Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetrakis(di-4-pyridylsulfane)dinitratocopper(II)

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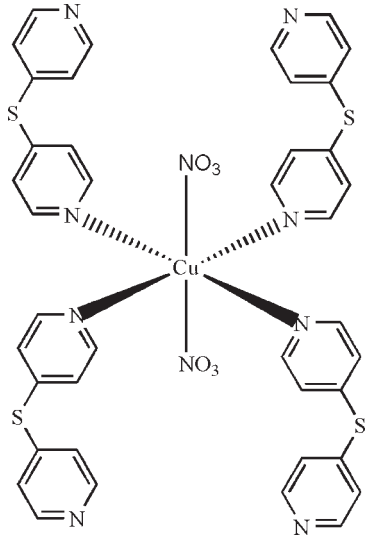
Received 13 March 2010; accepted 25 March 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.100; data-to-parameter ratio = 13.3.

In the title complex, $[Cu(NO_3)_2(C_{10}H_8N_2S)_4]$, the Cu^{II} atom (site symmetry $\overline{1}$) is coordinated by two monodentate nitrate ions and two monodentate di-4-pyridylsulfane ligands, resulting in a slightly distorted *trans*-arranged CuO_2N_4 octahedral geometry. Intramolecular C—H···O hydrogen bonds are present. In the crystal, adjacent molecules are linked *via* C—H···N hydrogen bonds into chains parallel to the *a* axis. Intermolecular C—H···O interactions also occur.

Related literature

For transition-metal complexes of di-4-pyridylsulfane, see: Wen *et al.* (2004); Muthu *et al.* (2005); Xu *et al.* (2007); Zhang *et al.* (2008).



Experimental

Crystal data

$[Cu(NO_3)_2(C_{10}H_8N_2S)_4]$
M_r = 940.59
Triclinic, $P\overline{1}$
a = 9.299 (4) Å
b = 10.765 (5) Å
c = 10.978 (5) Å
α = 84.408 (6)°
β = 73.759 (6)°
γ = 79.180 (6)°
V = 1035.1 (8) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 296 K
0.21 × 0.19 × 0.17 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.847, T_{max} = 0.874
7479 measured reflections
3728 independent reflections
2392 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.100
S = 0.90
3679 reflections
277 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O1^{i}	0.93	2.52	3.063 (4)	118
C5—H5···O2^{i}	0.93	2.49	3.419 (4)	174
C5—H5···O1^{i}	0.93	2.51	3.193 (4)	130
C14—H14···N4^{ii}	0.93	2.47	3.279 (5)	146
C1—H1···O1	0.93	2.27	3.008 (4)	135

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $x+1, y, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2428).

References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2000). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Muthu, S., Ni, Z. & Vittal, J. J. (2005). *Inorg. Chim. Acta*, **358**, 595–605
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wen, Y.-H., Cheng, J.-K., Zhang, J., Li, Z.-J. & Yao, Y.-G. (2004). *Acta Cryst.* C**60**, m618–m619.
Xu, Q.-F., Zhou, Q.-X., Lu, J.-M., Xia, X.-W., Wang, L.-H. & Zhang, Y. (2007). *Polyhedron*, **26**, 4849–4859
Zhang, J., Cheng, J.-K., Qin, Y.-Y., Li, Z.-J. & Yao, Y.-G. (2008). *Inorg. Chem. Commun.* **11**, 164–166

supporting information

Acta Cryst. (2010). E**66**, m487 [https://doi.org/10.1107/S1600536810011414]

Tetrakis(di-4-pyridylsulfane)dinitratocopper(II)

Rong-Hua Gao and Li-Li Yang

S1. Comment

Flexible ligands are interesting due to their smaller steric effects, which contribute to the construction of novel complexes. Compared to the widely investigated 4,4′-bipy, the dps (di-4-pyridylsulfane) ligand is more flexible and the two pyridine rings can rotate freely. There are only few complexes of metal-organic compounds with dps (Xu *et al.*, 2007; Wen *et al.*, 2004; Muthu *et al.*, 2005; Zhang *et al.*, 2008). Herein, we report the synthesis and structure of the title compound, dinitratotetrakis(di-4-pyridylsulfane)copper(II).

