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Poly[aquahexabenzimidazoleocta- μ -cyanido-octacyanidotricopper(II)-ditungstate(V)]

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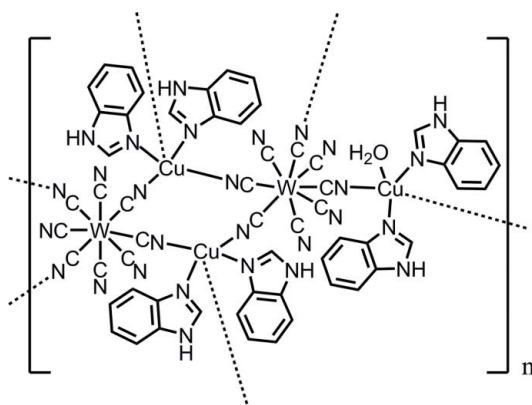
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.030; wR factor = 0.085; data-to-parameter ratio = 17.4.

In the polymeric title compound, $[\text{Cu}_3\text{W}_2(\text{CN})_{16}(\text{C}_7\text{H}_6\text{N}_2)_6(\text{H}_2\text{O})_6]_n$, the coordination geometry of the W(V) atom is eight-coordinate dodecahedral, where four CN groups of $[\text{W}(\text{CN})_8]$ are bridged to Cu^{II} ions, and the other four CN groups are not bridged. The coordination geometries of the Cu^{II} ions are five-coordinate pseudo-square-based pyramidal. There are two distinct Cu sites, which build and link the cyanido-bridged Cu–W ladder chains. Successive connections lead to the formation of a two-dimensional network. The H atoms of a coordinated water molecule and the imino groups form hydrogen bonds to the N atoms of non-bridged CN groups.

Related literature

For general background to molecule-based magnets, see: Catala *et al.* (2005); Garde *et al.* (1999); Herrera *et al.* (2004, 2008); Kosaka *et al.* (2009); Leipoldt *et al.* (1994); Ohkoshi *et al.* (2006, 2007, 2008); Sieklucka *et al.* (2009); Zhong *et al.* (2000). For related structures, see: Ohkoshi *et al.* (2003); Podgajny *et al.* (2002); Kaneko *et al.* (2007).



Experimental

Crystal data

$[\text{Cu}_3\text{W}_2(\text{CN})_{16}(\text{C}_7\text{H}_6\text{N}_2)_6(\text{H}_2\text{O})_6]$	$V = 6394.3$ (3) Å ³
$M_r = 1701.46$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 32.0103$ (8) Å	$\mu = 4.63$ mm ⁻¹
$b = 10.2389$ (3) Å	$T = 296$ K
$c = 19.5533$ (5) Å	$0.45 \times 0.12 \times 0.08$ mm
$\beta = 93.8269$ (8)°	

Data collection

Rigaku R-Axis RAPID diffractometer	31073 measured reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	7321 independent reflections
$T_{\text{min}} = 0.327$, $T_{\text{max}} = 0.690$	6376 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.059$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.085$	$\Delta\rho_{\text{max}} = 1.85$ e Å ⁻³
$S = 1.02$	$\Delta\rho_{\text{min}} = -1.08$ e Å ⁻³
7321 reflections	
421 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1 \cdots N6	1.05 (12)	2.20 (12)	3.178 (7)	154 (10)
N10–H10N \cdots N5 ⁱ	0.86	1.97	2.802 (5)	163
N12–H12N \cdots N8 ⁱⁱ	0.86	2.04	2.888 (5)	169
N14–H14N \cdots N7 ⁱⁱⁱ	0.86	2.18	2.973 (5)	154

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *VESTA* (Momma & Izumi, 2006); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2226).

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supporting information

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Poly[aqua hexabenzimidazole octa- μ -cyanido-octacyanidotricopper(II)ditungstate(V)]

Kenta Imoto, Souhei Kaneko, Yoshihide Tsunobuchi, Koji Nakabayashi and Shin-ichi Ohkoshi

