metal-organic compounds

CrossMark

Diaquabis(ethylenediamine-$\kappa^2 N,N'$)-copper(II) bis(sulfamerazinate)

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The asymmetric unit of the title compound, [Cu(C₂H₈N₂)₂(H₂O)₂](C₁₁H₁₁N₄O₂S)₂, contains one sulfamerazinate anion in a general position and one half-cation that is located on a center of inversion. The Cuᴵᴵ cation shows a strong Jahn–Teller distortion. It is coordinated by four N atoms of two ethylenediamine ligands in the basal plane and two O atoms at much longer distances in the axial positions in a bipyramidal coordination. In the crystal, the building blocks are connected by N—H⋯N, O—H⋯N, N—H⋯O and O—H⋯O hydrogen bonding into a two-dimensional network parallel to (001).

Related literature

For the antibacterial activity of sulfonamides, see: Anand (1980); Kratz *et al.* (2000); Grave *et al.* (2010). For uses of sulfamerazine, see: Murphy *et al.* (1943); Clark *et al.* (1943); Earle (1944); Forbes *et al.* (1946). The crystal structure of sulfamerazine was reported by Acharya *et al.* (1982). For a related compound in which sulfathiazole acts as a deprotonated counter-ion, see: Anacona *et al.* (2002).
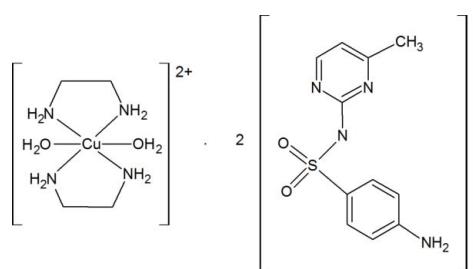
Experimental

Crystal data

[Cu(C₂H₈N₂)₂(H₂O)₂]-(C₁₁H₁₁N₄O₂S)₂	$\beta = 82.800\ (5)°$
$M_r = 746.41$	$\gamma = 78.873\ (5)°$
Triclinic, $P\bar{1}$	$V = 866.40\ (9)$ Å³
$a = 7.5429\ (4)$ Å	$Z = 1$
$b = 8.1800\ (5)$ Å	Mo $K\alpha$ radiation
$c = 14.8434\ (8)$ Å	$\mu = 0.81$ mm⁻¹
$\alpha = 75.299\ (5)°$	$T = 293$ K
	$0.41 \times 0.36 \times 0.17$ mm

Data collection

Oxford Diffraction Gemini diffractometer	4738 measured reflections
Absorption correction: analytical (de Meulenaer & Tompa, 1965)	4020 independent reflections
$T_{min} = 0.723$, $T_{max} = 0.869$	3361 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.097$	
$S = 1.05$	$\Delta\rho_{max} = 0.33$ e Å⁻³
4020 reflections	$\Delta\rho_{min} = -0.38$ e Å⁻³
215 parameters	

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1NA⋯O2ⁱ	0.97	2.09	3.022 (3)	162
O1W—H1W⋯O1	0.85	2.07	2.816 (2)	145
N1—H1NB⋯O1	0.97	2.41	3.219 (2)	140
O1W—H2W⋯N11ⁱⁱ	0.95	1.92	2.858 (2)	171
N2—H2NA⋯O2ⁱⁱ	0.97	2.33	3.189 (3)	147
N2—H2NA⋯N11ⁱⁱ	0.97	2.47	3.319 (3)	145
N2—H2NB⋯O2ⁱⁱⁱ	0.97	2.42	3.277 (3)	147
N14—H14A⋯N12ⁱᵛ	0.93	2.09	3.003 (3)	166
N14—H14B⋯O1ᵛ	0.95	2.21	2.993 (3)	140
N14—H14B⋯N13ᵛ	0.95	2.44	3.215 (3)	139

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

Data collection: *GEMINI* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Supporting information for this paper is available from the IUCr electronic archives (Reference: NC2325).

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supporting information

Diaquabis(ethylenediamine-*κ²N,N′*)copper(II) bis(sulfamerazinate)

Amani Direm, Wahiba Falek, Guillaume Pilet and Nourredine Benali-Cherif

S1. Comment

It is well known that many sulfonamide derivatives possess antibacterial activity (Anand, 1980; Kratz *et al.*, 2000; Grave *et al.*, 2010) including sulfamerazine which is widely used to treat susceptible microbial infections (Murphy *et al.*, 1943; Clark *et al.*, 1943). Faster absorption, low overall excretion rate by the kidneys, and an equal therapeutic and toxic effect of sulfamerazine compared to other sulfonamide drugs, such as sulfadiazine and sulfathiazole, have been claimed for its wider usage (Earle, 1944; Forbes *et al.*, 1946).