The title compound (Fig. 1) crystallizes in the monoclinic space group $P\bar{1}$. The copper(II) ion lies on a crystallography inversion centre and adopts a slightly distorted octahedral provided by four N atoms from two dps ligands in the equatorial plane and two O atoms from two nitrate ions in the axial position. In the equatorial plane, the Cu1—N1 and Cu1—N3 bond lengths are 2.047 (3) and 2.023 (3) Å respectively, while the Cu1—O1 axial bond length is 2.558 (3) Å. The conformation of the complex molecule is stabilized by intramolecular C—H···O hydrogen bonds (Table 1). In the crystal structure (Fig. 2), intermolecular C—H···N hydrogen interactions link molecules into chains parallel to the *a* axis.

S2. Experimental

The title compound was prepared by adding a solution of copper(II) nitrate hexahydrate (0.1 mmol) in water (6 ml) to a solution of di-4-pyridylsulfane (0.2 mmol) in CH_3OH (5 ml) with gentle stirring. After several days, block-shaped blue crystals suitable for X-ray analysis were obtained on slow evaporation of the solvent (Yield 30 mg; 31.9%, based on Cu). Anal. calcd for $C_{40}H_{32}CuN_{10}O_6S_4$ (940.59): C 51.08, H 3.43, N 14.89%; found: C 51.23, H 3.45, N 14.93%.

S3. Refinement

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å, and with U_{iso} (H) = 1.2U_{eq}(C). The anisotropic displacement parameters of atoms O1 and N5 were restrained to be similar (i.e. the SIMU restraint was applied).

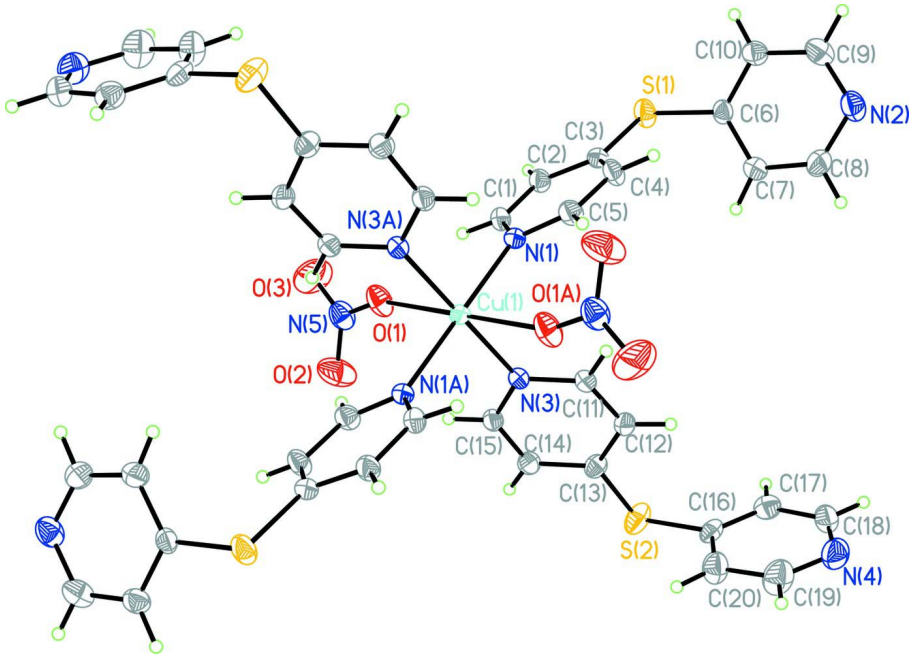


Figure 1

The molecular structure of the title compound with atomic labeling scheme and displacement ellipsoids drawn at the 50% probability level [symmetry code: (A) -x+1,-y+2,-z+1].

