) | N20—C46—C47 | 122.3 (7) |
| C16—N8—H8 | 124.0 | N20—C46—C48 | 106.4 (7) |
| N10—N9—Cu2 | 118.5 (4) | C48—C46—C47 | 131.2 (8) |
| C24—N9—Cu2 | 135.4 (5) | C46—C47—H47A | 109.5 |
| C24—N9—N10 | 104.5 (5) | C46—C47—H47B | 109.4 |
| N9—N10—H10 | 123.6 | C46—C47—H47C | 109.6 |
| C21—N10—N9 | 112.9 (6) | H47A—C47—H47B | 109.4 |
| C21—N10—H10 | 123.6 | H47A—C47—H47C | 109.5 |
| N12—N11—Cu2 | 116.3 (4) | H47B—C47—H47C | 109.4 |
| C29—N11—Cu2 | 136.8 (5) | C46—C48—H48 | 126.9 |
| C29—N11—N12 | 106.9 (6) | C46—C48—C49 | 106.2 (7) |
| N11—N12—H12 | 124.6 | C49—C48—H48 | 126.9 |
| N11—N12—C26 | 110.8 (6) | N19—C49—C48 | 109.7 (6) |
| C26—N12—H12 | 124.6 | N19—C49—C50 | 121.5 (7) |
| N14—N13—Cu2 | 118.9 (4) | C48—C49—C50 | 128.8 (7) |
| C34—N13—Cu2 | 135.7 (5) | C49—C50—H50A | 109.5 |
| C34—N13—N14 | 104.7 (6) | C49—C50—H50B | 109.5 |
| N13—N14—H14 | 123.1 | C49—C50—H50C | 109.5 |
| C31—N14—N13 | 113.9 (6) | H50A—C50—H50B | 109.5 |
| C31—N14—H14 | 123.1 | H50A—C50—H50C | 109.5 |
| N16—N15—Cu2 | 117.2 (5) | H50B—C50—H50C | 109.5 |
| C39—N15—Cu2 | 136.0 (5) | N22—C51—C52 | 122.4 (7) |
| C39—N15—N16 | 106.5 (6) | N22—C51—C53 | 106.0 (6) |
| N15—N16—H16 | 124.4 | C53—C51—C52 | 131.5 (8) |
| C36—N16—N15 | 111.3 (6) | C51—C52—H52A | 109.4 |
| C36—N16—H16 | 124.4 | C51—C52—H52B | 109.5 |
| N18—N17—Cu3 | 119.4 (4) | C51—C52—H52C | 109.5 |
| C44—N17—Cu3 | 135.2 (5) | H52A—C52—H52B | 109.5 |
| C44—N17—N18 | 105.1 (6) | H52A—C52—H52C | 109.5 |
| N17—N18—H18 | 123.4 | H52B—C52—H52C | 109.5 |
| C41—N18—N17 | 113.1 (6) | C51—C53—H53 | 126.9 |
| C41—N18—H18 | 123.4 | C51—C53—C54 | 106.3 (7) |
| N20—N19—Cu3 | 116.8 (4) | C54—C53—H53 | 126.9 |
| C49—N19—Cu3 | 137.3 (5) | N21—C54—C53 | 110.6 (6) |
| C49—N19—N20 | 105.9 (6) | N21—C54—C55 | 121.8 (7) |
| N19—N20—H20 | 124.1 | C53—C54—C55 | 127.6 (7) |
| C46—N20—N19 | 111.8 (6) | C54—C55—H55A | 109.5 |
| C46—N20—H20 | 124.1 | C54—C55—H55B | 109.5 |
| N22—N21—Cu3 | 119.5 (4) | C54—C55—H55C | 109.5 |
| C54—N21—Cu3 | 135.7 (5) | H55A—C55—H55B | 109.5 |
| C54—N21—N22 | 103.7 (6) | H55A—C55—H55C | 109.5 |
| N21—N22—H22 | 123.4 | H55B—C55—H55C | 109.5 |

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| C51—N22—N21 | 113.2 (6) | N24—C56—C57 | 121.8 (10) |
| C51—N22—H22 | 123.4 | N24—C56—C58 | 105.5 (7) |