The first crystal structure of sulfamerazine have been reported by (Acharya *et al.*, 1982). The presence of several potential donor sites, namely the amino, pyrimidine and sulfonamide N atoms and the sulfonyl O atoms, make this ligand a versatile complexing agent.

As part of our efforts to investigate metal(II) complexes based on sulfonamides, we report herein the crystal structure of the new copper(II) complex: Diaquabis(ethylenediamine-*κ*2 N,*N′*)copper(II) bis(sulfamerazinate).

The asymmetric unit of the title compound contains one sulfamerazinate counter-ion and a half $[Cu(en)_2(H_2O)_2]^{2+}$ cation (en = ethylenediamine) (Fig. 1). The metal ion is located in a ML6 environment and coordinated by four N atoms of two ethylenediamine ligands and two O atoms of two water molecules. The four N atoms of the ligands in the equatorial plane form a square-planar arrangement, while the 6-fold coordination is completed by the two water O atoms in the axial positions. The apical Cu—O bridging separation is 2.513 (2) Å while the equatorial Cu—N bridging bond lengths are 2.0168 (19) Å and 2.0016 (18) Å, which is typical for a Jahn-Teller distortion. A sulfamerazine anion that is deprotonated at the N11 N atom is present in the structure (Fig. 1). To the best of our knowledge, a search in the Cambridge Structural Database reveal, that this is the first crystal structure where a sulfamerazinate anion act as a counter ion. A similar situation is observed in $[Cu(en)_2(OH_2)_2](Stz)_2 \cdot 2H_2O$ (Anacona *et al.*, 2002) where a sulfathiazole acts as a deprotonated counter ion too.

In the crystal strcuture of the title compound every complex cation is linked *via* O—H⋯N, N—H⋯O and O—H⋯O hydrogen bonding to the counter cations, while the cations are interconnected *via* the N—H⋯N interaction, which lead to the formation of a two dimensional network (Fig. 2).

S2. Experimental

The single crystals of $[Cu(C_2H_8N_2)_2(H_2O)_2](C_{11}H_{12}N_4SO_2)_2$ were formed in a methanolic solution (50 ml) of $Cu(CH_3CO_2)_2$ (0.362 g, 2 mmol) and sulfamerazine (1.057 g, 4 mmol) by adding ethylenediamine (0.5 ml, 7.3 mmol). The precipitate obtained immediately was filtred out and the resulting filtrate was left to slowly evaporate at room temperature which lead to the formation of blue single crystals suitable for X-Ray diffraction.