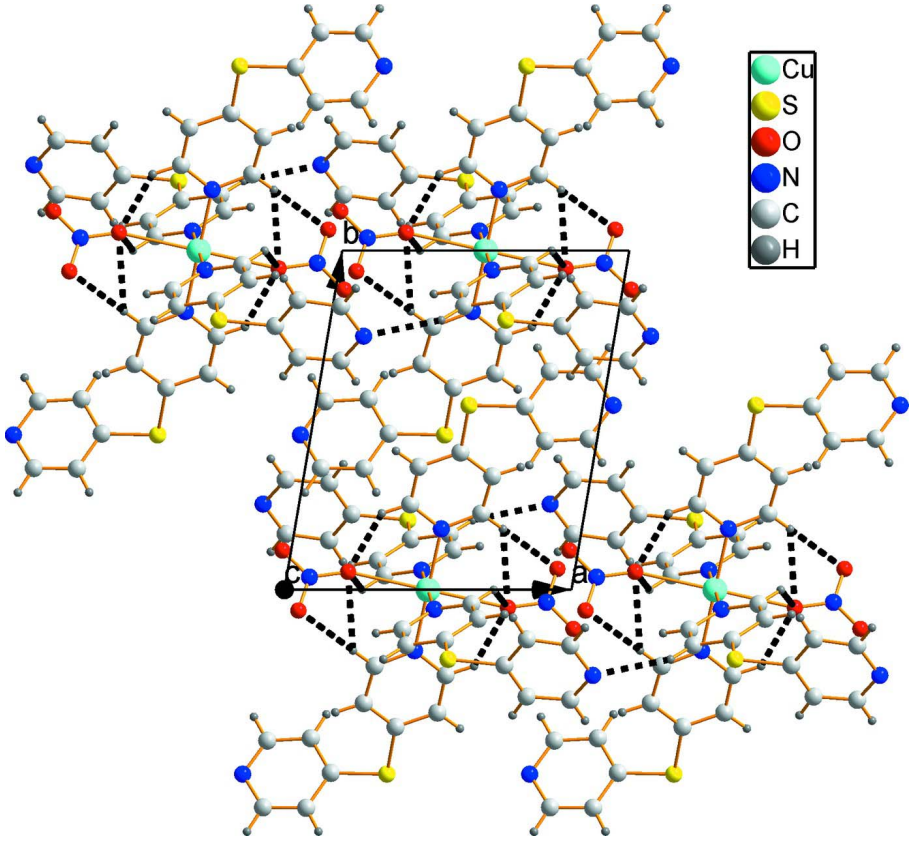


Figure 2

Crystal packing of the title compound viewed along the *c* axis. Hydrogen bonds are drawn as dashed lines.

Tetrakis(di-4-pyridylsulfane)dinitratocopper(II)

Crystal data

$[Cu(NO_3)_2(C_{10}H_8N_2S)_4]$
$M_r = 940.59$
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$c = 10.978$ (5) Å
$\alpha = 84.408$ (6)°
$\beta = 73.759$ (6)°
$\gamma = 79.180$ (6)°
$V = 1035.1$ (8) Å^3
$Z = 1$
$F(000) = 483$
$D_x = 1.509$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4796 reflections
$\theta = 2.3$–28.2°
$\mu = 0.79$ mm^{-1}
$T = 296$ K
Block, blue
0.21 × 0.19 × 0.17 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.847$, $T_{max} = 0.874$
7479 measured reflections
3728 independent reflections
2392 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 25.2°$, $\theta_{min} = 1.9°$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.100$
$S = 0.90$
3679 reflections
277 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor wR and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) etc. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	1.0000	0.5000	0.03494 (19)
S1	0.46635 (10)	0.45645 (8)	0.29541 (10)	0.0526 (3)
S2	0.38860 (11)	1.20522 (11)	−0.05513 (9)	0.0609 (3)
O1	0.7889 (3)	0.9473 (2)	0.4138 (2)	0.0586 (7)
O2	0.9388 (3)	1.0613 (3)	0.2949 (3)	0.0869 (10)
O3	1.0298 (3)	0.8845 (3)	0.3704 (3)	0.1064 (12)
N1	0.4896 (3)	0.8203 (2)	0.4611 (2)	0.0337 (6)
N2	−0.0360 (3)	0.4563 (3)	0.3369 (3)	0.0556 (9)
N3	0.4666 (3)	1.0575 (2)	0.3276 (2)	0.0327 (6)
N4	−0.1253 (4)	1.2525 (3)	0.0096 (3)	0.0642 (9)
N5	0.9202 (4)	0.9628 (3)	0.3612 (3)	0.0538 (7)
C1	0.6125 (4)	0.7481 (3)	0.3889 (3)	0.0381 (8)
H1	0.7061	0.7748	0.3711	0.046*
C2	0.6058 (4)	0.6377 (3)	0.3409 (3)	0.0381 (8)
H2	0.6937	0.5908	0.2917	0.046*
C3	0.4684 (4)	0.5955 (3)	0.3654 (3)	0.0359 (8)
C4	0.3437 (4)	0.6656 (3)	0.4452 (3)	0.0433 (9)
H4	0.2500	0.6385	0.4682	0.052*
C5	0.3596 (4)	0.7753 (3)	0.4899 (3)	0.0413 (9)
H5	0.2746	0.8210	0.5436	0.050*
C6	0.2705 (3)	0.4599 (3)	0.3124 (3)	0.0385 (8)
C7	0.1802 (4)	0.5620 (3)	0.2676 (4)	0.0510 (10)
H7	0.2205	0.6326	0.2270	0.061*
C8	0.0298 (4)	0.5550 (4)	0.2851 (4)	0.0560 (10)
H8	−0.0309	0.6253	0.2586	0.067*

