Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N—H···S and N—H···O hydrogen bonding in tetra-*n*-butylammonium (imidazolidine-2-thione-2κS)dioxo-1$\kappa^2 O$-di-μ-sulfido-1:2$\kappa^4 S$:*S*-copper(I)tungstate(VI)

Azizolla Beheshti,[a]* William Clegg,[b]* Sophie H. Dale[b] and Ahmad Solimankhani[a]

[a]Department of Chemistry, Faculty of Science, Shahid Chamran University, Ahvaz, Iran, and [b]School of Natural Sciences (Chemistry), University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU, England

Correspondence e-mail: beheshti_a@hotmail.com, w.clegg@ncl.ac.uk

Received 5 July 2005
Accepted 6 July 2005
Online 9 July 2005

In the title complex, $(C_{16}H_{36}N)[WCuO_2S_2(C_3H_6N_2S)]$, the W and Cu atoms have tetrahedral and trigonal-planar coordination, respectively. Two sulfide ligands bridge the two metal centres; tungsten is additionally coordinated by two terminal oxo ligands and copper by the exocyclic S atom of imidazolidine-2-thione. There is an intramolecular N—H···S hydrogen bond in the anion, and anions are linked into chains by N—H···O intermolecular hydrogen bonds. The more loosely held cation is disordered.

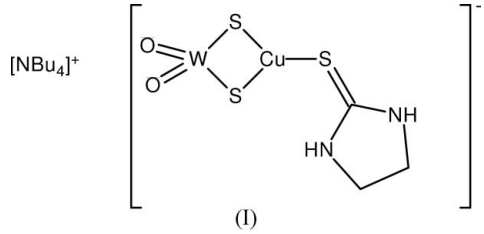
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.007 Å
Disorder in solvent or counterion
R factor = 0.033
wR factor = 0.073
Data-to-parameter ratio = 16.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The formation of hydrogen bonds, including intramolecular N—H···S hydrogen bonds, in many biological macromolecules such as azurin and rubredoxin, has been confirmed by X-ray crystallography, vibrational and NMR spectroscopic studies (Houseman *et al.*, 1992; Adman, 1991; Backes *et al.*, 1991; Blake *et al.*, 1992; Watenpaugh *et al.*, 1979; Tsukihara *et al.*, 1981; Adman *et al.*, 1975; Baker, 1988). We present here a copper(I) complex, (I), with two kinds of hydrogen bonds, namely intramolecular N—H···S and intermolecular N—H···O.



(I)

The structure of the bimetallic anion is shown in Fig. 1 and selected geometric parameters are given in Table 1. The disordered cation is geometrically unexceptional. In the $[O_2WS_2Cu(Imt)]^-$ anion (Imt is imidazolidine-2-thione), the coordination environments of tungsten(VI) and copper(I) are slightly distorted tetrahedral and rather more strongly

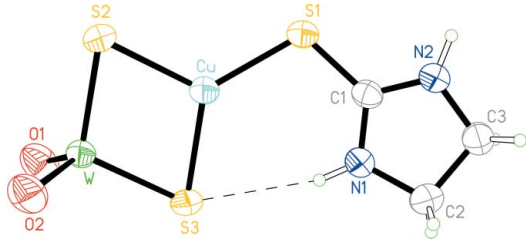


Figure 1
The structure of the anion with atom labels and 50% probability displacement ellipsoids for non-H atoms. The intramolecular hydrogen bond is shown as a dashed line.

distorted trigonal planar, respectively. The angular deviations around the Cu atom may be attributed to steric effects and the constraints of the WS_2Cu four-membered ring. Copper is coordinated by two bridging S and a terminal, monodentate S-donating Imt ligand. The bridging angles at S are the smallest angles in the complex and are only slightly larger than the value required for regular edge-sharing tetrahedra (70.5°; Summerville & Hoffman, 1976). Narrowing of the bridging angle is inevitably accompanied by a reduction in the W···Cu separation distance, which is not, however, considered as indicating a direct metal-metal bond. The Cu—S1 distance and Cu—S—C angle are typical of terminal monodentate S-donating thiones attached to trigonal planar Cu(I) (Beheshti *et al.*, 2004). In common with other thione complexes, a slight lengthening of the S—C distance occurs, relative to that of the C═S bond length in the free Imt ligand, due to a reduction in the π-bond character of the thione linkage accompanying metal-thione coordination. The Cu—S2 and Cu—S3 distances are in the range [2.168 (9)–2.340 (9) Å] reported for $(Et_4N)[WO_2S_2Cu(Hmimt)]$, where Hmimt is the closely related ligand 1-methylimidazole-2(3*H*)-thione (Beheshti *et al.*, 2004).

Although there are many crystallographically characterized examples of complexes in which Cu^I is bonded across S···S edges of $[WS_4]^{2-}$ and $[OWS_3]^{2-}$ tetrahedra, the title complex appears to be only the third case for $[O_2WS_2]^{2-}$, the others being the closely related Cu(Hmimt) complex mentioned above (Beheshti *et al.*, 2004) and a $CuPPh_3$ complex (Beheshti *et al.*, 2001).

The striking feature of the structure of the anion is the orientation of the thione ligand; this brings one NH group of the heterocyclic ligand into a position close to one bridging sulfur atom of the WO_2S_2 group, with the formation of an intramolecular N—H···S hydrogen bond (Fig.1 and Table 2). In addition to the intramolecular N—H···S hydrogen bond, the second NH group of Imt forms an intermolecular hydrogen bond with an oxo ligand attached to tungsten in a neighbouring anion (Fig. 2 and Table 2). This hydrogen bond generates a chain of anions. Such hydrogen bonds have been found to play important roles in regulating the properties of metal-sulfur proteins as well as their model complexes (Houseman *et al.*, 1992; Sun *et al.*, 1993).