| N24—N23—Cu3 | 119.3 (5) | C58—C56—C57 | 132.6 (9) |
| C59—N23—Cu3 | 135.0 (5) | C56—C57—H57A | 109.4 |
| C59—N23—N24 | 105.7 (6) | C56—C57—H57B | 109.4 |
| N23—N24—H24 | 124.0 | C56—C57—H57C | 109.7 |
| C56—N24—N23 | 111.9 (7) | H57A—C57—H57B | 109.5 |
| C56—N24—H24 | 124.0 | H57A—C57—H57C | 109.4 |
| N26—N25—Cu4 | 119.4 (4) | H57B—C57—H57C | 109.5 |
| N26—N25—C64 | 105.1 (6) | C56—C58—H58 | 126.9 |
| C64—N25—Cu4 | 135.5 (5) | C59—C58—C56 | 106.2 (8) |
| N25—N26—H26 | 123.6 | C59—C58—H58 | 126.9 |
| C61—N26—N25 | 112.8 (6) | N23—C59—C58 | 110.7 (8) |
| C61—N26—H26 | 123.6 | N23—C59—C60 | 123.7 (7) |
| N28—N27—Cu4 | 118.3 (4) | C58—C59—C60 | 125.6 (8) |
| C69—N27—Cu4 | 135.8 (5) | C59—C60—H60A | 109.4 |
| C69—N27—N28 | 105.9 (6) | C59—C60—H60B | 109.5 |
| N27—N28—H28 | 123.9 | C59—C60—H60C | 109.5 |
| C66—N28—N27 | 112.2 (6) | H60A—C60—H60B | 109.5 |
| C66—N28—H28 | 123.9 | H60A—C60—H60C | 109.5 |
| N30—N29—Cu4 | 117.1 (4) | H60B—C60—H60C | 109.5 |
| C71—N29—Cu4 | 138.3 (5) | N26—C61—C62 | 121.3 (8) |
| C71—N29—N30 | 104.5 (6) | N26—C61—C63 | 105.9 (7) |
| N29—N30—H30 | 124.0 | C63—C61—C62 | 132.8 (8) |
| C74—N30—N29 | 112.0 (6) | C61—C62—H62A | 109.5 |
| C74—N30—H30 | 124.0 | C61—C62—H62B | 109.5 |
| N32—N31—Cu4 | 119.4 (4) | C61—C62—H62C | 109.5 |
| N32—N31—C79 | 105.4 (5) | H62A—C62—H62B | 109.5 |
| C79—N31—Cu4 | 134.2 (5) | H62A—C62—H62C | 109.5 |
| N31—N32—H32 | 123.9 | H62B—C62—H62C | 109.5 |
| C76—N32—N31 | 112.3 (6) | C61—C63—H63 | 126.2 |
| C76—N32—H32 | 123.9 | C61—C63—C64 | 107.6 (7) |
| N2—C1—C2 | 119.3 (8) | C64—C63—H63 | 126.2 |
| N2—C1—C3 | 106.9 (7) | N25—C64—C63 | 108.6 (7) |
| C3—C1—C2 | 133.8 (8) | N25—C64—C65 | 121.0 (7) |
| C1—C2—H2A | 109.3 | C63—C64—C65 | 130.4 (7) |
| C1—C2—H2B | 109.4 | C64—C65—H65A | 109.6 |
| C1—C2—H2C | 109.6 | C64—C65—H65B | 109.5 |
| H2A—C2—H2B | 109.5 | C64—C65—H65C | 109.4 |
| H2A—C2—H2C | 109.5 | H65A—C65—H65B | 109.5 |
| H2B—C2—H2C | 109.5 | H65A—C65—H65C | 109.5 |
| C1—C3—H3 | 126.6 | H65B—C65—H65C | 109.5 |
| C1—C3—C4 | 106.8 (7) | N28—C66—C67 | 123.4 (7) |
| C4—C3—H3 | 126.6 | N28—C66—C68 | 104.4 (7) |
| N1—C4—C3 | 109.5 (7) | C68—C66—C67 | 132.1 (8) |
| N1—C4—C5 | 123.2 (7) | C66—C67—H67A | 109.7 |
| C3—C4—C5 | 127.3 (8) | C66—C67—H67B | 109.4 |
| C4—C5—H5A | 109.4 | C66—C67—H67C | 109.4 |