C9	0.0547 (4)	0.3585 (3)	0.3756 (4)	0.0556 (10)
H9	0.0133	0.2866	0.4105	0.067*
C10	0.2053 (4)	0.3570 (3)	0.3674 (3)	0.0453 (9)
H10	0.2621	0.2871	0.3987	0.054*
C11	0.3401 (4)	1.0425 (3)	0.2976 (3)	0.0365 (8)
H11	0.2705	1.0005	0.3569	0.044*
C12	0.3082 (4)	1.0855 (3)	0.1852 (3)	0.0386 (8)
H12	0.2191	1.0726	0.1693	0.046*
C13	0.4103 (4)	1.1485 (3)	0.0953 (3)	0.0389 (8)
C14	0.5424 (4)	1.1637 (3)	0.1250 (3)	0.0404 (9)
H14	0.6140	1.2051	0.0671	0.049*
C15	0.5658 (4)	1.1175 (3)	0.2396 (3)	0.0369 (8)
H15	0.6547	1.1281	0.2575	0.044*
C16	0.1889 (4)	1.2224 (3)	−0.0291 (3)	0.0415 (9)
C17	0.1259 (4)	1.1460 (3)	−0.0847 (3)	0.0504 (10)
H17	0.1873	1.0824	−0.1364	0.061*
C18	−0.0290 (5)	1.1645 (4)	−0.0632 (4)	0.0592 (11)
H18	−0.0694	1.1118	−0.1022	0.071*
C19	0.0927 (4)	1.3150 (4)	0.0459 (4)	0.0603 (11)
H19	0.1307	1.3701	0.0843	0.072*
C20	−0.0611 (5)	1.3244 (4)	0.0630 (4)	0.0725 (13)
H20	−0.1250	1.3859	0.1161	0.087*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0427 (4)	0.0243 (3)	0.0432 (4)	−0.0055 (2)	−0.0207 (3)	0.0000 (3)
S1	0.0416 (6)	0.0364 (5)	0.0856 (8)	−0.0001 (4)	−0.0239 (5)	−0.0226 (5)
S2	0.0406 (6)	0.0945 (8)	0.0442 (6)	−0.0093 (5)	−0.0137 (5)	0.0163 (6)
O1	0.0421 (14)	0.0601 (14)	0.0723 (17)	−0.0193 (12)	−0.0018 (13)	−0.0171 (13)
O2	0.073 (2)	0.064 (2)	0.107 (3)	−0.0221 (16)	0.0062 (18)	0.0106 (18)
O3	0.069 (2)	0.089 (2)	0.148 (3)	0.0266 (18)	−0.036 (2)	0.000 (2)
N1	0.0358 (16)	0.0265 (14)	0.0415 (17)	−0.0050 (12)	−0.0151 (14)	−0.0005 (12)
N2	0.0396 (18)	0.052 (2)	0.076 (2)	−0.0107 (16)	−0.0115 (17)	−0.0103 (18)
N3	0.0353 (16)	0.0287 (14)	0.0370 (17)	−0.0077 (12)	−0.0128 (14)	−0.0015 (12)
N4	0.045 (2)	0.073 (2)	0.072 (3)	−0.0104 (19)	−0.0154 (19)	0.006 (2)
N5	0.0412 (16)	0.0535 (16)	0.0649 (18)	−0.0102 (15)	−0.0065 (15)	−0.0127 (14)
C1	0.0317 (19)	0.0398 (19)	0.046 (2)	−0.0101 (16)	−0.0133 (17)	−0.0003 (17)
C2	0.035 (2)	0.0339 (19)	0.047 (2)	−0.0037 (15)	−0.0122 (17)	−0.0078 (16)
C3	0.040 (2)	0.0269 (17)	0.044 (2)	−0.0049 (15)	−0.0170 (17)	−0.0005 (15)
C4	0.0293 (19)	0.0364 (19)	0.065 (3)	−0.0094 (15)	−0.0092 (18)	−0.0096 (18)
C5	0.037 (2)	0.0347 (19)	0.051 (2)	−0.0030 (16)	−0.0087 (18)	−0.0083 (17)
C6	0.038 (2)	0.0345 (18)	0.048 (2)	−0.0056 (15)	−0.0179 (17)	−0.0093 (16)
C7	0.049 (2)	0.040 (2)	0.069 (3)	−0.0125 (17)	−0.023 (2)	0.0068 (19)
C8	0.050 (2)	0.046 (2)	0.077 (3)	−0.0013 (19)	−0.030 (2)	−0.001 (2)
C9	0.054 (3)	0.044 (2)	0.065 (3)	−0.0131 (19)	−0.006 (2)	−0.004 (2)
C10	0.047 (2)	0.0341 (19)	0.054 (2)	−0.0027 (17)	−0.0130 (19)	−0.0068 (17)
C11	0.0350 (19)	0.0340 (18)	0.042 (2)	−0.0104 (15)	−0.0114 (17)	0.0008 (16)