In the solid state, infrared spectroscopy may also be used to probe the mode of coordination of Imt and $[WO_2S_2]^{2-}$ ligands. Uncoordinated Imt exhibits N—H stretching and C═S bands at 3200 and 510 cm^{-1}, respectively. The corresponding N—H and C═S vibration bands were observed at 3308 and 500 cm^{-1} for the complex. The shifts of ν(N—H) (108 cm^{-1} upwards) and ν(C═S) (10 cm^{-1} downwards) and the absence of a ν(S—H) band at 2500 cm^{-1} clearly indicate that the Imt ligand is coordinated only *via* the thione sulfur in the complex. The W═O stretching frequencies of the $[WO_2S_2]^{2-}$ ligand in the complex (918 and 867 cm^{-1}) are shifted to higher values than for the free $[WO_2S_2]^{2-}$ anion (850 and 795 cm^{-1} in the ammonium salt; McDonald *et al.*, 1983); this indicates that the $[WO_2S_2]^{2-}$ ligand is coordinated through its sulfur atoms. The band at 437 cm^{-1} is assigned to the bridging W—S bonds.

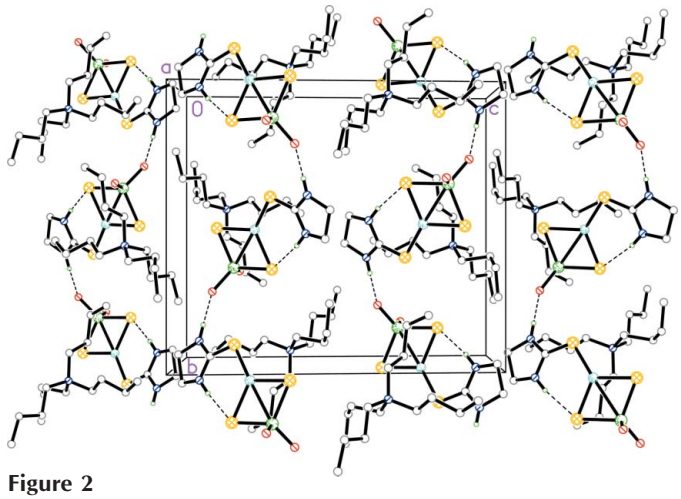


Figure 2
A section of the packing, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines, and other H atoms have been omitted, together with minor disorder components.

Thus, the infrared spectroscopic results are consistent with the X-ray structural analysis.

Experimental

$(NH_4)_2[WO_2S_2]$ (0.316 g, 1.0 mmol) was dissolved in acetone (40 ml) and solid (n-Bu_4N)Br (0.676 g, 2.1 mmol) was added. The mixture was stirred at room temperature for 5 min. CuCl (0.099 g, 1 mmol) was added and the mixture was stirred for 1 h. Imt (0.112 g, 1.1 mmol) was added and the mixture was stirred at room temperature for 4 h and then filtered. The filtrate was evaporated under vacuum. The oily residue was dissolved in dichloromethane (25 ml) and the solution filtered to remove any insoluble material. The filtrate was evaporated to dryness under vacuum. The residue was washed with distilled water (2 × 2 ml), 2-propanol (2 × 2 ml) and diethyl ether (2 × 5 ml) and dried *in vacuo* to give a pale-brown powder. The yield at this stage was 0.43 g (46%). Crystals were obtained by diffusing diethyl ether into a saturated solution in acetone. On leaving the solution to stand in a refrigerator overnight, air-stable orange crystals were deposited, which are soluble in common organic solvents. ^{1}H NMR (DMSO-d_6, 300 K): δ 8.38 (*s*, N—H), 3.68 (*s*, CH_2); ^{13}C NMR (DMSO-d_6, 300 K): δ 180.23 (C1), 45.41 (C2 and C3) (using the atom numbering of Fig. 1). In the ^{1}H NMR spectrum of the complex, the ligand signals are shifted down-field from their positions in the spectrum of the free ligand (N—H,7.94 and CH_2 3.505 p.p.m.), but in the ^{13}C NMR spectrum of the complex, the C═S signal is shifted up-field from its position in the spectrum of the free ligand (183.35 p.p.m.), due to the reduction of the C═S bond order upon coordination and a shift of electron density producing partial double bond character in the C—N bond. These observations indicate that, in DMSO-d_6, the ligand remains coordinated to the metal.

Crystal data

$(C_{16}H_{36}N)[WCuO_2S_2(C_3H_6N_2S)]$
M_r = 688.13
Monoclinic, $P2_1/c$
a = 10.6925 (16) Å
b = 14.875 (2) Å
c = 17.2342 (8) Å
β = 94.742 (7)°
V = 2731.7 (6) Å^3
Z = 4
D_x = 1.673 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 227 reflections
θ = 2.5–27.5°
μ = 5.23 mm^{-1}
T = 150 (2) K
Block, orange
0.77 × 0.43 × 0.31 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: numerical (*SHELXTL*; Sheldrick, 2001)
T_{min} = 0.100, T_{max} = 0.239
28801 measured reflections
6215 independent reflections
4881 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 27.5°
$h = -13 \rightarrow 13$
$k = -19 \rightarrow 18$
$l = -22 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.074
S = 1.07
6215 reflections
378 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0159P)^2 + 6.5317P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.029
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.00053 (11)

Table 1
Selected geometric parameters (Å, °).

W—Cu	2.6755 (6)	Cu—S3	2.2459 (14)
W—O1	1.731 (4)	S1—C1	1.711 (5)
W—O2	1.750 (3)	C1—N1	1.338 (6)
W—S2	2.2652 (13)	C1—N2	1.326 (6)
W—S3	2.2670 (13)	N1—C2	1.471 (6)
Cu—S1	2.2047 (13)	C2—C3	1.543 (7)
Cu—S2	2.2385 (14)	C3—N2	1.453 (6)
O1—W—O2	109.42 (18)	S1—C1—N1	126.8 (4)
O1—W—S2	109.53 (14)	S1—C1—N2	123.3 (3)
O1—W—S3	109.63 (15)	N1—C1—N2	109.9 (4)
O2—W—S2	110.36 (13)	C1—N1—C2	111.5 (4)
O2—W—S3	111.47 (13)	N1—C2—C3	101.2 (4)
S2—W—S3	106.37 (5)	C2—C3—N2	102.5 (4)
S1—Cu—S2	123.40 (5)	C1—N2—C3	112.0 (4)
S1—Cu—S3	128.57 (5)	W—S2—Cu	72.89 (4)
S2—Cu—S3	108.02 (5)	W—S3—Cu	72.72 (4)
Cu—S1—C1	106.99 (16)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···S3	0.87 (1)	2.66 (2)	3.490 (4)	160 (5)
N2—H2···O2^{i}	0.87 (1)	1.87 (1)	2.729 (5)	174 (5)

