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Synthesis and crystal structure of poly[(2,6-dimethylpyrazine-κN^4)(μ_3-thiocyanato-$\kappa^3 N$:S:S)-copper(I)]

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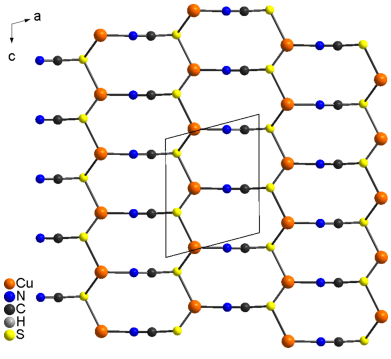
Crystals of the title compound, $[Cu(NCS)(C_6H_8N_2)]_n$ ($C_6H_8N_2$ = 2,6-dimethylpyrazine), were prepared by the reaction of CuNCS and 2,6-dimethylpyrazine in acetonitrile. The asymmetric unit consists of one Cu^I cation, one thiocyanate anion and one 2,6-dimethylpyrazine ligand with all atoms lying on general positions. The copper cations are tetrahedrally coordinated by two S- and one N-bonded thiocyanate anions and one 2,6-dimethylpyrazine ligand, which s coordinated to the metal center with the N atom that is not adjacent to the methyl groups. The copper cations are linked by the μ-1,3,3 (N,S,S) bridging thiocyanate anions into layers that lie parallel to the *ac* plane. The layers are stacked perpendicular to the *b*-axis direction and are separated by the 2,6-dimethylpyrazine ligands. The title crystal structure is compared with those of related CuNCS compounds with isomeric dimethylpyrazine ligands.

1. Chemical context

Coordination compounds based on copper(I) halides with chloride, bromide and iodide anions and N-donor coligands show an extremely large structural variability (*e.g.*, Kromp & Sheldrick, 1999; Näther *et al.*, 2001, 2002; Li *et al.*, 2005; Peng *et al.*, 2010). They usually consist of a variety of CuX substructures such as monomeric and dimeric units, chains or layers that can be further linked if bridging ligands are used. This might also be one reason why several polymorphs or isomers are reported (Näther & Jess, 2003; Park *et al.*, 2012; Peng *et al.*, 2010; Näther *et al.*, 2003). For many of these compounds, a different ratio between the copper(I) halide and the N-donor coligands is observed and thermal treatment of the coligand-rich compounds usually leads to the transformation into coligand-deficient compounds that show more condensed CuX substructures (Näther & Jess, 2001, 2002).

Such coordination compounds can also be prepared with copper(I) pseudohalides such as cyanide, azide or thiocyanate anions and many of them are reported in the literature because of their luminescence properties (Chesnut *et al.*, 1999; Lemos *et al.*, 2001; Starosta *et al.*, 2012; Nitsch *et al.*, 2015). As is the case for the copper(I) halide coordination compounds, they also show typical CuX substructures (X = pseudohalide), which, especially for cyanides, are very often more complicated than those in copper(I) halides. The different CuX substructures can further be connected into more condensed networks if bridging coligands such as, for example, pyrazine derivatives are used. If a database search is limited to the isomeric dimethylpyrazine ligands and copper(I), a number of compounds with cyanide, azide and thiocyanate anions are

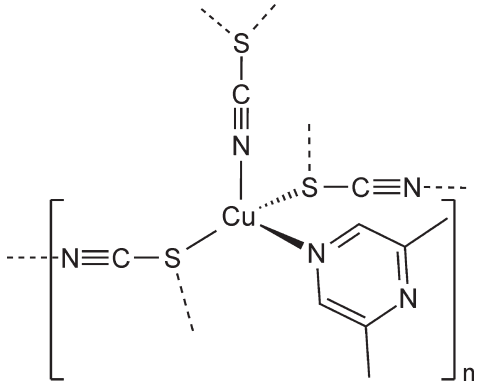


reported in the CSD (Version 5.43, 2025; Groom *et al.*, 2016) using CONQUEST (Bruno *et al.*, 2002).