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| C4—C5—H5B | 109.6 | H67A—C67—H67B | 109.5 |
| C4—C5—H5C | 109.6 | H67A—C67—H67C | 109.5 |
| H5A—C5—H5B | 109.5 | H67B—C67—H67C | 109.5 |
| H5A—C5—H5C | 109.5 | C66—C68—H68 | 125.5 |
| H5B—C5—H5C | 109.3 | C69—C68—C66 | 109.1 (7) |
| N4—C6—C7 | 121.2 (7) | C69—C68—H68 | 125.5 |
| N4—C6—C8 | 106.6 (7) | N27—C69—C68 | 108.4 (7) |
| C8—C6—C7 | 132.1 (8) | N27—C69—C70 | 121.9 (7) |
| C6—C7—H7A | 109.4 | C68—C69—C70 | 129.7 (7) |
| C6—C7—H7B | 109.6 | C69—C70—H70A | 109.4 |
| C6—C7—H7C | 109.5 | C69—C70—H70B | 109.4 |
| H7A—C7—H7B | 109.4 | C69—C70—H70C | 109.6 |
| H7A—C7—H7C | 109.5 | H70A—C70—H70B | 109.5 |
| H7B—C7—H7C | 109.5 | H70A—C70—H70C | 109.5 |
| C6—C8—H8A | 126.4 | H70B—C70—H70C | 109.5 |
| C6—C8—C9 | 107.2 (7) | N29—C71—C72 | 120.3 (7) |
| C9—C8—H8A | 126.4 | N29—C71—C73 | 111.4 (7) |
| N3—C9—C8 | 108.8 (6) | C73—C71—C72 | 128.3 (7) |
| N3—C9—C10 | 122.6 (7) | C71—C72—H72A | 109.5 |
| C8—C9—C10 | 128.6 (7) | C71—C72—H72B | 109.5 |
| C9—C10—H10A | 109.1 | C71—C72—H72C | 109.5 |
| C9—C10—H10B | 109.8 | H72A—C72—H72B | 109.4 |
| C9—C10—H10C | 109.6 | H72A—C72—H72C | 109.5 |
| H10A—C10—H10B | 109.5 | H72B—C72—H72C | 109.5 |
| H10A—C10—H10C | 109.5 | C71—C73—H73 | 127.2 |
| H10B—C10—H10C | 109.5 | C74—C73—C71 | 105.6 (7) |
| N6—C11—C12 | 121.8 (7) | C74—C73—H73 | 127.2 |
| N6—C11—C13 | 104.9 (7) | N30—C74—C73 | 106.6 (7) |
| C13—C11—C12 | 133.3 (8) | N30—C74—C75 | 121.0 (8) |
| C11—C12—H12A | 109.6 | C73—C74—C75 | 132.4 (8) |
| C11—C12—H12B | 109.4 | C74—C75—H75A | 109.4 |
| C11—C12—H12C | 109.5 | C74—C75—H75B | 109.7 |
| H12A—C12—H12B | 109.5 | C74—C75—H75C | 109.3 |
| H12A—C12—H12C | 109.5 | H75A—C75—H75B | 109.5 |
| H12B—C12—H12C | 109.4 | H75A—C75—H75C | 109.5 |
| C11—C13—H13 | 126.2 | H75B—C75—H75C | 109.5 |
| C11—C13—C14 | 107.7 (7) | N32—C76—C77 | 121.2 (7) |
| C14—C13—H13 | 126.2 | N32—C76—C78 | 106.2 (6) |
| N5—C14—C13 | 109.4 (7) | C78—C76—C77 | 132.6 (8) |
| N5—C14—C15 | 122.5 (7) | C76—C77—H77A | 109.4 |
| C13—C14—C15 | 128.1 (7) | C76—C77—H77B | 109.5 |
| C14—C15—H15A | 109.3 | C76—C77—H77C | 109.6 |
| C14—C15—H15B | 109.6 | H77A—C77—H77B | 109.4 |
| C14—C15—H15C | 109.5 | H77A—C77—H77C | 109.5 |
| H15A—C15—H15B | 109.5 | H77B—C77—H77C | 109.5 |