Symmetry code: (i) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

The cation is disordered. Most C atoms could be resolved into two components with sensible connectivities. Separate occupancy factors were refined for the components of each *n*-butyl group, giving values of 0.747 (9), 0.660 (12), 0.690 (9) and 0.817 (10) for the major sites; similarity restraints were applied to the displacement parameters and bond lengths. The remaining C atoms may also be disordered, to a smaller extent, but this could not be resolved. H atoms bonded to N were located in a difference map and refined with a restrained N—H distance of 0.87 (2) Å, and with U_{iso}(H) = 1.2U_{eq}(N). Other H atoms were positioned geometrically and refined with a riding model, with C—H = 0.95–0.99 Å, and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

We thank the EPSRC (UK) and Shahid Chamran University for financial support.

References

Adman, E. T. (1991). *Adv. Protein Chem.* **42**, 145–197.
Adman, E., Watenpaugh, K. D. & Jensen, L. H. (1975). *Proc. Natl Acad. Sci. USA*, **72**, 4854–4858.
Backes, G., Mino, Y., Loehr, T. M., Meyer, T. E., Cusanovich, M. A., Sweeney, W. V., Adman, E. T. & Sanders-Loehr, J. (1991). *J. Am. Chem. Soc.* **113**, 2055–2064.
Baker, E. N. (1988). *J. Mol. Biol.* **203**, 1071–1095.
Beheshti, A., Brooks, N. R., Clegg, W. & Khorrmdin, R. (2004). *Acta Cryst.* E**60**, m1923–m1926.
Beheshti, A., Clegg, W. & Fallah, H. (2001). *Inorg. Chim. Acta*, **322**, 1–6.
Blake, P. R., Park, J. B., Adams, M. W. W. & Summers, M. F. (1992). *J. Am. Chem. Soc.* **114**, 4931–4933.
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
Houseman, A. L. P., Oh, B. H., Kennedy, M. C., Fan, C., Werst, M. M., Beinert, H., Markley, J. L. & Hoffman, B. M. (1992). *Biochemistry*, **31**, 2073–2080.
McDonald, J. W., Friesen, G. D., Rosenhein, L. D. & Newton, W. E. (1983). *Inorg. Chim. Acta*, **72**, 205–210.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Sheldrick, G. M. (2001). *SHELXTL*. Version 5. Bruker AXS Inc., Madison, Wisconsin, USA.
Summerville, R. H. & Hoffman, R. (1976). *J. Am. Chem. Soc.* **98**, 7240–7254.
Sun, W.-Y., Ueyama, N. & Nakamura, A. (1993). *Inorg. Chem.* **32**, 1095–1100.
Tsukihara, T., Fukuyama, K., Nakamura, M., Katsube, Y., Tanaka, N., Kakudo, M., Wada, K., Hase, T. & Matsubara, H. (1981). *J. Biochem.* **90**, 1763–1773.
Watenpaugh, K. D., Sieker, L. C. & Jensen, L. H. (1979). *J. Mol. Biol.* **131**, 509–522.

supporting information

Acta Cryst. (2005). E**61**, m1509–m1511 [https://doi.org/10.1107/S1600536805021628]

N—H···S and N—H···O hydrogen bonding in tetra-*n*-butylammonium (imidazolidine-2-thione-2κS)dioxo-1$\kappa^2 O$-di-μ-sulfido-1:2$\kappa^4 S$:*S*-copper(I)tungstate(VI)

Azizolla Beheshti, William Clegg, Sophie H. Dale and Ahmad Solimankhani

tetra-n-butylammonium (imidazolidine-2-thione-2κS)dioxo-1$\kappa^2 O$-di-μ-sulfido-1:2$\kappa^4 S$:*S*- copper(I)tungstate(VI)