S3. Refinement

All C-H and all N-H H atoms of the ethylenediamine molecules were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and were refined isotropic with $[U_{iso}(H) = 1.2\ U_{eq}\ (C,N)]$ (1.5 for methyl H atoms) using a riding odel with C—H = 0.93, 0.96 and 0.97 Å (for aromatic, methyl and methylene H atoms and N—H = 0.97 Å for amino H atoms. The N-H and the O-H water H atoms were located in difference map and refined with varying coordinates and fixed isotropic displacement parameters.
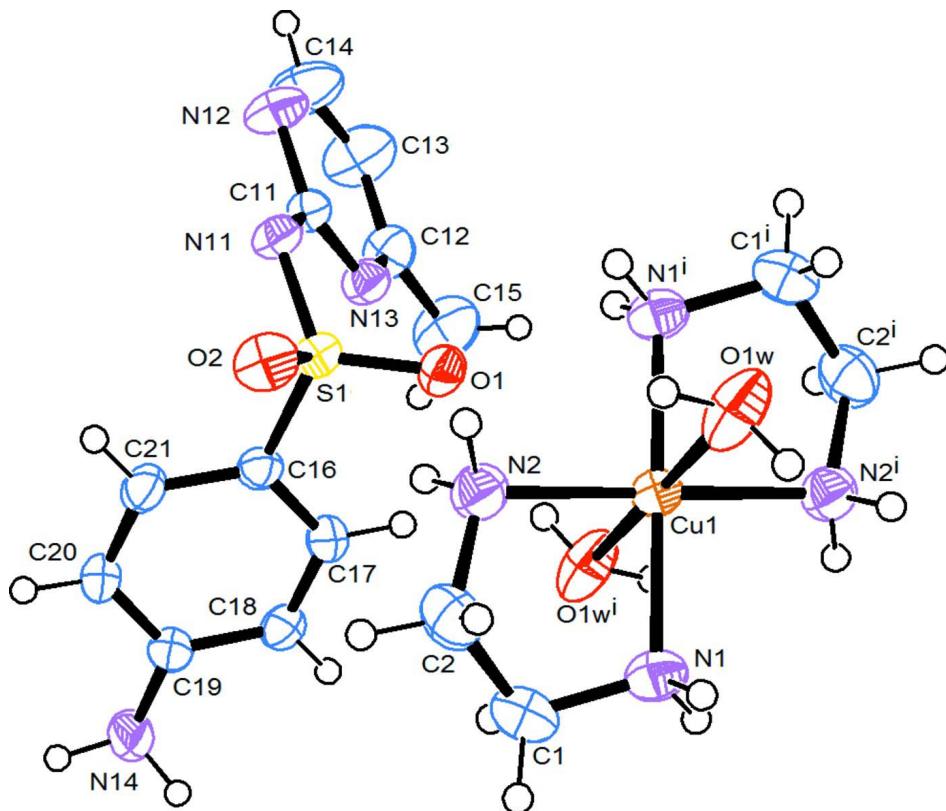
Figure 1

Crystal structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level.
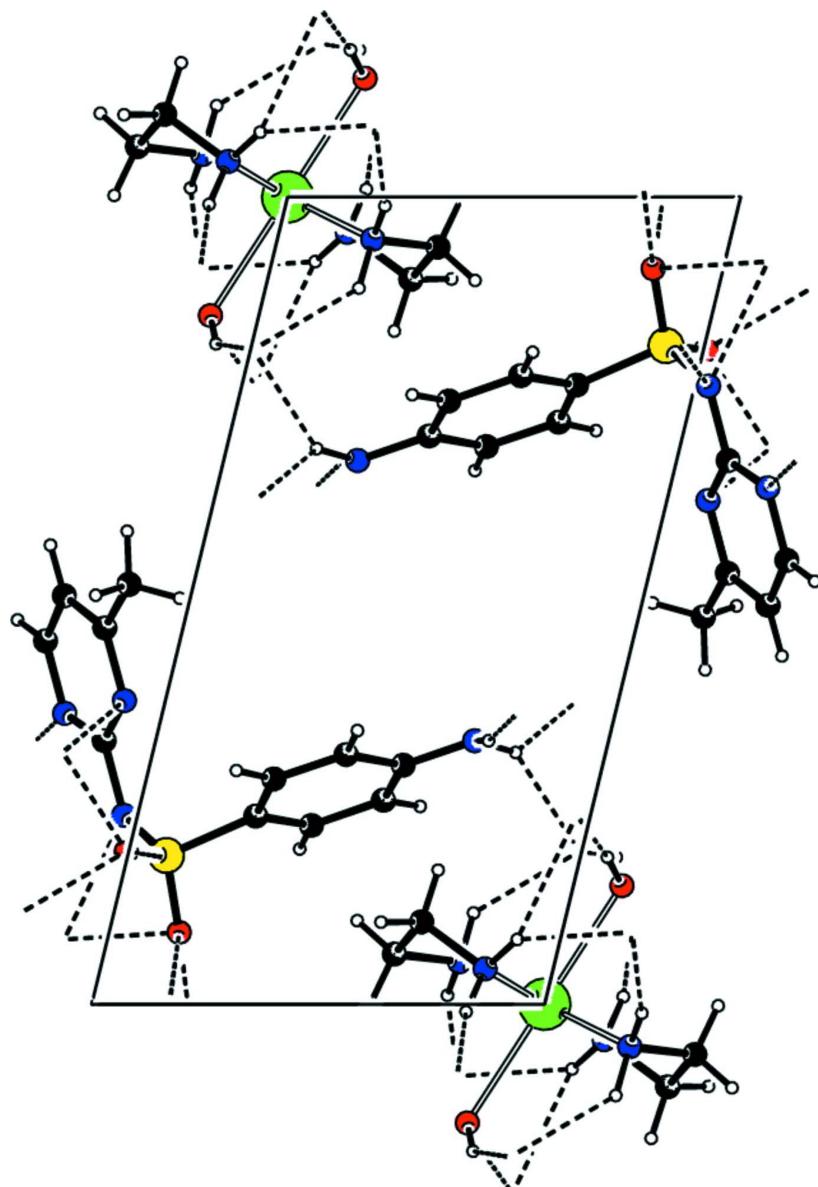
Figure 2

Crystal packing of the title compound, shown through the *a* axis, with hydrogen bonding drawn as dashed lines.