C12	0.0321 (19)	0.0406 (19)	0.045 (2)	−0.0078 (15)	−0.0133 (17)	0.0028 (17)
C13	0.0323 (19)	0.044 (2)	0.037 (2)	−0.0021 (16)	−0.0084 (17)	−0.0008 (16)
C14	0.034 (2)	0.043 (2)	0.042 (2)	−0.0099 (16)	−0.0081 (17)	0.0042 (17)
C15	0.0321 (19)	0.0322 (18)	0.049 (2)	−0.0054 (15)	−0.0136 (18)	−0.0035 (17)
C16	0.037 (2)	0.050 (2)	0.036 (2)	−0.0015 (17)	−0.0137 (17)	0.0079 (17)
C17	0.053 (2)	0.045 (2)	0.051 (3)	−0.0016 (18)	−0.015 (2)	−0.0030 (19)
C18	0.062 (3)	0.061 (3)	0.068 (3)	−0.024 (2)	−0.032 (2)	0.006 (2)
C19	0.053 (3)	0.068 (3)	0.065 (3)	−0.006 (2)	−0.021 (2)	−0.018 (2)
C20	0.053 (3)	0.079 (3)	0.080 (3)	0.008 (2)	−0.015 (3)	−0.024 (3)

Geometric parameters (Å, º)

Cu1—N3^{i}	2.023 (3)	C4—H4	0.9300
Cu1—N3	2.023 (3)	C5—H5	0.9300
Cu1—N1^{i}	2.047 (3)	C6—C10	1.370 (4)
Cu1—N1	2.047 (3)	C6—C7	1.390 (4)
Cu1—O1	2.558 (3)	C7—C8	1.373 (5)
Cu1—O1^{i}	2.558 (3)	C7—H7	0.9300
S1—C3	1.754 (3)	C8—H8	0.9300
S1—C6	1.772 (3)	C9—C10	1.375 (5)
S2—C13	1.757 (3)	C9—H9	0.9300
S2—C16	1.775 (3)	C10—H10	0.9300
O1—N5	1.231 (3)	C11—C12	1.366 (4)
O2—N5	1.238 (4)	C11—H11	0.9300
O3—N5	1.216 (4)	C12—C13	1.387 (4)
N1—C5	1.331 (4)	C12—H12	0.9300
N1—C1	1.348 (4)	C13—C14	1.397 (4)
N2—C8	1.326 (4)	C14—C15	1.367 (4)
N2—C9	1.334 (4)	C14—H14	0.9300
N3—C15	1.344 (4)	C15—H15	0.9300
N3—C11	1.347 (4)	C16—C17	1.367 (4)
N4—C20	1.326 (5)	C16—C19	1.374 (5)
N4—C18	1.329 (5)	C17—C18	1.372 (5)
C1—C2	1.365 (4)	C17—H17	0.9300
C1—H1	0.9300	C18—H18	0.9300
C2—C3	1.383 (4)	C19—C20	1.375 (5)
C2—H2	0.9300	C19—H19	0.9300
C3—C4	1.383 (4)	C20—H20	0.9300
C4—C5	1.370 (4)		