With azide anions, no copper(I) compounds with 2,3-dimethylpyrazine are reported but one three-dimensional compound with the composition $Cu_2(N_3)_2$(2,5-dimethylpyrazine) is known that shows a complicated Cu–azide substructure, in which the azide anions act as μ-1,1,3 bridging ligands (Guang *et al.*, 2012). Furthermore, $Cu_2(N_3)_2$(2,6-dimethylpyrazine) is also found (Fan *et al.*, 2015*a*,*b*).

Copper(I) compounds with cyanide anions are reported with all three isomers of dimethylpyrazine. These include $Cu_3(CN)_3$(2,3-dimethylpyrazine) (Greve & Näther, 2004), $Cu_6(CN)_6$(2,3-dimethylpyrazine) (Chesnut *et al.*, 2001) and $Cu_2(CN)_2$(2,5-dimethylpyrazine) (Chesnut *et al.*, 2001). Finally, two isomers of $Cu_2(CN)_2$(2,6-dimethylpyrazine) are reported. In one of them, the copper cations are linked by bridging cyanide anions into $Cu_4(CN)_4$ units that condense into layers by way of $Cu_2(CN)_2$ four-membered rings (Näther, 2025), whereas in the second modification a one-dimensional copper(I) cyanide network is found that consists of alternating twelve- and four-membered rings (Chesnut *et al.*, 2001).

With thiocyanate anions and 2,5-dimethylpyrazine, a compound with the composition $Cu_2(NCS)_2$(2,5-dimethylpyrazine) is found, in which CuNCS layers are observed, that are linked by the 2,5-dimethylpyrazine ligands into a three-dimensional network (Näther *et al.*, 2003; Otieno *et al.*, 2003). A three-dimensional structure is also found for $Cu_2(NCS)_2$(2,3-dimethylpyrazine), even if the layer topology is different from that of the 2,5-dimethylpyrazine compound (Näther *et al.*, 2003). Compounds with a 1:1 ratio of copper(I) thiocyanate and 2,6-dimethylpyrazine are unknown and we therefore tried to prepare such compounds by the reaction of CuNCS and 2,6-dimethylpyrazine. In the course of these investigations we obtained crystals of the title compound, (**I**), that were characterized by single-crystal X-ray diffraction.



2. Structural commentary

The asymmetric unit of (**I**), Cu(NCS)($C_6H_8N_2$) ($C_6H_8N_2$ = 2,6-dimethylpyrazine), consists of one copper(I) cation, one thiocyanate anion and one 2,6-dimethylpyrazine ligand, with all of the atoms located in general positions (Fig. 1) in space group $P2_1/c$. The metal cations are fourfold coordinated by one N- and two S-bonded thiocyanate anions and one 2,6-dimethylpyrazine ligand. Because of steric repulsion between the metal cation and the methyl groups of the 2,6-dimethylpyrazine ligand, this ligand is only coordinated with the N atom that does not lie between the two methyl groups (Fig. 1). The two Cu—S bond lengths are only slightly different and the bond angles deviate from the ideal values, which shows that the tetrahedra are slightly distorted (Table 1). As expected, the C—N—Cu angle is close to linearity, whereas the C—S—Cu angles roughly correspond to a tetrahedral angle (Table 1).

Table 1
Selected geometric parameters (Å, °).