S1. Comment

In molecule-based magnets, preparing compounds with a high Curie temperature (T_C) is a challenging issue. From this view point, octacyanometalate $[M(CN)_8]$ ($M = Mo, W, Nb$)-based magnets have been aggressively studied due to their high T_C (Garde *et al.*, 1999; Zhong *et al.*, 2000; Herrera *et al.*, 2008; Sieklucka *et al.*, 2009; Kosaka *et al.*, 2009) and properties such as photomagnetism (Herrera *et al.*, 2004; Catala *et al.*, 2005; Ohkoshi *et al.*, 2006; Ohkoshi *et al.*, 2008) and chemically sensitive magnetism (Ohkoshi *et al.*, 2007). Octacyanometalates, $[M(CN)_8]$ ($M = Mo, W, Nb$), a versatile class of building blocks, can adopt different spatial configurations depending on their chemical environment, *e.g.*, square antiprism (D_{4d}), dodecahedron (D_{2d}), and bicapped trigonal prism (C_{2v}) (Leipoldt *et al.*, 1994). Thus, crystal structures of their complexes have various coordination geometries. Several octacyanometalate-based magnets of Cu—W systems such as $\{[Cu_3[W(CN)_8]_2]3.4H_2O\}_n$ (3-dimensional network complex, 3-D) (Garde *et al.*, 1999), $\{[Cu_3[W(CN)_8]_2(pyrimidine)_2]8H_2O\}_n$ (3-D) (Ohkoshi *et al.*, 2007), $\{[(tetrenH_5)_{0.8}Cu_4[W(CN)_8]_4]7.2H_2O\}_n$ (2-D) (Sieklucka *et al.*, 2009), $\{[Cu_3[W(CN)_8]_2(3-cyanopyridine)_6]4H_2O\}_n$ (2-D), and $\{[Cu_3[W(CN)_8]_2(4-cyanopyridine)_6]8H_2O\}_n$ (2-D) (Ohkoshi *et al.*, 2003), have been reported.

The asymmetric unit of the present compound consists of a $[W(CN)_8]^{3-}$ anion, a $[CuI(benzimidazole)_2]^{2+}$ cation and one-half of $[Cu2(benzimidazole)(H_2O)]^{2+}$ cation (Fig. 1). The coordination geometry of W is an 8-coordinated dodecahedron, where four CN groups of $[W(CN)_8]$ are bridged to Cu ions (three Cu1 and one Cu2), and other four CN groups are not bridged. The coordination geometries of the two types of Cu^{II} ions (Cu1 and Cu2) are 5-coordinated pseudo-square pyramidal. The Cu1 atom is coordinated to three nitrogen atoms of CN groups and two nitrogen atoms of benzimidazole molecules. The Cu2 atom is coordinated to two nitrogen atoms of CN groups, two nitrogen atoms of benzimidazole molecules, and an oxygen atom of an H₂O molecule. The cyano-bridged-Cu1—W ladder chains are linked by Cu2 pillar units (Fig. 2). The benzimidazole molecules coordinated to Cu1 are aligned alternately between the layers with the intermolecular shortest distance of 3.452 (7) Å.

The field-cooled magnetization (FCM) curve at 10 Oe showed that the magnetization value gradually increased below 10 K and then drastically dropped below 7.5 K with decreasing temperature. The magnetization vs. external magnetic field (M - H) curve at 2 K showed a spin-flip transition with the critical magnetic field of 900 Oe and the saturation magnetization (M_s) value of 5.2 μ_B . This M_s value is close to the expected value of 5.0 μ_B for the ferromagnetic ordering of W^V ($S = 1/2$) ions and Cu^{II} ($S = 1/2$) ions. These FCM and M - H curves indicate that this compound is a metamagnet.

S2. Experimental

The title compound was prepared by reacting an aqueous solution of $Cs_3[W(CN)_8]2H_2O$ (1.2×10^{-2} mol dm^{-3}) with a mixed aqueous solution of $CuCl_2 \cdot 2H_2O$ (1.8×10^{-2} mol dm^{-3}) and benzimidazole (2.0×10^{-2} mol dm^{-3}) at room temperature. The prepared compound was a deep blue rod-shaped crystal. Elemental analyses: calculated for

$\text{Cu}_3[\text{W}(\text{CN})_8]_2(\text{benzimidazole})_6(\text{H}_2\text{O})$, Calculated: Cu, 11.20; W, 21.61; C, 40.94; H, 2.25; N, 23.05. Found: Cu, 11.32; W, 21.78; C, 40.65; H, 2.42; N, 23.15.

In the Infrared (IR) spectra, cyano stretching peaks were observed at 2206, 2201, 2186, 2183, and 2165 cm^{-1} .

S3. Refinement

The H atoms of the benzimidazole molecules were placed in calculated positions, with $\text{C—H} = 0.95 \text{ \AA}$, and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. The maximum and minimum residual electron density peaks were located 0.83 and 0.93 \AA , respectively from the W1 atom. A plausible water hydrogen was found in a difference map, and was refined freely. The second water hydrogen is a symmetry equivalent of the first, because the water oxygen O1 lies on the crystallographic 2-fold.