Crystal data

$(C_{16}H_{36}N)[WCuO_2S_2(C_3H_6N_2S)]$
$M_r = 688.13$
Monoclinic, $P2_1/c$
$a = 10.6925\ (16)$ Å
$b = 14.875\ (2)$ Å
$c = 17.2342\ (8)$ Å
$\beta = 94.742\ (7)°$
$V = 2731.7\ (6)$ Å^3
$Z = 4$
$F(000) = 1376$
$D_x = 1.673$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 227 reflections
$\theta = 2.5–27.5°$
$\mu = 5.23$ mm^{-1}
$T = 150$ K
Block, orange
0.77 × 0.43 × 0.31 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: numerical (SHELXTL; Sheldrick, 2001)
$T_{min} = 0.100$, $T_{max} = 0.239$
28801 measured reflections
6215 independent reflections
4881 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 27.5°$, $\theta_{min} = 4.0°$
$h = -13\rightarrow13$
$k = -19\rightarrow18$
$l = -22\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.074$
$S = 1.07$
6215 reflections
378 parameters
623 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0159P)^2 + 6.5317P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.029$
$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -0.96$ e Å^{-3}
Extinction correction: SHELXTL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00053 (11)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
W	0.713367 (17)	0.642794 (12)	0.184549 (11)	0.03394 (7)	
Cu	0.85205 (5)	0.50990 (4)	0.25158 (3)	0.03535 (14)	
S1	0.96624 (11)	0.39730 (8)	0.30142 (7)	0.0405 (3)	
C1	1.0637 (4)	0.4403 (3)	0.3761 (3)	0.0342 (10)	
N1	1.0582 (4)	0.5224 (3)	0.4072 (2)	0.0439 (10)	
H1	1.016 (4)	0.563 (3)	0.380 (3)	0.053*	
C2	1.1657 (5)	0.5394 (3)	0.4642 (3)	0.0469 (12)	
H2A	1.1388	0.5665	0.5126	0.056*	
H2B	1.2287	0.5789	0.4424	0.056*	
C3	1.2168 (5)	0.4433 (3)	0.4784 (3)	0.0458 (12)	
H3A	1.3093	0.4416	0.4780	0.055*	
H3B	1.1928	0.4190	0.5286	0.055*	
N2	1.1563 (4)	0.3938 (3)	0.4130 (2)	0.0416 (9)	
H2	1.176 (5)	0.3388 (14)	0.402 (3)	0.050*	
O1	0.5557 (4)	0.6585 (3)	0.1964 (3)	0.0608 (11)	
O2	0.7641 (4)	0.7254 (2)	0.1219 (2)	0.0548 (9)	
S2	0.74285 (13)	0.50400 (9)	0.13514 (8)	0.0479 (3)	
S3	0.82482 (15)	0.64692 (9)	0.30226 (8)	0.0535 (3)	
N3	0.2927 (3)	0.4345 (2)	0.1444 (2)	0.0425 (8)	
C4	0.3881 (5)	0.4170 (4)	0.0858 (3)	0.0557 (12)	
H4A	0.3539	0.4404	0.0346	0.067*	
H4B	0.4650	0.4517	0.1017	0.067*	
C5	0.4243 (6)	0.3196 (4)	0.0759 (4)	0.0765 (17)	
H5A	0.3523	0.2838	0.0531	0.092*	0.747 (9)
H5B	0.4559	0.2926	0.1263	0.092*	0.747 (9)
H5C	0.3452	0.2881	0.0849	0.092*	0.253 (9)
H5D	0.4799	0.3087	0.1238	0.092*	0.253 (9)
C6	0.5292 (7)	0.3255 (6)	0.0195 (5)	0.067 (2)	0.747 (9)
H6A	0.4976	0.3566	−0.0290	0.081*	0.747 (9)
H6B	0.6013	0.3600	0.0439	0.081*	0.747 (9)
C7	0.5704 (10)	0.2307 (7)	0.0010 (6)	0.093 (3)	0.747 (9)
H7A	0.6126	0.2034	0.0479	0.139*	0.747 (9)
H7B	0.6284	0.2328	−0.0401	0.139*	0.747 (9)
H7C	0.4967	0.1947	−0.0167	0.139*	0.747 (9)
C6X	0.4808 (19)	0.2572 (16)	0.0178 (14)	0.073 (3)	0.253 (9)
H6C	0.4920	0.1955	0.0388	0.088*	0.253 (9)
H6D	0.4283	0.2550	−0.0323	0.088*	0.253 (9)
C7X	0.606 (2)	0.302 (2)	0.0086 (18)	0.083 (5)	0.253 (9)
H7D	0.5926	0.3656	−0.0050	0.124*	0.253 (9)
H7E	0.6480	0.2721	−0.0328	0.124*	0.253 (9)
H7F	0.6592	0.2979	0.0576	0.124*	0.253 (9)
C8	0.3408 (5)	0.4008 (4)	0.2244 (3)	0.0495 (11)	
H8A	0.2717	0.4048	0.2591	0.059*	0.660 (12)
H8B	0.3631	0.3365	0.2201	0.059*	0.660 (12)
H8C	0.3287	0.3349	0.2263	0.059*	0.340 (12)

H8D	0.2897	0.4281	0.2636	0.059*	0.340 (12)
C9	0.4529 (10)	0.4502 (7)	0.2623 (5)	0.065 (2)	0.660 (12)
H9A	0.4324	0.5143	0.2699	0.078*	0.660 (12)
H9B	0.5245	0.4464	0.2295	0.078*	0.660 (12)
C10	0.4848 (10)	0.4045 (7)	0.3401 (5)	0.062 (2)	0.660 (12)
H10A	0.4109	0.4063	0.3711	0.075*	0.660 (12)
H10B	0.5061	0.3407	0.3315	0.075*	0.660 (12)
C11	0.5946 (11)	0.4507 (9)	0.3848 (6)	0.086 (4)	0.660 (12)
H11A	0.6733	0.4252	0.3693	0.129*	0.660 (12)
H11B	0.5895	0.4416	0.4407	0.129*	0.660 (12)
H11C	0.5920	0.5152	0.3732	0.129*	0.660 (12)
C9X	0.4797 (10)	0.4220 (17)	0.2469 (11)	0.064 (3)	0.340 (12)
H9C	0.5291	0.3835	0.2138	0.076*	0.340 (12)
H9D	0.4936	0.4849	0.2308	0.076*	0.340 (12)
C10X	0.539 (2)	0.4127 (14)	0.3300 (9)	0.069 (3)	0.340 (12)
H10C	0.5105	0.3561	0.3528	0.083*	0.340 (12)
H10D	0.6316	0.4095	0.3292	0.083*	0.340 (12)
C11X	0.505 (3)	0.4914 (14)	0.3806 (11)	0.080 (5)	0.340 (12)
H11D	0.5448	0.5464	0.3628	0.120*	0.340 (12)
H11E	0.5353	0.4795	0.4349	0.120*	0.340 (12)
H11F	0.4140	0.4991	0.3766	0.120*	0.340 (12)
C12	0.1712 (4)	0.3831 (3)	0.1232 (3)	0.0477 (11)	
H12A	0.1089	0.4010	0.1597	0.057*	0.690 (9)
H12B	0.1878	0.3181	0.1308	0.057*	0.690 (9)
H12C	0.1214	0.3850	0.1691	0.057*	0.310 (9)
H12D	0.1940	0.3194	0.1154	0.057*	0.310 (9)
C13	0.1135 (7)	0.3978 (8)	0.0399 (5)	0.063 (2)	0.690 (9)
H13A	0.1645	0.3666	0.0028	0.076*	0.690 (9)
H13B	0.1128	0.4628	0.0274	0.076*	0.690 (9)
C14	−0.0226 (7)	0.3607 (5)	0.0317 (7)	0.068 (2)	0.690 (9)
H14A	−0.0664	0.3767	0.0783	0.081*	0.690 (9)
H14B	−0.0698	0.3870	−0.0147	0.081*	0.690 (9)
C15	−0.0157 (10)	0.2602 (5)	0.0237 (7)	0.077 (3)	0.690 (9)
H15A	0.0487	0.2447	−0.0114	0.116*	0.690 (9)
H15B	−0.0972	0.2371	0.0023	0.116*	0.690 (9)
H15C	0.0061	0.2332	0.0749	0.116*	0.690 (9)
C13X	0.085 (2)	0.4117 (13)	0.0527 (11)	0.065 (3)	0.310 (9)
H13C	0.1326	0.4442	0.0148	0.077*	0.310 (9)
H13D	0.0176	0.4517	0.0689	0.077*	0.310 (9)
C14X	0.0277 (18)	0.3248 (14)	0.0162 (12)	0.069 (3)	0.310 (9)
H14C	−0.0066	0.3355	−0.0382	0.082*	0.310 (9)
H14D	0.0917	0.2767	0.0165	0.082*	0.310 (9)
C15X	−0.0763 (18)	0.2993 (16)	0.0669 (13)	0.076 (5)	0.310 (9)
H15D	−0.0410	0.2916	0.1208	0.114*	0.310 (9)
H15E	−0.1150	0.2428	0.0481	0.114*	0.310 (9)
H15F	−0.1398	0.3469	0.0646	0.114*	0.310 (9)
C16	0.2708 (5)	0.5361 (3)	0.1449 (4)	0.0576 (12)	
H16A	0.2542	0.5565	0.0903	0.069*	0.817 (10)