N3^{i}—Cu1—N3	180.000 (1)	C10—C6—S1	119.4 (3)
N3^{i}—Cu1—N1^{i}	87.75 (10)	C7—C6—S1	122.4 (3)
N3—Cu1—N1^{i}	92.25 (10)	C8—C7—C6	117.8 (3)
N3^{i}—Cu1—N1	92.25 (10)	C8—C7—H7	121.1
N3—Cu1—N1	87.75 (10)	C6—C7—H7	121.1
N1^{i}—Cu1—N1	180.00 (14)	N2—C8—C7	125.3 (3)
N3^{i}—Cu1—O1	86.21 (9)	N2—C8—H8	117.3
N3—Cu1—O1	93.79 (9)	C7—C8—H8	117.3

N1^{i}—Cu1—O1	91.99 (9)	N2—C9—C10	124.3 (3)
N1—Cu1—O1	88.01 (9)	N2—C9—H9	117.9
N3^{i}—Cu1—O1^{i}	93.79 (9)	C10—C9—H9	117.9
N3—Cu1—O1^{i}	86.21 (9)	C6—C10—C9	119.0 (3)
N1^{i}—Cu1—O1^{i}	88.01 (9)	C6—C10—H10	120.5
N1—Cu1—O1^{i}	91.99 (9)	C9—C10—H10	120.5
O1—Cu1—O1^{i}	180.000 (1)	N3—C11—C12	123.8 (3)
C3—S1—C6	103.18 (15)	N3—C11—H11	118.1
C13—S2—C16	101.57 (15)	C12—C11—H11	118.1
N5—O1—Cu1	159.3 (2)	C11—C12—C13	119.2 (3)
C5—N1—C1	116.5 (3)	C11—C12—H12	120.4
C5—N1—Cu1	122.5 (2)	C13—C12—H12	120.4
C1—N1—Cu1	120.4 (2)	C12—C13—C14	117.5 (3)
C8—N2—C9	115.3 (3)	C12—C13—S2	124.7 (3)
C15—N3—C11	116.8 (3)	C14—C13—S2	117.8 (3)
C15—N3—Cu1	121.7 (2)	C15—C14—C13	119.6 (3)
C11—N3—Cu1	121.4 (2)	C15—C14—H14	120.2
C20—N4—C18	115.0 (3)	C13—C14—H14	120.2
O3—N5—O1	122.4 (4)	N3—C15—C14	123.1 (3)
O3—N5—O2	119.9 (4)	N3—C15—H15	118.4
O1—N5—O2	117.7 (3)	C14—C15—H15	118.4
N1—C1—C2	122.9 (3)	C17—C16—C19	117.9 (3)
N1—C1—H1	118.5	C17—C16—S2	121.4 (3)
C2—C1—H1	118.5	C19—C16—S2	120.7 (3)
C1—C2—C3	120.0 (3)	C16—C17—C18	119.1 (4)
C1—C2—H2	120.0	C16—C17—H17	120.4
C3—C2—H2	120.0	C18—C17—H17	120.4
C4—C3—C2	117.2 (3)	N4—C18—C17	124.5 (4)
C4—C3—S1	125.1 (3)	N4—C18—H18	117.7
C2—C3—S1	117.7 (2)	C17—C18—H18	117.7
C5—C4—C3	119.3 (3)	C16—C19—C20	118.4 (4)
C5—C4—H4	120.4	C16—C19—H19	120.8
C3—C4—H4	120.4	C20—C19—H19	120.8
N1—C5—C4	123.9 (3)	N4—C20—C19	125.0 (4)
N1—C5—H5	118.1	N4—C20—H20	117.5
C4—C5—H5	118.1	C19—C20—H20	117.5
C10—C6—C7	118.1 (3)		