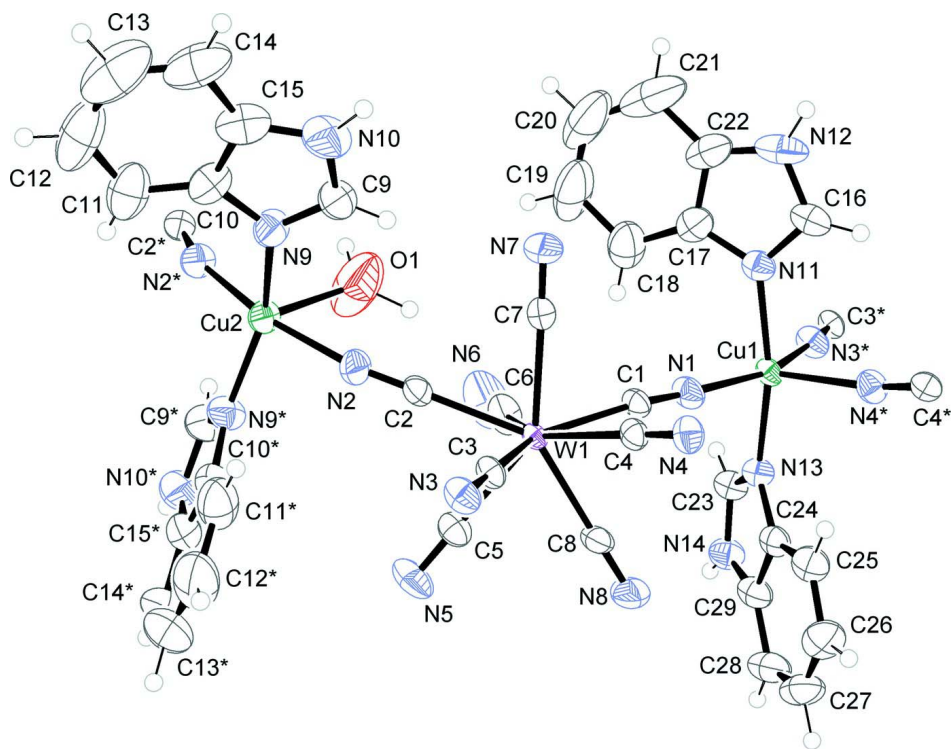


Figure 1

Thermal ellipsoid plots (50% probability level) of $\text{Cu}_3[\text{W}(\text{CN})_8]_2(\text{C}_7\text{H}_6\text{N}_2)_6(\text{H}_2\text{O})$. Magenta, Green, gray, light blue, red, and white circle represent W, Cu, C, N, O, and H atoms, respectively. The asterisks indicate the atoms generated by symmetry operations.

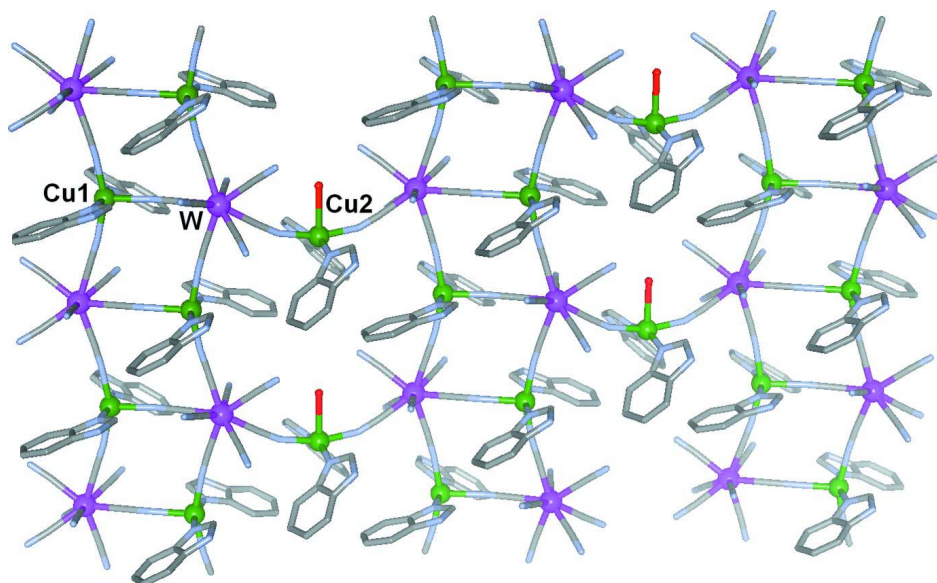


Figure 2

A structure diagram of $\text{Cu}_3[\text{W}(\text{CN})_8]_2(\text{C}_7\text{H}_6\text{N}_2)_6(\text{H}_2\text{O})$. Magenta, Green, gray, light blue, and red represent W, Cu, C, N, and O atoms, respectively. Hydrogen atoms are omitted for clarity.