Cu1—N11^{i}	1.963 (2)	Cu1—S1	2.3238 (8)
Cu1—N2	2.094 (2)	Cu1—S1^{ii}	2.3809 (8)
N11^{i}—Cu1—N2	105.53 (10)	S1—Cu1—S1^{ii}	114.74 (3)
N11^{i}—Cu1—S1	118.22 (7)	C11—S1—Cu1	107.96 (9)
N2—Cu1—S1	110.30 (7)	C11—S1—Cu1^{iii}	96.46 (10)
N11^{i}—Cu1—S1^{ii}	105.40 (8)	Cu1—S1—Cu1^{iii}	105.06 (3)
N2—Cu1—S1^{ii}	100.90 (7)	C11—N11—Cu1^{iv}	168.0 (3)

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

In the extended structure, the copper(I) cations are connected by μ-1,1,3(*S*,*S*,*N*)-bridging thiocyanate anions into ten-membered rings built up of three cations and three thiocyanate anions, condensing into corrugated layers that lie parallel to the *ac* plane (Fig. 2). It is noted that this layer topology is completely different from that in $Cu_2(NCS)_2$(2,3-dimethylpyrazine) (Näther *et al.*, 2003), where tetranuclear units built up of four copper(I) cations and four thiocyanate anions are observed, which condense into layers by way of

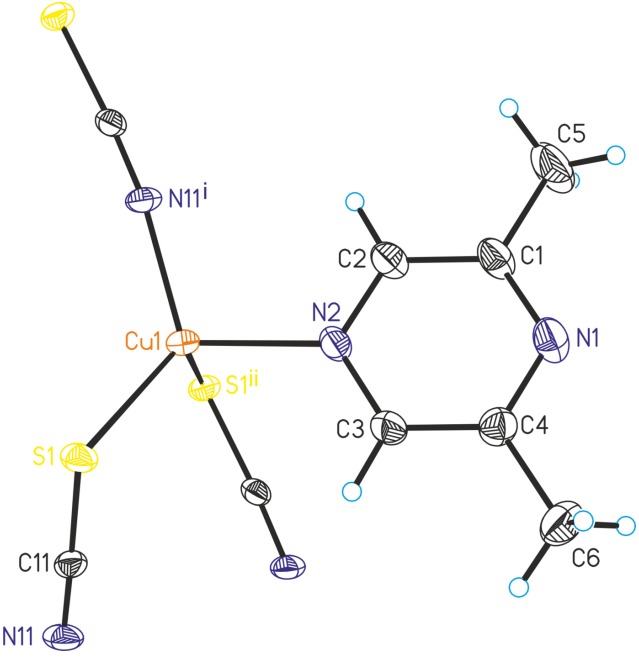


Figure 1
The asymmetric unit of (**I**) expanded to show the full metal coordination sphere with labeling of selected atoms and displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i) $x-1, -y+\frac{1}{2}, z$ - 1/2; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

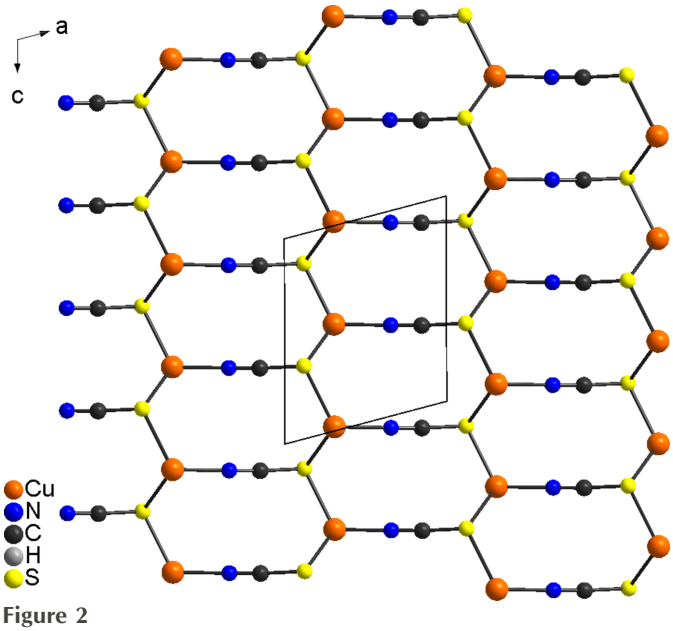


Figure 2
Crystal structure of (**I**) with a view onto the CuNCS layers along the crystallographic *b*-axis direction. The 2,6-dimethylpyrazine ligands are omitted for clarity.