H16B	0.3492	0.5656	0.1663	0.069*	0.817 (10)
H16C	0.3496	0.5669	0.1341	0.069*	0.183 (10)
H16D	0.2065	0.5515	0.1023	0.069*	0.183 (10)
C17	0.1630 (7)	0.5687 (4)	0.1912 (6)	0.0682 (19)	0.817 (10)
H17A	0.0823	0.5488	0.1644	0.082*	0.817 (10)
H17B	0.1711	0.5404	0.2434	0.082*	0.817 (10)
C18	0.1602 (8)	0.6708 (4)	0.2010 (5)	0.070 (2)	0.817 (10)
H18A	0.1702	0.6990	0.1498	0.084*	0.817 (10)
H18B	0.0768	0.6884	0.2169	0.084*	0.817 (10)
C19	0.2605 (7)	0.7082 (6)	0.2600 (5)	0.064 (2)	0.817 (10)
H19A	0.2420	0.6902	0.3125	0.097*	0.817 (10)
H19B	0.2614	0.7739	0.2564	0.097*	0.817 (10)
H19C	0.3427	0.6844	0.2490	0.097*	0.817 (10)
C17X	0.228 (4)	0.5713 (16)	0.2212 (12)	0.065 (3)	0.183 (10)
H17C	0.2842	0.5517	0.2668	0.078*	0.183 (10)
H17D	0.1404	0.5547	0.2286	0.078*	0.183 (10)
C18X	0.243 (4)	0.6711 (17)	0.203 (2)	0.066 (3)	0.183 (10)
H18C	0.3297	0.6854	0.1920	0.079*	0.183 (10)
H18D	0.1843	0.6897	0.1587	0.079*	0.183 (10)
C19X	0.210 (4)	0.716 (3)	0.278 (2)	0.069 (5)	0.183 (10)
H19D	0.1369	0.6860	0.2977	0.104*	0.183 (10)
H19E	0.1896	0.7795	0.2681	0.104*	0.183 (10)
H19F	0.2813	0.7119	0.3175	0.104*	0.183 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
W	0.03594 (11)	0.02814 (10)	0.03732 (12)	−0.00322 (8)	0.00050 (7)	0.00084 (8)
Cu	0.0374 (3)	0.0294 (3)	0.0387 (3)	−0.0017 (2)	−0.0002 (2)	−0.0011 (2)
S1	0.0453 (7)	0.0279 (6)	0.0470 (7)	−0.0012 (5)	−0.0032 (5)	−0.0037 (5)
C1	0.039 (2)	0.029 (2)	0.035 (2)	0.0003 (18)	0.0072 (19)	0.0018 (19)
N1	0.050 (2)	0.035 (2)	0.044 (2)	0.0071 (18)	−0.0077 (19)	−0.0027 (19)
C2	0.053 (3)	0.040 (3)	0.046 (3)	−0.001 (2)	−0.004 (2)	−0.006 (2)
C3	0.049 (3)	0.046 (3)	0.042 (3)	0.008 (2)	−0.002 (2)	−0.005 (2)
N2	0.046 (2)	0.033 (2)	0.044 (2)	0.0052 (18)	−0.0031 (19)	−0.0035 (19)
O1	0.046 (2)	0.051 (2)	0.086 (3)	0.0042 (17)	0.009 (2)	0.009 (2)
O2	0.067 (2)	0.042 (2)	0.056 (2)	−0.0083 (18)	0.0093 (18)	0.0126 (18)
S2	0.0622 (8)	0.0368 (7)	0.0424 (7)	0.0020 (6)	−0.0098 (6)	−0.0093 (6)
S3	0.0791 (9)	0.0342 (6)	0.0439 (7)	0.0075 (6)	−0.0151 (6)	−0.0121 (6)
N3	0.0447 (19)	0.0399 (19)	0.044 (2)	−0.0052 (16)	0.0082 (14)	0.0101 (17)
C4	0.044 (2)	0.085 (3)	0.039 (2)	0.000 (2)	0.007 (2)	0.005 (3)
C5	0.063 (3)	0.102 (4)	0.065 (3)	0.011 (3)	0.007 (3)	−0.028 (3)
C6	0.048 (4)	0.086 (5)	0.067 (4)	0.002 (3)	−0.002 (3)	−0.030 (4)
C7	0.088 (6)	0.101 (6)	0.089 (6)	0.020 (5)	0.011 (5)	−0.042 (6)
C6X	0.056 (6)	0.095 (6)	0.068 (6)	−0.001 (6)	0.004 (6)	−0.029 (6)
C7X	0.073 (9)	0.093 (11)	0.086 (10)	−0.015 (8)	0.025 (8)	−0.033 (10)
C8	0.072 (3)	0.041 (3)	0.037 (2)	−0.010 (2)	0.0070 (19)	0.006 (2)
C9	0.090 (5)	0.060 (5)	0.042 (4)	−0.023 (4)	−0.007 (3)	0.002 (3)