N3^{i}—Cu1—O1—N5	−120.2 (7)	C3—S1—C6—C10	−127.2 (3)
N3—Cu1—O1—N5	59.8 (7)	C3—S1—C6—C7	55.2 (3)
N1^{i}—Cu1—O1—N5	−32.6 (7)	C10—C6—C7—C8	2.2 (5)
N1—Cu1—O1—N5	147.4 (7)	S1—C6—C7—C8	179.8 (3)
N3—Cu1—N1—C5	−89.3 (3)	C9—N2—C8—C7	1.1 (6)
O1—Cu1—N1—C5	176.8 (3)	C6—C7—C8—N2	−3.0 (6)
O1^{i}—Cu1—N1—C5	−3.2 (3)	C8—N2—C9—C10	1.6 (6)
N3^{i}—Cu1—N1—C1	−98.5 (2)	C7—C6—C10—C9	0.2 (5)
N3—Cu1—N1—C1	81.5 (2)	S1—C6—C10—C9	−177.4 (3)
O1—Cu1—N1—C1	−12.3 (2)	N2—C9—C10—C6	−2.3 (6)

O1^{i}—Cu1—N1—C1	167.7 (2)	C15—N3—C11—C12	−0.6 (4)
N1^{i}—Cu1—N3—C15	57.4 (2)	Cu1—N3—C11—C12	176.5 (2)
N1—Cu1—N3—C15	−122.6 (2)	N3—C11—C12—C13	0.0 (5)
O1—Cu1—N3—C15	−34.7 (2)	C11—C12—C13—C14	0.5 (5)
O1^{i}—Cu1—N3—C15	145.3 (2)	C11—C12—C13—S2	178.0 (2)
N1^{i}—Cu1—N3—C11	−119.5 (2)	C16—S2—C13—C12	23.8 (3)
N1—Cu1—N3—C11	60.5 (2)	C16—S2—C13—C14	−158.6 (3)
O1—Cu1—N3—C11	148.3 (2)	C12—C13—C14—C15	−0.3 (5)
O1^{i}—Cu1—N3—C11	−31.7 (2)	S2—C13—C14—C15	−178.0 (2)
Cu1—O1—N5—O3	166.9 (5)	C11—N3—C15—C14	0.8 (4)
Cu1—O1—N5—O2	−14.5 (9)	Cu1—N3—C15—C14	−176.3 (2)
C5—N1—C1—C2	3.5 (5)	C13—C14—C15—N3	−0.4 (5)
Cu1—N1—C1—C2	−167.9 (2)	C13—S2—C16—C17	−111.6 (3)
N1—C1—C2—C3	0.1 (5)	C13—S2—C16—C19	69.8 (3)
C1—C2—C3—C4	−3.6 (5)	C19—C16—C17—C18	−0.2 (5)
C1—C2—C3—S1	177.4 (2)	S2—C16—C17—C18	−179.0 (3)
C6—S1—C3—C4	16.6 (3)	C20—N4—C18—C17	−0.3 (6)
C6—S1—C3—C2	−164.5 (3)	C16—C17—C18—N4	−0.3 (6)
C2—C3—C4—C5	3.5 (5)	C17—C16—C19—C20	1.2 (5)
S1—C3—C4—C5	−177.6 (3)	S2—C16—C19—C20	179.9 (3)
C1—N1—C5—C4	−3.6 (5)	C18—N4—C20—C19	1.4 (6)
Cu1—N1—C5—C4	167.5 (2)	C16—C19—C20—N4	−1.9 (7)
C3—C4—C5—N1	0.2 (5)		

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1^{i}	0.93	2.52	3.063 (4)	118
C5—H5···O2^{i}	0.93	2.49	3.419 (4)	174
C5—H5···O1^{i}	0.93	2.51	3.193 (4)	130
C14—H14···N4^{ii}	0.93	2.47	3.279 (5)	146
C1—H1···O1	0.93	2.27	3.008 (4)	135

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1; (ii) *x*+1, *y*, *z*.