Cu_2S_2 rings (Fig. 3: top). In contrast, in $Cu_2(NCS)_2$(2,5-dimethylpyrazine) (Näther *et al.*, 2003; Otieno *et al.*, 2003), ten-membered rings are also found but the orientation of the two thiocyanate anions within these rings is reversed and the rings are therefore more distorted (Fig. 3: bottom).

Concerning the overall structural discussion, it must be kept in mind that in the 2,3- and 2,5-dimethylpyrazine compounds, the ratio between the CuNCS component and the dimethylpyrazine derivative is different, but this difference only originates from the fact that the coligand is only terminally

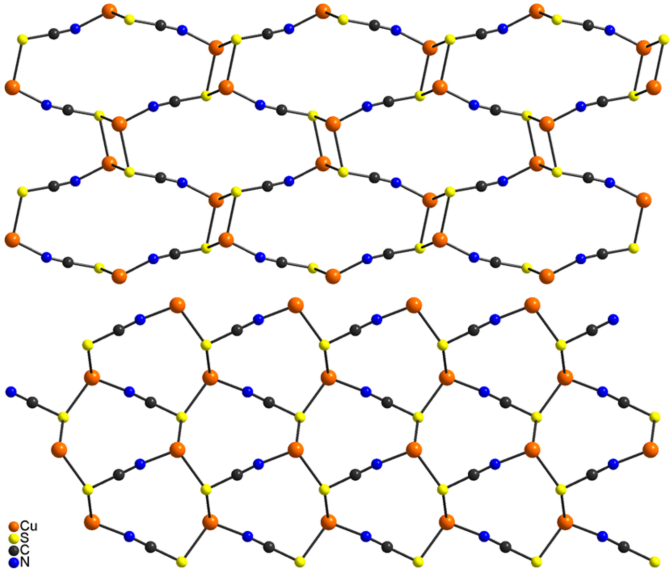


Figure 3
View of the CuNCS networks in $Cu_2(NCS)_2$(2,3-dimethylpyrazine) (top) and $Cu_2(NCS)_2$(2,5-dimethylpyrazine) (bottom) reported in the literature (Näther *et al.*, 2003; Otieno *et al.*, 2003).

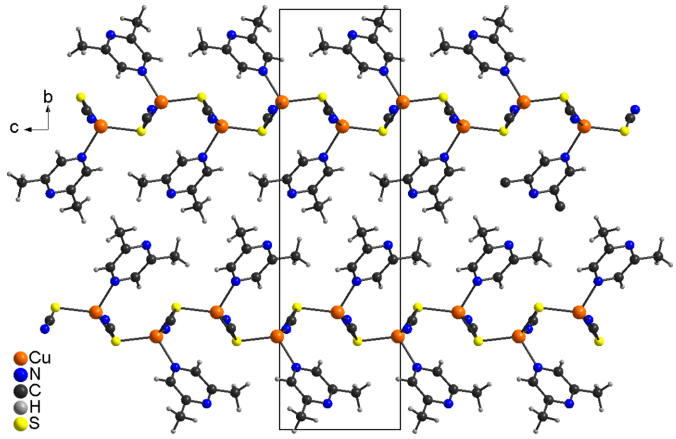


Figure 4
Crystal structure of (**I**) with a view along the crystallographic *a*-axis direction.

coordinating in (**I**), whereas it act as a bridging ligand in the compounds with the two other isomers. In this context, it is noted that no CuNCS compounds with 2,3- or 2,5-dimethylpyrazine are reported, in which the ratio between CuNCS and coligand is identical to that in (**I**), which indicates that for these ligands a terminal coordination is not favored. In contrast, in (**I**), one of the coordinating N atoms of the 2,6-dimethylpyrazine ligand is shielded by the two neighbouring methyl groups, which means that a compound with a bridging coordination of the neutral coligand, similar to that in the thiocyanate compounds with 2,3- and 2,5-dimethylpyrazine, might not exist.