C10	0.075 (5)	0.067 (5)	0.043 (4)	−0.028 (4)	−0.004 (4)	0.003 (3)
C11	0.085 (7)	0.109 (8)	0.060 (5)	−0.041 (6)	−0.020 (5)	0.011 (6)
C9X	0.087 (5)	0.054 (6)	0.047 (5)	−0.019 (5)	−0.014 (4)	0.003 (5)
C10X	0.091 (6)	0.069 (6)	0.046 (5)	−0.025 (6)	−0.009 (5)	0.010 (5)
C11X	0.099 (10)	0.094 (9)	0.047 (7)	−0.025 (9)	0.007 (8)	0.000 (7)
C12	0.043 (2)	0.033 (2)	0.067 (3)	−0.0051 (18)	0.0109 (19)	0.008 (2)
C13	0.044 (4)	0.051 (4)	0.090 (4)	−0.003 (3)	−0.015 (3)	0.015 (4)
C14	0.045 (4)	0.045 (4)	0.110 (5)	0.004 (3)	−0.011 (4)	0.003 (4)
C15	0.082 (6)	0.046 (4)	0.098 (7)	0.001 (4)	−0.031 (5)	0.000 (5)
C13X	0.048 (5)	0.046 (5)	0.096 (5)	−0.004 (4)	−0.012 (4)	0.013 (5)
C14X	0.051 (6)	0.052 (6)	0.101 (6)	−0.001 (5)	−0.013 (5)	0.005 (5)
C15X	0.060 (8)	0.059 (9)	0.107 (10)	−0.013 (7)	−0.010 (7)	0.004 (9)
C16	0.055 (3)	0.037 (2)	0.082 (3)	−0.008 (2)	0.009 (2)	0.014 (2)
C17	0.055 (4)	0.039 (3)	0.112 (5)	−0.002 (3)	0.017 (3)	0.005 (3)
C18	0.055 (4)	0.037 (3)	0.119 (5)	0.003 (3)	0.010 (4)	0.001 (3)
C19	0.064 (5)	0.052 (4)	0.079 (5)	0.013 (4)	0.017 (4)	−0.003 (4)
C17X	0.056 (6)	0.039 (4)	0.101 (6)	0.001 (5)	0.010 (5)	0.001 (5)
C18X	0.052 (7)	0.041 (5)	0.106 (7)	−0.001 (7)	0.012 (7)	0.003 (5)
C19X	0.062 (12)	0.043 (8)	0.102 (10)	0.003 (11)	0.006 (10)	0.001 (8)

Geometric parameters (Å, º)

W—Cu	2.6755 (6)	C11—H11C	0.980
W—O1	1.731 (4)	C9X—H9C	0.990
W—O2	1.750 (3)	C9X—H9D	0.990
W—S2	2.2652 (13)	C9X—C10X	1.525 (8)
W—S3	2.2670 (13)	C10X—H10C	0.990
Cu—S1	2.2047 (13)	C10X—H10D	0.990
Cu—S2	2.2385 (14)	C10X—C11X	1.522 (8)
Cu—S3	2.2459 (14)	C11X—H11D	0.980
S1—C1	1.711 (5)	C11X—H11E	0.980
C1—N1	1.338 (6)	C11X—H11F	0.980
C1—N2	1.326 (6)	C12—H12A	0.990
N1—H1	0.868 (10)	C12—H12B	0.990
N1—C2	1.471 (6)	C12—H12C	0.990
C2—H2A	0.990	C12—H12D	0.990
C2—H2B	0.990	C12—C13	1.531 (7)
C2—C3	1.543 (7)	C12—C13X	1.525 (8)
C3—H3A	0.990	C13—H13A	0.990
C3—H3B	0.990	C13—H13B	0.990
C3—N2	1.453 (6)	C13—C14	1.552 (7)
N2—H2	0.867 (10)	C14—H14A	0.990
N3—C4	1.517 (5)	C14—H14B	0.990
N3—C8	1.516 (5)	C14—C15	1.504 (7)
N3—C12	1.525 (5)	C15—H15A	0.980
N3—C16	1.530 (5)	C15—H15B	0.980
C4—H4A	0.990	C15—H15C	0.980
C4—H4B	0.990	C13X—H13C	0.990

C4—C5	1.513 (6)	C13X—H13D	0.990
C5—H5A	0.990	C13X—C14X	1.541 (8)
C5—H5B	0.990	C14X—H14C	0.990
C5—H5C	0.990	C14X—H14D	0.990
C5—H5D	0.990	C14X—C15X	1.518 (8)
C5—C6	1.547 (7)	C15X—H15D	0.980
C5—C6X	1.527 (8)	C15X—H15E	0.980
C6—H6A	0.990	C15X—H15F	0.980
C6—H6B	0.990	C16—H16A	0.990
C6—C7	1.518 (7)	C16—H16B	0.990
C7—H7A	0.980	C16—H16C	0.990
C7—H7B	0.980	C16—H16D	0.990
C7—H7C	0.980	C16—C17	1.535 (6)
C6X—H6C	0.990	C16—C17X	1.520 (8)
C6X—H6D	0.990	C17—H17A	0.990
C6X—C7X	1.519 (8)	C17—H17B	0.990
C7X—H7D	0.980	C17—C18	1.528 (6)
C7X—H7E	0.980	C18—H18A	0.990
C7X—H7F	0.980	C18—H18B	0.990
C8—H8A	0.990	C18—C19	1.521 (7)
C8—H8B	0.990	C19—H19A	0.980
C8—H8C	0.990	C19—H19B	0.980
C8—H8D	0.990	C19—H19C	0.980
C8—C9	1.507 (7)	C17X—H17C	0.990
C8—C9X	1.536 (8)	C17X—H17D	0.990
C9—H9A	0.990	C17X—C18X	1.526 (8)
C9—H9B	0.990	C18X—H18C	0.990
C9—C10	1.518 (7)	C18X—H18D	0.990
C10—H10A	0.990	C18X—C19X	1.523 (8)
C10—H10B	0.990	C19X—H19D	0.980
C10—C11	1.514 (7)	C19X—H19E	0.980
C11—H11A	0.980	C19X—H19F	0.980
C11—H11B	0.980		