| H15A—C15—H15C | 109.5 | C76—C78—H78 | 126.4 |
| H15B—C15—H15C | 109.4 | C76—C78—C79 | 107.1 (7) |
| N8—C16—C17 | 121.2 (7) | C79—C78—H78 | 126.4 |

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| N8—C16—C18 | 105.8 (6) | N31—C79—C78 | 108.9 (6) |
| C18—C16—C17 | 133.0 (7) | N31—C79—C80 | 122.6 (6) |
| C16—C17—H17A | 109.5 | C78—C79—C80 | 128.5 (7) |
| C16—C17—H17B | 109.5 | C79—C80—H80A | 109.5 |
| C16—C17—H17C | 109.5 | C79—C80—H80B | 109.5 |
| H17A—C17—H17B | 109.5 | C79—C80—H80C | 109.3 |
| H17A—C17—H17C | 109.5 | H80A—C80—H80B | 109.5 |
| H17B—C17—H17C | 109.5 | H80A—C80—H80C | 109.5 |
| C16—C18—H18A | 126.8 | H80B—C80—H80C | 109.5 |

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| Cu1—N1—N2—C1 | −174.0 (5) | N15—N16—C36—C37 | −178.2 (8) |
| Cu1—N1—C4—C3 | 172.4 (6) | N15—N16—C36—C38 | 1.6 (9) |
| Cu1—N1—C4—C5 | −9.5 (12) | N16—N15—C39—C38 | 1.3 (8) |
| Cu1—N3—N4—C6 | 178.9 (5) | N16—N15—C39—C40 | −179.1 (7) |
| Cu1—N3—C9—C8 | −179.3 (5) | N16—C36—C38—C39 | −0.7 (9) |
| Cu1—N3—C9—C10 | 0.8 (11) | N17—N18—C41—C42 | −178.0 (7) |
| Cu1—N5—N6—C11 | −175.4 (5) | N17—N18—C41—C43 | 0.4 (9) |
| Cu1—N5—C14—C13 | 173.2 (6) | N18—N17—C44—C43 | −0.1 (8) |
| Cu1—N5—C14—C15 | −7.5 (12) | N18—N17—C44—C45 | −180.0 (7) |
| Cu1—N7—N8—C16 | 175.9 (5) | N18—C41—C43—C44 | −0.4 (9) |
| Cu1—N7—C19—C18 | −174.7 (6) | N19—N20—C46—C47 | −176.9 (7) |
| Cu1—N7—C19—C20 | 5.7 (12) | N19—N20—C46—C48 | 1.2 (8) |
| Cu2—N9—N10—C21 | 166.0 (5) | N20—N19—C49—C48 | 1.9 (8) |
| Cu2—N9—C24—C23 | −164.1 (5) | N20—N19—C49—C50 | 179.4 (7) |
| Cu2—N9—C24—C25 | 16.4 (11) | N20—C46—C48—C49 | 0.0 (9) |
| Cu2—N11—N12—C26 | −176.7 (5) | N21—N22—C51—C52 | −175.8 (7) |
| Cu2—N11—C29—C28 | 176.4 (6) | N21—N22—C51—C53 | 2.0 (8) |
| Cu2—N11—C29—C30 | −2.8 (12) | N22—N21—C54—C53 | −0.7 (8) |
| Cu2—N13—N14—C31 | −173.2 (5) | N22—N21—C54—C55 | 178.3 (7) |
| Cu2—N13—C34—C33 | 170.5 (5) | N22—C51—C53—C54 | −2.3 (8) |
| Cu2—N13—C34—C35 | −11.9 (11) | N23—N24—C56—C57 | −177.0 (7) |
| Cu2—N15—N16—C36 | 173.1 (5) | N23—N24—C56—C58 | 1.5 (9) |
| Cu2—N15—C39—C38 | −172.1 (6) | N24—N23—C59—C58 | 0.4 (9) |
| Cu2—N15—C39—C40 | 7.4 (12) | N24—N23—C59—C60 | 179.1 (7) |
| Cu3—N17—N18—C41 | 174.2 (5) | N24—C56—C58—C59 | −1.2 (10) |
| Cu3—N17—C44—C43 | −173.2 (5) | N25—N26—C61—C62 | 178.9 (7) |