Diaquabis(ethylenediamine-*κ²N,N′*)copper(II) bis[(4-aminophenylsulfonyl)(4-methylpyrimidin-2-yl)azanide]

Crystal data
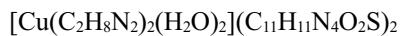
[Cu(C₂H₈N₂)₂(H₂O)₂](C₁₁H₁₁N₄O₂S)₂	$\gamma = 78.873\ (5)°$
$M_r = 746.41$	$V = 866.40\ (9)$ Å³
Triclinic, $P\bar{1}$	$Z = 1$
Hall symbol: -P 1	$F(000) = 391$
$a = 7.5429\ (4)$ Å	$D_x = 1.431$ Mg m⁻³
$b = 8.1800\ (5)$ Å	Mo *Kα* radiation, $\lambda = 0.71069$ Å
$c = 14.8434\ (8)$ Å	Cell parameters from 3709 reflections
$\alpha = 75.299\ (5)°$	$\theta = 3$–$29°$
$\beta = 82.800\ (5)°$	$\mu = 0.81$ mm⁻¹

T = 293 K

Block, blue

0.41 × 0.36 × 0.17 mm

Data collection

Oxford Diffraction Gemini diffractometer	4738 measured reflections
Radiation source: fine-focus sealed tube	4020 independent reflections
Graphite monochromator	3361 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	R_{int} = 0.019
Absorption correction: analytical (de Meulenaer & Tompa, 1965)	θ_{max} = 29.3°, θ_{min} = 2.9°
	$h = -10 \rightarrow 7$
T_{min} = 0.723, T_{max} = 0.869	$k = -9 \rightarrow 11$
	$l = -20 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.097	
S = 1.05	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2 + 0.4528P]$
4020 reflections	where $P = (F_o^2 + 2F_c^2)/3$
215 parameters	$(\Delta/\sigma)_{max} < 0.001$
0 restraints	$\Delta\rho_{max}$ = 0.33 e Å⁻³
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min}$ = −0.38 e Å⁻³

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems open-flow nitrogen cryostat (Cosier & Glazer, 1986) with a nominal stability of 0.1 K.
Cosier, J. & Glazer, A·*M*., 1986. J. Appl. Cryst. 105–107.

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	0.5	0	0	0.03130 (12)
S1	0.93674 (7)	0.08503 (7)	0.18420 (3)	0.03012 (13)
O1	0.7864 (2)	−0.0053 (2)	0.18937 (11)	0.0387 (4)
O2	1.0053 (2)	0.1546 (2)	0.08903 (10)	0.0428 (4)
C20	0.8897 (3)	0.5351 (3)	0.25274 (16)	0.0355 (5)
H20	0.9615	0.6189	0.2451	0.043*
N13	0.9256 (2)	−0.0906 (2)	0.37617 (12)	0.0347 (4)
C21	0.9576 (3)	0.3893 (3)	0.22151 (15)	0.0346 (5)
H21	1.0743	0.3759	0.1924	0.041*
C16	0.8532 (3)	0.2613 (3)	0.23311 (14)	0.0291 (4)
O1W	0.4227 (2)	0.1071 (3)	0.14692 (12)	0.0552 (5)
C12	0.9149 (3)	−0.1728 (3)	0.46614 (16)	0.0435 (6)