Cu—W—O1	124.00 (13)	C8—C9X—H9D	106.7
Cu—W—O2	126.57 (13)	C8—C9X—C10X	122.5 (15)
Cu—W—S2	53.09 (4)	H9C—C9X—H9D	106.6
Cu—W—S3	53.28 (4)	H9C—C9X—C10X	106.7
O1—W—O2	109.42 (18)	H9D—C9X—C10X	106.7
O1—W—S2	109.53 (14)	C9X—C10X—H10C	109.3
O1—W—S3	109.63 (15)	C9X—C10X—H10D	109.3
O2—W—S2	110.36 (13)	C9X—C10X—C11X	111.6 (17)
O2—W—S3	111.47 (13)	H10C—C10X—H10D	108.0
S2—W—S3	106.37 (5)	H10C—C10X—C11X	109.3
W—Cu—S1	177.30 (4)	H10D—C10X—C11X	109.3
W—Cu—S2	54.02 (4)	C10X—C11X—H11D	109.5
W—Cu—S3	54.01 (4)	C10X—C11X—H11E	109.5
S1—Cu—S2	123.40 (5)	C10X—C11X—H11F	109.5

S1—Cu—S3	128.57 (5)	H11D—C11X—H11E	109.5
S2—Cu—S3	108.02 (5)	H11D—C11X—H11F	109.5
Cu—S1—C1	106.99 (16)	H11E—C11X—H11F	109.5
S1—C1—N1	126.8 (4)	N3—C12—H12A	108.5
S1—C1—N2	123.3 (3)	N3—C12—H12B	108.5
N1—C1—N2	109.9 (4)	N3—C12—H12C	107.3
C1—N1—H1	118 (4)	N3—C12—H12D	107.3
C1—N1—C2	111.5 (4)	N3—C12—C13	115.0 (5)
H1—N1—C2	125 (4)	N3—C12—C13X	120.0 (9)
N1—C2—H2A	111.5	H12A—C12—H12B	107.5
N1—C2—H2B	111.5	H12A—C12—C13	108.5
N1—C2—C3	101.2 (4)	H12B—C12—C13	108.5
H2A—C2—H2B	109.4	H12C—C12—H12D	106.9
H2A—C2—C3	111.5	H12C—C12—C13X	107.4
H2B—C2—C3	111.5	H12D—C12—C13X	107.3
C2—C3—H3A	111.3	C12—C13—H13A	109.7
C2—C3—H3B	111.3	C12—C13—H13B	109.8
C2—C3—N2	102.5 (4)	C12—C13—C14	109.6 (7)
H3A—C3—H3B	109.2	H13A—C13—H13B	108.2
H3A—C3—N2	111.3	H13A—C13—C14	109.7
H3B—C3—N2	111.3	H13B—C13—C14	109.8
C1—N2—C3	112.0 (4)	C13—C14—H14A	110.1
C1—N2—H2	125 (4)	C13—C14—H14B	110.1
C3—N2—H2	123 (4)	C13—C14—C15	108.0 (9)
W—S2—Cu	72.89 (4)	H14A—C14—H14B	108.4
W—S3—Cu	72.72 (4)	H14A—C14—C15	110.1
C4—N3—C8	110.7 (4)	H14B—C14—C15	110.1
C4—N3—C12	111.1 (4)	C12—C13X—H13C	110.4
C4—N3—C16	106.5 (4)	C12—C13X—H13D	110.4
C8—N3—C12	105.7 (3)	C12—C13X—C14X	106.6 (13)
C8—N3—C16	111.2 (4)	H13C—C13X—H13D	108.6
C12—N3—C16	111.6 (4)	H13C—C13X—C14X	110.4
N3—C4—H4A	108.4	H13D—C13X—C14X	110.4
N3—C4—H4B	108.4	C13X—C14X—H14C	110.8
N3—C4—C5	115.6 (4)	C13X—C14X—H14D	110.7
H4A—C4—H4B	107.4	C13X—C14X—C15X	104.9 (19)
H4A—C4—C5	108.4	H14C—C14X—H14D	108.8
H4B—C4—C5	108.4	H14C—C14X—C15X	110.8
C4—C5—H5A	111.2	H14D—C14X—C15X	110.8
C4—C5—H5B	111.2	C14X—C15X—H15D	109.5
C4—C5—H5C	101.8	C14X—C15X—H15E	109.5
C4—C5—H5D	101.8	C14X—C15X—H15F	109.5
C4—C5—C6	102.9 (5)	H15D—C15X—H15E	109.5
C4—C5—C6X	140.8 (12)	H15D—C15X—H15F	109.5
H5A—C5—H5B	109.1	H15E—C15X—H15F	109.5
H5A—C5—C6	111.2	N3—C16—H16A	108.3
H5B—C5—C6	111.2	N3—C16—H16B	108.3
H5C—C5—H5D	104.7	N3—C16—H16C	108.8