3. Supramolecular features

The layers in (**I**) are stacked perpendicular to the *b*-axis direction and are separated by the 2,6-dimethylpyrazine ligands (Fig. 4). The coligands of neighboring layers point towards each other, which means that the layers are only linked by van der Waals interactions. There are no directional intermolecular interactions. This is completely different to the 2,3- and 2,5-dimethylpyrazine compounds $Cu_2(NCS)_2$(2,3-dimethylpyrazine) and $Cu_2(NCS)_2$(2,5-dimethylpyrazine) in which the layers are connected by bridging 2,3- and 2,5-dimethylpyrazine ligands into a three-dimensional network (Näther *et al.*, 2003; Otieno *et al.*, 2003). As mentioned above, this might be traced back to the fact that in 2,3- and 2,5-dimethylpyrazine, only one methyl group is adjacent to the coordinating N atom, whereas in 2,6-dimethylpyrazine the two methyl groups effectively shield one of the N atoms, which makes metal coordination much more difficult.

4. Database survey

As mentioned above, with 2,6-dimethylpyrazine and copper(I) thiocyanate no compounds are reported but there is one mixed copper(I/II) pseudohalide compound with the composition $[Cu_8^{I}Cu_2^{II}(CN)_4(NCS)_8$(2,6-dimethylpyrazine)$_7]$ that

shows a three-dimensional coordination network (Jess & Näther, 2006).

With copper(I) halides, two compounds with 2,6-dimethylpyrazine are known. This includes Cu_2Cl_2(2,6-dimethylpyrazine), in which the copper cations are tetrahedrally coordinated by three chloride anions and one 2,6-dimethylpyrazine ligand and are linked by μ-1,1 bridging chloride anions into double chains that are further connected into layers by bridging 2,6-dimethylpyrazine ligands (Fan *et al.*, 2015). CuI(2,6-dimethylpyrazine) shows a structure similar to that of Cu_2Cl_2(2,6-dimethylpyrazine) mentioned above, but in this compound, the 2,6-dimethylpyrazine ligand is only terminally coordinated (Kitada & Ishida, 2014; Zhang *et al.*, 2014).

Finally, it is noted that with divalent copper(II) cations, two different polymorphs with the composition $CuBr_2$(2,6-dimethylpyrazine) are reported, in which the copper cations are linked into chains by bridging 2,6-dimethylpyrazine ligands (Ding *et al.*, 2021).

5. Synthesis and crystallization

Copper(I) thiocyanate and 2,6-dimethylpyrazine were purchased from Sigma-Aldrich: 1.000 mmol (121.6 mg) of copper(I) thiocyanate and 1.000 mmol (108.1 mg) of 2,6-dimethylpyrazine were reacted in 3 ml of acetonitrile. Within 3 d, colourless blocks of (**I**) suitable for single crystal X-ray diffraction were obtained.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C—H hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and were refined isotropically with $U_{iso}(H) = 1.2U_{eq}(C)$ (1.5 for methyl H atoms).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu(NCS)(C_6H_8N_2)]$
M_r	229.76
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	200
a, b, c (Å)	5.6765 (4), 23.4382 (14), 6.9655 (6)
β (°)	104.620 (9)
V (Å^3)	896.73 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.61
Crystal size (mm)	0.20 × 0.19 × 0.15
Data collection	
Diffractometer	Stoe *IPDS*-II
Absorption correction	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2008)
T_{min}, T_{max}	0.470, 0.620
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6594, 2163, 1704
R_{int}	0.047
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.661
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.096, 1.03
No. of reflections	2163
No. of parameters	112
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.62

Computer programs: *X-AREA* (Stoe, 2008), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 1999) and *XP* in *SHELXTL-PC* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

Acknowledgements

Financial support by the State of Schleswig-Holstein is gratefully acknowledged.