| Cu3—N17—C44—C45 | 6.9 (12) | N25—N26—C61—C63 | 0.8 (9) |
| Cu3—N19—N20—C46 | −179.8 (5) | N26—N25—C64—C63 | 1.0 (8) |
| Cu3—N19—C49—C48 | 179.1 (5) | N26—N25—C64—C65 | −179.7 (7) |
| Cu3—N19—C49—C50 | −3.5 (12) | N26—C61—C63—C64 | −0.1 (9) |
| Cu3—N21—N22—C51 | 169.4 (5) | N27—N28—C66—C67 | −175.1 (7) |
| Cu3—N21—C54—C53 | −168.5 (5) | N27—N28—C66—C68 | 1.9 (8) |
| Cu3—N21—C54—C55 | 10.6 (11) | N28—N27—C69—C68 | 0.3 (8) |
| Cu3—N23—N24—C56 | 176.5 (5) | N28—N27—C69—C70 | 179.0 (6) |
| Cu3—N23—C59—C58 | −176.8 (6) | N28—C66—C68—C69 | −1.6 (8) |
| Cu3—N23—C59—C60 | 1.9 (12) | N29—N30—C74—C73 | 1.0 (9) |
| Cu4—N25—N26—C61 | −178.7 (5) | N29—N30—C74—C75 | 179.5 (7) |
| Cu4—N25—C64—C63 | 178.0 (5) | N29—C71—C73—C74 | 0.9 (9) |

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| Cu4—N25—C64—C65 | −2.7 (12) | N30—N29—C71—C72 | 179.5 (7) |
| Cu4—N27—N28—C66 | 178.2 (4) | N30—N29—C71—C73 | −0.3 (8) |
| Cu4—N27—C69—C68 | −179.2 (5) | N31—N32—C76—C77 | 178.7 (8) |
| Cu4—N27—C69—C70 | −0.5 (11) | N31—N32—C76—C78 | 0.2 (9) |
| Cu4—N29—N30—C74 | −177.8 (5) | N32—N31—C79—C78 | 0.8 (8) |
| Cu4—N29—C71—C72 | −4.0 (12) | N32—N31—C79—C80 | −178.5 (7) |
| Cu4—N29—C71—C73 | 176.2 (6) | N32—C76—C78—C79 | 0.4 (9) |
| Cu4—N31—N32—C76 | 169.6 (5) | C1—C3—C4—N1 | −0.8 (9) |
| Cu4—N31—C79—C78 | −167.3 (5) | C1—C3—C4—C5 | −178.7 (8) |
| Cu4—N31—C79—C80 | 13.3 (11) | C2—C1—C3—C4 | 178.7 (9) |
| O1—S1—O2—Cu2 | 170.6 (6) | C4—N1—N2—C1 | −1.0 (7) |
| O2—S1—O1—Cu1 | 177.8 (5) | C6—C8—C9—N3 | 0.5 (9) |
| O3—S1—O1—Cu1 | −62.2 (7) | C6—C8—C9—C10 | −179.6 (7) |
| O3—S1—O2—Cu2 | 51.6 (8) | C7—C6—C8—C9 | 176.2 (8) |
| O4—S1—O1—Cu1 | 58.3 (7) | C9—N3—N4—C6 | −0.5 (7) |
| O4—S1—O2—Cu2 | −68.4 (8) | C11—C13—C14—N5 | −1.0 (10) |
| O5—S2—O6—Cu3 | 170.8 (5) | C11—C13—C14—C15 | 179.8 (8) |
| O6—S2—O5—Cu2 | −177.9 (4) | C12—C11—C13—C14 | −178.9 (10) |
| O7—S2—O5—Cu2 | −58.5 (6) | C14—N5—N6—C11 | −1.9 (8) |
| O7—S2—O6—Cu3 | 51.8 (7) | C16—C18—C19—N7 | 0.6 (9) |
| O8—S2—O5—Cu2 | 62.5 (5) | C16—C18—C19—C20 | −179.9 (8) |
| O8—S2—O6—Cu3 | −68.5 (7) | C17—C16—C18—C19 | −179.0 (9) |
| O9—S3—O10—Cu4 | 166.2 (6) | C19—N7—N8—C16 | 0.2 (8) |
| O10—S3—O9—Cu3 | 177.9 (5) | C21—C23—C24—N9 | 0.9 (9) |
| O11—S3—O9—Cu3 | −62.7 (7) | C21—C23—C24—C25 | −179.6 (7) |