C11	1.0858 (3)	−0.1138 (3)	0.32650 (15)	0.0310 (4)
N11	1.1063 (2)	−0.0306 (2)	0.23427 (12)	0.0325 (4)
N12	1.2372 (3)	−0.2157 (3)	0.36031 (14)	0.0469 (5)
C15	0.7356 (4)	−0.1427 (5)	0.5202 (2)	0.0659 (8)
H15A	0.6836	−0.0235	0.5029	0.099*
H15B	0.752	−0.1751	0.5858	0.099*
H15C	0.656	−0.2102	0.5066	0.099*
C13	1.0634 (4)	−0.2794 (4)	0.5060 (2)	0.0652 (9)
H13	1.0572	−0.3371	0.5686	0.078*
C14	1.2192 (4)	−0.2967 (4)	0.4501 (2)	0.0658 (9)
H14	1.3198	−0.3699	0.4761	0.079*
C17	0.6811 (3)	0.2811 (3)	0.27905 (14)	0.0323 (5)
H17	0.6123	0.1942	0.2895	0.039*
N14	0.6421 (3)	0.7043 (3)	0.32650 (17)	0.0488 (5)
C19	0.7133 (3)	0.5595 (3)	0.29608 (15)	0.0328 (5)
C18	0.6118 (3)	0.4279 (3)	0.30924 (15)	0.0343 (5)
H18	0.4955	0.44	0.3389	0.041*
N1	0.6743 (3)	−0.2106 (2)	0.05258 (13)	0.0382 (4)
H1NA	0.7839	−0.2193	0.011	0.046*
H1NB	0.7067	−0.2059	0.113	0.046*
N2	0.3086 (3)	−0.1504 (2)	0.04393 (14)	0.0394 (4)
H2NA	0.2099	−0.0953	0.0802	0.047*
H2NB	0.2601	−0.1696	−0.0093	0.047*
C1	0.5849 (4)	−0.3587 (3)	0.06228 (18)	0.0455 (6)
H1A	0.6484	−0.4586	0.1035	0.055*
H1B	0.5857	−0.384	0.0018	0.055*
C2	0.3928 (4)	−0.3160 (3)	0.10211 (18)	0.0476 (6)
H2A	0.3254	−0.4055	0.1017	0.057*
H2B	0.3916	−0.3071	0.1661	0.057*
H14A	0.5169	0.7352	0.3264	0.05*
H14B	0.7011	0.801	0.3119	0.05*
H1W	0.5101	0.0795	0.182	0.05*
H2W	0.3232	0.0599	0.182	0.05*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0291 (2)	0.0302 (2)	0.0334 (2)	−0.00225 (15)	−0.00634 (15)	−0.00569 (15)
S1	0.0257 (3)	0.0345 (3)	0.0295 (3)	−0.0024 (2)	−0.0030 (2)	−0.0079 (2)
O1	0.0305 (8)	0.0411 (9)	0.0488 (9)	−0.0061 (7)	−0.0087 (7)	−0.0156 (7)
O2	0.0432 (9)	0.0525 (10)	0.0277 (8)	−0.0025 (8)	0.0009 (7)	−0.0066 (7)
C20	0.0292 (11)	0.0323 (12)	0.0452 (12)	−0.0109 (9)	−0.0030 (9)	−0.0056 (10)
N13	0.0300 (9)	0.0369 (10)	0.0354 (10)	−0.0041 (8)	−0.0007 (8)	−0.0071 (8)
C21	0.0246 (10)	0.0390 (12)	0.0381 (12)	−0.0075 (9)	0.0004 (9)	−0.0051 (9)
C16	0.0275 (10)	0.0282 (10)	0.0294 (10)	−0.0025 (8)	−0.0047 (8)	−0.0035 (8)
O1W	0.0365 (9)	0.0874 (14)	0.0414 (10)	−0.0189 (9)	−0.0090 (7)	−0.0056 (9)
C12	0.0428 (13)	0.0493 (15)	0.0367 (12)	−0.0103 (11)	0.0000 (10)	−0.0068 (11)
C11	0.0270 (10)	0.0300 (11)	0.0366 (11)	−0.0028 (8)	−0.0029 (8)	−0.0099 (9)