H5C—C5—C6X	101.8	N3—C16—H16D	108.8
H5D—C5—C6X	101.8	N3—C16—C17	115.9 (4)
C5—C6—H6A	110.0	N3—C16—C17X	113.7 (10)
C5—C6—H6B	110.0	H16A—C16—H16B	107.4
C5—C6—C7	108.5 (7)	H16A—C16—C17	108.3
H6A—C6—H6B	108.4	H16B—C16—C17	108.3
H6A—C6—C7	110.0	H16C—C16—H16D	107.7
H6B—C6—C7	110.0	H16C—C16—C17X	108.8
C5—C6X—H6C	111.4	H16D—C16—C17X	108.8
C5—C6X—H6D	111.4	C16—C17—H17A	108.9
C5—C6X—C7X	101.6 (15)	C16—C17—H17B	108.9
H6C—C6X—H6D	109.3	C16—C17—C18	113.2 (6)
H6C—C6X—C7X	111.4	H17A—C17—H17B	107.8
H6D—C6X—C7X	111.5	H17A—C17—C18	108.9
C6X—C7X—H7D	109.5	H17B—C17—C18	108.9
C6X—C7X—H7E	109.5	C17—C18—H18A	108.6
C6X—C7X—H7F	109.5	C17—C18—H18B	108.6
H7D—C7X—H7E	109.5	C17—C18—C19	114.7 (7)
H7D—C7X—H7F	109.5	H18A—C18—H18B	107.6
H7E—C7X—H7F	109.5	H18A—C18—C19	108.6
N3—C8—H8A	108.4	H18B—C18—C19	108.6
N3—C8—H8B	108.4	C18—C19—H19A	109.5
N3—C8—H8C	108.7	C18—C19—H19B	109.5
N3—C8—H8D	108.7	C18—C19—H19C	109.5
N3—C8—C9	115.5 (5)	H19A—C19—H19B	109.5
N3—C8—C9X	114.2 (8)	H19A—C19—H19C	109.5
H8A—C8—H8B	107.5	H19B—C19—H19C	109.5
H8A—C8—C9	108.4	C16—C17X—H17C	112.4
H8B—C8—C9	108.4	C16—C17X—H17D	112.4
H8C—C8—H8D	107.6	C16—C17X—C18X	96.8 (17)
H8C—C8—C9X	108.7	H17C—C17X—H17D	110.0
H8D—C8—C9X	108.7	H17C—C17X—C18X	112.4
C8—C9—H9A	110.5	H17D—C17X—C18X	112.4
C8—C9—H9B	110.5	C17X—C18X—H18C	111.2
C8—C9—C10	106.1 (6)	C17X—C18X—H18D	111.2
H9A—C9—H9B	108.7	C17X—C18X—C19X	103 (2)
H9A—C9—C10	110.5	H18C—C18X—H18D	109.1
H9B—C9—C10	110.5	H18C—C18X—C19X	111.2
C9—C10—H10A	109.5	H18D—C18X—C19X	111.2
C9—C10—H10B	109.5	C18X—C19X—H19D	109.5
C9—C10—C11	110.8 (7)	C18X—C19X—H19E	109.5
H10A—C10—H10B	108.1	C18X—C19X—H19F	109.5
H10A—C10—C11	109.5	H19D—C19X—H19E	109.5
H10B—C10—C11	109.5	H19D—C19X—H19F	109.5
C8—C9X—H9C	106.7	H19E—C19X—H19F	109.5
O1—W—Cu—S1	107.0 (9)	N3—C4—C5—C6	−175.0 (5)
O1—W—Cu—S2	89.88 (18)	N3—C4—C5—C6X	158.8 (14)

O1—W—Cu—S3	−90.14 (18)	C4—C5—C6—C7	−177.1 (7)
O2—W—Cu—S1	−72.0 (9)	C4—C5—C6X—C7X	58 (3)
O2—W—Cu—S2	−89.12 (16)	C4—N3—C8—C9	66.7 (8)
O2—W—Cu—S3	90.86 (17)	C4—N3—C8—C9X	42.3 (12)
S2—W—Cu—S1	17.1 (9)	C12—N3—C8—C9	−172.9 (7)
S2—W—Cu—S3	179.99 (7)	C12—N3—C8—C9X	162.7 (11)
S3—W—Cu—S1	−162.9 (9)	C16—N3—C8—C9	−51.6 (8)
S3—W—Cu—S2	−179.99 (7)	C16—N3—C8—C9X	−75.9 (11)
W—Cu—S1—C1	147.5 (9)	N3—C8—C9—C10	−179.2 (7)
S2—Cu—S1—C1	164.09 (16)	C8—C9—C10—C11	−178.3 (12)
S3—Cu—S1—C1	−14.74 (18)	N3—C8—C9X—C10X	166.5 (17)
Cu—S1—C1—N1	10.3 (5)	C8—C9X—C10X—C11X	−78 (3)
Cu—S1—C1—N2	−171.4 (4)	C4—N3—C12—C13	−52.7 (7)
S1—C1—N1—C2	−173.5 (4)	C4—N3—C12—C13X	−70.8 (13)
N2—C1—N1—C2	7.9 (6)	C8—N3—C12—C13	−172.9 (6)
C1—N1—C2—C3	−15.3 (5)	C8—N3—C12—C13X	169.1 (13)
N1—C2—C3—N2	16.0 (5)	C16—N3—C12—C13	66.0 (7)
S1—C1—N2—C3	−174.6 (4)	C16—N3—C12—C13X	48.0 (13)
N1—C1—N2—C3	4.0 (6)	N3—C12—C13—C14	−166.9 (7)
C2—C3—N2—C1	−13.1 (6)	C12—C13—C14—C15	−78.5 (12)
S1—Cu—S2—W	−179.05 (5)	N3—C12—C13X—C14X	144.5 (14)
S3—Cu—S2—W	−0.01 (6)	C12—C13X—C14X—C15X	79 (2)
O1—W—S2—Cu	−118.40 (15)	C4—N3—C16—C17	171.3 (6)
O2—W—S2—Cu	121.07 (14)	C4—N3—C16—C17X	−153.7 (18)
S3—W—S2—Cu	0.01 (6)	C8—N3—C16—C17	−68.0 (7)
S1—Cu—S3—W	178.99 (5)	C8—N3—C16—C17X	−33.1 (18)
S2—Cu—S3—W	0.01 (6)	C12—N3—C16—C17	49.9 (7)
O1—W—S3—Cu	118.33 (14)	C12—N3—C16—C17X	84.8 (18)
O2—W—S3—Cu	−120.36 (14)	N3—C16—C17—C18	170.2 (6)
S2—W—S3—Cu	−0.01 (6)	C16—C17—C18—C19	−74.8 (11)
C8—N3—C4—C5	58.8 (6)	N3—C16—C17X—C18X	169.6 (18)
C12—N3—C4—C5	−58.3 (6)	C16—C17X—C18X—C19X	−177 (3)
C16—N3—C4—C5	179.9 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···S3	0.87 (1)	2.66 (2)	3.490 (4)	160 (5)
N2—H2···O2^{i}	0.87 (1)	1.87 (1)	2.729 (5)	174 (5)

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