| O11—S3—O10—Cu4 | 47.1 (7) | C22—C21—C23—C24 | 176.1 (8) |
| O12—S3—O9—Cu3 | 58.7 (7) | C24—N9—N10—C21 | −1.7 (8) |
| O12—S3—O10—Cu4 | −73.3 (8) | C26—C28—C29—N11 | 0.1 (9) |
| O13—S4—O14—Cu1$^{ii}$ | 163.1 (6) | C26—C28—C29—C30 | 179.3 (8) |
| O13—S4—O14—Cu1$^{i}$ | −9.3 (4) | C27—C26—C28—C29 | −179.5 (10) |
| O14—S4—O13—Cu4 | 178.2 (4) | C29—N11—N12—C26 | 1.2 (8) |
| O15—S4—O13—Cu4 | 57.9 (5) | C31—C33—C34—N13 | −0.1 (9) |
| O15—S4—O14—Cu1$^{ii}$ | −75.2 (8) | C31—C33—C34—C35 | −177.6 (7) |
| O15—S4—O14—Cu1$^{i}$ | 112.4 (6) | C32—C31—C33—C34 | 177.3 (8) |
| O16—S4—O13—Cu4 | −62.9 (5) | C34—N13—N14—C31 | −1.5 (8) |
| O16—S4—O14—Cu1$^{i}$ | −127.3 (6) | C36—C38—C39—N15 | −0.4 (10) |
| O16—S4—O14—Cu1$^{ii}$ | 45.1 (8) | C36—C38—C39—C40 | −179.9 (8) |
| N1—N2—C1—C2 | −178.3 (7) | C37—C36—C38—C39 | 179.1 (9) |
| N1—N2—C1—C3 | 0.5 (8) | C39—N15—N16—C36 | −1.8 (8) |
| N2—N1—C4—C3 | 1.0 (8) | C41—C43—C44—N17 | 0.3 (9) |
| N2—N1—C4—C5 | 179.1 (7) | C41—C43—C44—C45 | −179.8 (8) |
| N2—C1—C3—C4 | 0.1 (9) | C42—C41—C43—C44 | 177.7 (9) |
| N3—N4—C6—C7 | −176.6 (6) | C44—N17—N18—C41 | −0.2 (8) |
| N3—N4—C6—C8 | 0.8 (8) | C46—C48—C49—N19 | −1.3 (9) |
| N4—N3—C9—C8 | 0.0 (8) | C46—C48—C49—C50 | −178.5 (8) |
| N4—N3—C9—C10 | −179.9 (6) | C47—C46—C48—C49 | 177.9 (8) |
| N4—C6—C8—C9 | −0.8 (9) | C49—N19—N20—C46 | −2.0 (8) |
| N5—N6—C11—C12 | −179.9 (8) | C51—C53—C54—N21 | 1.9 (9) |

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| N5—N6—C11—C13 | 1.3 (9) | C51—C53—C54—C55 | −177.0 (7) |
| N6—N5—C14—C13 | 1.7 (8) | C52—C51—C53—C54 | 175.2 (8) |
| N6—N5—C14—C15 | −179.1 (7) | C54—N21—N22—C51 | −0.8 (8) |
| N6—C11—C13—C14 | −0.2 (10) | C56—C58—C59—N23 | 0.5 (10) |
| N7—N8—C16—C17 | 178.9 (7) | C56—C58—C59—C60 | −178.2 (8) |
| N7—N8—C16—C18 | 0.1 (8) | C57—C56—C58—C59 | 177.0 (9) |
| N8—N7—C19—C18 | −0.5 (8) | C59—N23—N24—C56 | −1.2 (8) |
| N8—N7—C19—C20 | 180.0 (7) | C61—C63—C64—N25 | −0.6 (9) |
| N8—C16—C18—C19 | −0.4 (9) | C61—C63—C64—C65 | −179.8 (9) |
| N9—N10—C21—C22 | −176.0 (6) | C62—C61—C63—C64 | −177.9 (9) |
| N9—N10—C21—C23 | 2.3 (9) | C64—N25—N26—C61 | −1.2 (8) |
| N10—N9—C24—C23 | 0.4 (8) | C66—C68—C69—N27 | 0.9 (9) |
| N10—N9—C24—C25 | −179.1 (7) | C66—C68—C69—C70 | −177.7 (7) |
| N10—C21—C23—C24 | −1.9 (9) | C67—C66—C68—C69 | 174.9 (8) |