N11	0.0231 (9)	0.0370 (10)	0.0342 (9)	−0.0004 (7)	−0.0007 (7)	−0.0066 (8)
N12	0.0329 (10)	0.0558 (13)	0.0437 (12)	0.0082 (9)	−0.0079 (9)	−0.0061 (10)
C15	0.0537 (17)	0.087 (2)	0.0487 (16)	−0.0136 (16)	0.0144 (13)	−0.0092 (15)
C13	0.0594 (18)	0.082 (2)	0.0379 (14)	0.0001 (16)	−0.0060 (13)	0.0082 (14)
C14	0.0506 (17)	0.078 (2)	0.0508 (17)	0.0136 (15)	−0.0142 (13)	0.0038 (15)
C17	0.0303 (11)	0.0299 (11)	0.0362 (11)	−0.0091 (9)	−0.0002 (9)	−0.0053 (9)
N14	0.0372 (11)	0.0357 (11)	0.0781 (15)	−0.0080 (9)	0.0029 (10)	−0.0239 (10)
C19	0.0316 (11)	0.0300 (11)	0.0357 (11)	−0.0049 (9)	−0.0051 (9)	−0.0050 (9)
C18	0.0252 (10)	0.0361 (12)	0.0397 (12)	−0.0047 (9)	0.0017 (9)	−0.0075 (9)
N1	0.0359 (10)	0.0388 (11)	0.0353 (10)	0.0005 (8)	−0.0066 (8)	−0.0037 (8)
N2	0.0352 (10)	0.0417 (11)	0.0429 (11)	−0.0046 (8)	−0.0037 (8)	−0.0141 (9)
C1	0.0549 (15)	0.0320 (12)	0.0446 (14)	−0.0010 (11)	−0.0043 (11)	−0.0047 (10)
C2	0.0555 (16)	0.0379 (14)	0.0468 (14)	−0.0136 (12)	0.0009 (12)	−0.0034 (11)

Geometric parameters (Å, º)

Cu1—N1	2.0016 (18)	C15—H15B	0.96
Cu1—N1i	2.0016 (18)	C15—H15C	0.96
Cu1—N2	2.0168 (19)	C13—C14	1.357 (4)
Cu1—N2i	2.0168 (19)	C13—H13	0.93
S1—O2	1.4524 (16)	C14—H14	0.93
S1—O1	1.4530 (16)	C17—C18	1.374 (3)
S1—N11	1.5806 (17)	C17—H17	0.93
S1—C16	1.752 (2)	N14—C19	1.364 (3)
C20—C21	1.373 (3)	N14—H14A	0.9300
C20—C19	1.404 (3)	N14—H14B	0.9500
C20—H20	0.93	C19—C18	1.399 (3)
N13—C12	1.334 (3)	C18—H18	0.93
N13—C11	1.341 (3)	N1—C1	1.465 (3)
C21—C16	1.393 (3)	N1—H1NA	0.97
C21—H21	0.93	N1—H1NB	0.97
C16—C17	1.389 (3)	N2—C2	1.481 (3)
O1W—H1W	0.8500	N2—H2NA	0.97
O1W—H2W	0.9500	N2—H2NB	0.97
C12—C13	1.376 (4)	C1—C2	1.505 (4)
C12—C15	1.494 (4)	C1—H1A	0.97
C11—N12	1.347 (3)	C1—H1B	0.97
C11—N11	1.370 (3)	C2—H2A	0.97
N12—C14	1.332 (3)	C2—H2B	0.97
C15—H15A	0.96		
N1—Cu1—N1i	180	N12—C14—C13	124.2 (2)
N1—Cu1—N2	85.23 (8)	N12—C14—H14	117.9
N1i—Cu1—N2	94.77 (8)	C13—C14—H14	117.9
N1—Cu1—N2i	94.77 (8)	C18—C17—C16	120.5 (2)
N1i—Cu1—N2i	85.23 (8)	C18—C17—H17	119.7
N2—Cu1—N2i	180	C16—C17—H17	119.7
O2—S1—O1	113.23 (10)	C19—N14—H14A	115.00