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supporting information

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Synthesis and crystal structure of poly[(2,6-dimethylpyrazine-κN^4)(μ_3-thiocyanato-$\kappa^3 N{:}S{:}S$)copper(I)]

Christian Näther

Computing details

Poly[(2,6-dimethylpyrazine-κN^4)(μ_3-thiocyanato-$\kappa^3 N{:}S{:}S$)copper(I)]

Crystal data

$[Cu(NCS)(C_6H_8N_2)]$
$M_r = 229.76$
Monoclinic, $P2_1/c$
$a = 5.6765$ (4) Å
$b = 23.4382$ (14) Å
$c = 6.9655$ (6) Å
$\beta = 104.620$ (9)°
$V = 896.73$ (12) Å^3
$Z = 4$
$F(000) = 464$
$D_x = 1.702$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5598 reflections
$\theta = 6.3$–$56.0°$
$\mu = 2.61$ mm^{-1}
$T = 200$ K
Block, colorless
0.20 × 0.19 × 0.15 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: numerical (X-Red and X-Shape; Stoe, 2008)
$T_{min} = 0.470$, $T_{max} = 0.620$
6594 measured reflections
2163 independent reflections
1704 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 28.0°$, $\theta_{min} = 3.2°$
$h = -7 \rightarrow 7$
$k = -29 \rightarrow 30$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.096$
$S = 1.03$
2163 reflections
112 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.010 (3)

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.69476 (6)	0.27873 (2)	0.52022 (5)	0.02275 (15)
N1	0.7931 (5)	0.43852 (12)	0.1025 (4)	0.0296 (6)
C1	0.5987 (6)	0.40441 (13)	0.0613 (4)	0.0281 (6)
C2	0.5679 (6)	0.36229 (13)	0.1940 (4)	0.0252 (6)
H2	0.423880	0.339862	0.163200	0.030*
N2	0.7354 (4)	0.35266 (11)	0.3629 (3)	0.0226 (5)
C3	0.9327 (5)	0.38613 (14)	0.4014 (4)	0.0259 (6)
H3	1.057102	0.379901	0.519348	0.031*
C4	0.9611 (6)	0.42982 (13)	0.2736 (4)	0.0253 (6)
C5	0.4140 (8)	0.41223 (19)	−0.1321 (6)	0.0507 (11)
H5A	0.396766	0.452951	−0.164523	0.076*
H5B	0.256982	0.396923	−0.121909	0.076*
H5C	0.467254	0.391925	−0.236799	0.076*
C6	1.1765 (7)	0.46912 (17)	0.3216 (5)	0.0373 (8)
H6A	1.226703	0.477786	0.200078	0.056*
H6B	1.311239	0.450682	0.417527	0.056*
H6C	1.132326	0.504568	0.378469	0.056*
S1	0.88125 (12)	0.29030 (3)	0.85550 (10)	0.02064 (18)
C11	1.1536 (5)	0.25913 (13)	0.9018 (4)	0.0187 (5)
N11	1.3454 (4)	0.23893 (12)	0.9428 (3)	0.0243 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01201 (19)	0.0303 (2)	0.0246 (2)	−0.00085 (13)	0.00210 (13)	0.00651 (13)
N1	0.0388 (15)	0.0256 (14)	0.0223 (12)	−0.0007 (11)	0.0039 (11)	0.0035 (9)
C1	0.0351 (16)	0.0231 (16)	0.0208 (13)	0.0000 (13)	−0.0028 (12)	0.0016 (11)
C2	0.0276 (14)	0.0204 (15)	0.0236 (13)	0.0012 (11)	−0.0012 (11)	0.0008 (11)
N2	0.0247 (12)	0.0197 (12)	0.0200 (11)	−0.0019 (9)	−0.0005 (9)	0.0043 (9)
C3	0.0243 (14)	0.0271 (16)	0.0218 (13)	−0.0043 (11)	−0.0023 (11)	0.0030 (10)
C4	0.0263 (15)	0.0246 (15)	0.0246 (14)	−0.0034 (12)	0.0053 (11)	−0.0017 (11)
C5	0.057 (2)	0.049 (2)	0.0310 (18)	−0.008 (2)	−0.0170 (17)	0.0144 (16)
C6	0.0353 (18)	0.038 (2)	0.0378 (18)	−0.0144 (15)	0.0071 (14)	0.0014 (13)
S1	0.0139 (3)	0.0280 (4)	0.0194 (3)	0.0041 (2)	0.0030 (2)	0.0007 (2)
C11	0.0148 (12)	0.0262 (14)	0.0146 (11)	−0.0048 (10)	0.0031 (9)	−0.0029 (9)
N11	0.0114 (10)	0.0392 (15)	0.0212 (11)	0.0020 (10)	0.0021 (8)	−0.0027 (10)