| N11—N12—C26—C27 | 179.0 (8) | C69—N27—N28—C66 | −1.4 (7) |
| N11—N12—C26—C28 | −1.1 (9) | C71—N29—N30—C74 | −0.4 (8) |
| N12—N11—C29—C28 | −0.7 (8) | C71—C73—C74—N30 | −1.1 (9) |
| N12—N11—C29—C30 | 180.0 (7) | C71—C73—C74—C75 | −179.4 (9) |
| N12—C26—C28—C29 | 0.6 (9) | C72—C71—C73—C74 | −178.9 (8) |
| N13—N14—C31—C32 | −176.9 (7) | C76—C78—C79—N31 | −0.8 (9) |
| N13—N14—C31—C33 | 1.4 (8) | C76—C78—C79—C80 | 178.6 (8) |
| N14—N13—C34—C33 | 0.9 (8) | C77—C76—C78—C79 | −177.9 (9) |
| N14—N13—C34—C35 | 178.5 (7) | C79—N31—N32—C76 | −0.6 (8) |
| N14—C31—C33—C34 | −0.8 (9) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O4 | 0.86 | 2.08 | 2.792 (7) | 139 |
| N6—H6···O3 | 0.86 | 2.04 | 2.889 (7) | 168 |
| N10—H10···O3 | 0.86 | 2.11 | 2.869 (7) | 146 |
| N12—H12···O4 | 0.86 | 2.12 | 2.951 (8) | 163 |
| N14—H14···O8 | 0.86 | 2.10 | 2.835 (7) | 143 |
| N16—H16···O5 | 0.86 | 2.44 | 2.889 (7) | 114 |
| N16—H16···O7 | 0.86 | 2.04 | 2.894 (8) | 173 |
| N18—H18···O6 | 0.86 | 2.39 | 2.866 (8) | 116 |
| N18—H18···O8 | 0.86 | 2.14 | 2.988 (7) | 169 |
| N20—H20···S3 | 0.86 | 2.76 | 3.504 (6) | 146 |
| N20—H20···O9 | 0.86 | 2.41 | 2.885 (9) | 115 |
| N20—H20···O11 | 0.86 | 2.08 | 2.933 (7) | 171 |
| N22—H22···O7 | 0.86 | 2.05 | 2.828 (7) | 150 |
| N24—H24···O12 | 0.86 | 2.16 | 2.840 (8) | 135 |
| N26—H26···O16 | 0.86 | 2.02 | 2.875 (7) | 171 |
| N28—H28···O15 | 0.86 | 2.07 | 2.803 (7) | 143 |
| N30—H30···O10 | 0.86 | 2.31 | 2.817 (8) | 118 |
| N30—H30···O12 | 0.86 | 2.24 | 3.083 (8) | 165 |

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|---|---|---|---|---|
| N32—H32···O11 | 0.86 | 2.12 | 2.857 (7) | 144 |
| C30—H30*C*···O5 | 0.96 | 2.39 | 3.213 (11) | 144 |
| C50—H50*A*···O6 | 0.96 | 2.23 | 3.124 (9) | 155 |
| C65—H65*B*···O10 | 0.96 | 2.27 | 3.192 (11) | 160 |
| C70—H70*B*···O10 | 0.96 | 2.35 | 3.116 (10) | 137 |
| C2—H2*A*···N16$^{iii}$ | 0.96 | 3.01 | 3.722 (10) | 132 |
| C2—H2*A*···O7$^{iii}$ | 0.96 | 28 | 3.806 (9) | 146 |
| C53—H53···N8$^{iv}$ | 0.93 | 3.07 | 3.66 (1) | 123 |
| C32—H32*B*···N32$^{v}$ | 0.96 | 3.00 | 3.792 (10) | 140 |
| C32—H32*B*···N31$^{v}$ | 0.96 | 3.17 | 3.984 (10) | 143 |
| C32—H32*B*···N28$^{v}$ | 0.96 | 2.87 | 3.735 (11) | 150 |

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