O2—S1—N11	105.46 (9)	C19—N14—H14B	122.00
O1—S1—N11	113.64 (10)	H14A—N14—H14B	112.00
O2—S1—C16	106.20 (10)	N14—C19—C18	120.2 (2)
O1—S1—C16	106.87 (10)	N14—C19—C20	122.0 (2)
N11—S1—C16	111.27 (10)	C18—C19—C20	117.8 (2)
C21—C20—C19	121.0 (2)	C17—C18—C19	121.1 (2)
C21—C20—H20	119.5	C17—C18—H18	119.5
C19—C20—H20	119.5	C19—C18—H18	119.5
C12—N13—C11	117.89 (19)	C1—N1—Cu1	107.55 (14)
C20—C21—C16	120.5 (2)	C1—N1—H1NA	110.2
C20—C21—H21	119.7	Cu1—N1—H1NA	110.2
C16—C21—H21	119.7	C1—N1—H1NB	110.2
C17—C16—C21	119.0 (2)	Cu1—N1—H1NB	110.2
C17—C16—S1	121.54 (16)	H1NA—N1—H1NB	108.5
C21—C16—S1	119.33 (16)	C2—N2—Cu1	108.34 (14)
H1W—O1W—H2W	107.00	C2—N2—H2NA	110
N13—C12—C13	120.8 (2)	Cu1—N2—H2NA	110
N13—C12—C15	116.8 (2)	C2—N2—H2NB	110
C13—C12—C15	122.4 (2)	Cu1—N2—H2NB	110
N13—C11—N12	124.9 (2)	H2NA—N2—H2NB	108.4
N13—C11—N11	120.69 (18)	N1—C1—C2	108.2 (2)
N12—C11—N11	114.39 (19)	N1—C1—H1A	110.1
C11—N11—S1	119.66 (14)	C2—C1—H1A	110.1
C14—N12—C11	115.0 (2)	N1—C1—H1B	110.1
C12—C15—H15A	109.5	C2—C1—H1B	110.1
C12—C15—H15B	109.5	H1A—C1—H1B	108.4
H15A—C15—H15B	109.5	N2—C2—C1	108.23 (19)
C12—C15—H15C	109.5	N2—C2—H2A	110.1
H15A—C15—H15C	109.5	C1—C2—H2A	110.1
H15B—C15—H15C	109.5	N2—C2—H2B	110.1
C14—C13—C12	117.2 (2)	C1—C2—H2B	110.1
C14—C13—H13	121.4	H2A—C2—H2B	108.4
C12—C13—H13	121.4		
C19—C20—C21—C16	−0.7 (3)	C16—S1—N11—C11	64.56 (19)
C20—C21—C16—C17	−1.8 (3)	N13—C11—N12—C14	0.1 (4)
C20—C21—C16—S1	174.88 (16)	N11—C11—N12—C14	179.7 (2)
O2—S1—C16—C17	129.97 (17)	N13—C12—C13—C14	0.0 (5)
O1—S1—C16—C17	8.82 (19)	C15—C12—C13—C14	−179.9 (3)
N11—S1—C16—C17	−115.76 (17)	C11—N12—C14—C13	−1.0 (5)
O2—S1—C16—C21	−46.61 (18)	C12—C13—C14—N12	1.0 (5)
O1—S1—C16—C21	−167.75 (16)	C21—C16—C17—C18	2.7 (3)
N11—S1—C16—C21	67.66 (18)	S1—C16—C17—C18	−173.90 (16)
C11—N13—C12—C13	−0.8 (4)	C21—C20—C19—N14	−179.1 (2)
C11—N13—C12—C15	179.1 (2)	C21—C20—C19—C18	2.2 (3)
C12—N13—C11—N12	0.8 (3)	C16—C17—C18—C19	−1.1 (3)
C12—N13—C11—N11	−178.8 (2)	N14—C19—C18—C17	180.0 (2)
N13—C11—N11—S1	−3.7 (3)	C20—C19—C18—C17	−1.3 (3)

N12—C11—N11—S1	176.63 (17)	Cu1—N1—C1—C2	−43.1 (2)
O2—S1—N11—C11	179.29 (17)	Cu1—N2—C2—C1	−35.0 (2)
O1—S1—N11—C11	−56.1 (2)	N1—C1—C2—N2	52.3 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*NA*···O2ii	0.97	2.09	3.022 (3)	162
O1*W*—H1*W*···O1	0.85	2.07	2.816 (2)	145
N1—H1*NB*···O1	0.97	2.41	3.219 (2)	140
O1*W*—H2*W*···N11iii	0.95	1.92	2.858 (2)	171
N2—H2*NA*···O2iii	0.97	2.33	3.189 (3)	147
N2—H2*NA*···N11iii	0.97	2.47	3.319 (3)	145
N2—H2*NB*···O2i	0.97	2.42	3.277 (3)	147
N14—H14*A*···N12iv	0.93	2.09	3.003 (3)	166
N14—H14*B*···O1v	0.95	2.21	2.993 (3)	140
N14—H14*B*···N13v	0.95	2.44	3.215 (3)	139
C17—H17···O1	0.93	2.55	2.915 (3)	104

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