Geometric parameters (Å, º)

Cu1—N11^{i}	1.963 (2)	C3—C4	1.393 (4)
Cu1—N2	2.094 (2)	C3—H3	0.9500
Cu1—S1	2.3238 (8)	C4—C6	1.500 (4)
Cu1—S1^{ii}	2.3809 (8)	C5—H5A	0.9800
N1—C1	1.334 (4)	C5—H5B	0.9800
N1—C4	1.341 (4)	C5—H5C	0.9800
C1—C2	1.393 (4)	C6—H6A	0.9800
C1—C5	1.495 (5)	C6—H6B	0.9800
C2—N2	1.332 (4)	C6—H6C	0.9800
C2—H2	0.9500	S1—C11	1.666 (3)
N2—C3	1.338 (4)	C11—N11	1.155 (4)
N11^{i}—Cu1—N2	105.53 (10)	N1—C4—C6	117.5 (3)
N11^{i}—Cu1—S1	118.22 (7)	C3—C4—C6	121.9 (3)
N2—Cu1—S1	110.30 (7)	C1—C5—H5A	109.5
N11^{i}—Cu1—S1^{ii}	105.40 (8)	C1—C5—H5B	109.5
N2—Cu1—S1^{ii}	100.90 (7)	H5A—C5—H5B	109.5
S1—Cu1—S1^{ii}	114.74 (3)	C1—C5—H5C	109.5
C1—N1—C4	117.7 (3)	H5A—C5—H5C	109.5
N1—C1—C2	121.2 (3)	H5B—C5—H5C	109.5
N1—C1—C5	118.3 (3)	C4—C6—H6A	109.5
C2—C1—C5	120.5 (3)	C4—C6—H6B	109.5
N2—C2—C1	121.7 (3)	H6A—C6—H6B	109.5
N2—C2—H2	119.2	C4—C6—H6C	109.5
C1—C2—H2	119.2	H6A—C6—H6C	109.5
C2—N2—C3	116.9 (3)	H6B—C6—H6C	109.5
C2—N2—Cu1	117.0 (2)	C11—S1—Cu1	107.96 (9)
C3—N2—Cu1	125.3 (2)	C11—S1—Cu1^{iii}	96.46 (10)
N2—C3—C4	122.0 (3)	Cu1—S1—Cu1^{iii}	105.06 (3)
N2—C3—H3	119.0	N11—C11—S1	176.6 (3)
C4—C3—H3	119.0	C11—N11—Cu1^{iv}	168.0 (3)
N1—C4—C3	120.6 (3)		
C4—N1—C1—C2	1.8 (5)	C2—N2—C3—C4	1.2 (4)
C4—N1—C1—C5	−177.9 (3)	Cu1—N2—C3—C4	170.5 (2)
N1—C1—C2—N2	−2.9 (5)	C1—N1—C4—C3	0.7 (5)
C5—C1—C2—N2	176.7 (3)	C1—N1—C4—C6	−178.6 (3)
C1—C2—N2—C3	1.3 (4)	N2—C3—C4—N1	−2.3 (5)
C1—C2—N2—Cu1	−168.9 (2)	N2—C3—C4—C6	177.0 (3)

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