Poly[aquahexabenzimidazoleocta- μ -cyanido- octacyanidotricopper(II)ditungstate(V)]

Crystal data

$[\text{Cu}_3\text{W}_2(\text{CN})_{16}(\text{C}_7\text{H}_6\text{N}_2)_6(\text{H}_2\text{O})]$

$M_r = 1701.46$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 32.0103\ (8)\ \text{\AA}$

$b = 10.2389\ (3)\ \text{\AA}$

$c = 19.5533\ (5)\ \text{\AA}$

$\beta = 93.8269\ (8)^\circ$

$V = 6394.3\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 3300.00$

$D_x = 1.767\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71075\ \text{\AA}$

Cell parameters from 24759 reflections

$\theta = 3.0\text{--}27.5^\circ$

$\mu = 4.63\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Stick, blue

$0.45 \times 0.12 \times 0.08\ \text{mm}$

Data collection

Rigaku R-AXIS RAPID
diffractometer

Detector resolution: $10.00\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.327$, $T_{\max} = 0.690$

31073 measured reflections

7321 independent reflections

6376 reflections with $F^2 > 2\sigma(F^2)$

$R_{\text{int}} = 0.059$

$\theta_{\max} = 27.5^\circ$

$h = -39 \rightarrow 41$

$k = -13 \rightarrow 13$

$l = -25 \rightarrow 24$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.030$

$wR(F^2) = 0.085$

$S = 1.02$

7321 reflections

421 parameters

0 restraints

H atoms treated by a mixture of independent
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 13.526P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$

$$\Delta\rho_{\max} = 1.85 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.08 \text{ e } \text{\AA}^{-3}$$

Special details

Refinement. Refinement was performed using all reflections. The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R -factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
W(1)	0.145909 (4)	0.677683 (13)	0.197487 (7)	0.01965 (5)
Cu(2)	0.0000	0.49203 (8)	0.2500	0.03412 (16)
Cu(1)	0.188606 (15)	1.17685 (4)	0.21356 (2)	0.02394 (11)
O(1)	0.0000	0.7293 (9)	0.2500	0.122 (3)
N(2)	0.05975 (11)	0.5193 (3)	0.23372 (18)	0.0370 (8)
N(1)	0.17619 (12)	0.9853 (3)	0.21299 (18)	0.0346 (7)
N(3)	0.17679 (12)	0.3708 (3)	0.21001 (18)	0.0342 (7)
N(4)	0.24430 (12)	0.6811 (3)	0.26064 (19)	0.0339 (8)
N(5)	0.10782 (14)	0.5221 (4)	0.0592 (2)	0.0526 (11)
N(6)	0.06447 (17)	0.8632 (4)	0.1550 (3)	0.0742 (16)
N(7)	0.13445 (14)	0.7107 (5)	0.36327 (19)	0.0533 (11)
N(8)	0.19927 (14)	0.7590 (4)	0.06671 (18)	0.0495 (10)
N(9)	0.01423 (12)	0.4524 (4)	0.34652 (19)	0.0422 (9)
N(10)	0.04890 (15)	0.4583 (5)	0.4471 (2)	0.0610 (12)
N(11)	0.17406 (12)	1.1776 (3)	0.31062 (18)	0.0334 (8)
N(12)	0.17738 (19)	1.1969 (4)	0.4229 (2)	0.0611 (13)
N(13)	0.18846 (12)	1.1756 (3)	0.11163 (18)	0.0306 (7)
N(14)	0.16506 (13)	1.2126 (4)	0.00448 (19)	0.0410 (8)
C(2)	0.09067 (13)	0.5704 (4)	0.22258 (19)	0.0295 (8)
C(1)	0.16532 (12)	0.8801 (3)	0.21138 (19)	0.0276 (8)
C(3)	0.16736 (12)	0.4779 (3)	0.20814 (18)	0.0253 (7)
C(4)	0.21022 (13)	0.6805 (3)	0.2396 (2)	0.0276 (8)
C(5)	0.12014 (14)	0.5790 (4)	0.1062 (2)	0.0339 (9)
C(6)	0.09391 (15)	0.8020 (4)	0.1676 (2)	0.0399 (10)
C(7)	0.13846 (14)	0.7019 (4)	0.3060 (2)	0.0334 (9)
C(8)	0.18115 (14)	0.7292 (4)	0.11189 (19)	0.0329 (8)
C(9)	0.04547 (15)	0.5048 (5)	0.3837 (2)	0.0499 (12)
C(10)	-0.00421 (16)	0.3619 (5)	0.3883 (2)	0.0478 (11)
C(11)	-0.03601 (18)	0.2733 (6)	0.3741 (3)	0.0692 (16)
C(12)	-0.0462 (2)	0.1936 (7)	0.4281 (5)	0.097 (2)
C(13)	-0.0237 (3)	0.2026 (9)	0.4940 (5)	0.111 (3)
C(14)	0.0073 (3)	0.2874 (8)	0.5065 (3)	0.086 (2)
C(15)	0.01723 (19)	0.3657 (6)	0.4523 (2)	0.0585 (14)
C(16)	0.19871 (18)	1.2102 (5)	0.3653 (2)	0.0452 (11)
C(17)	0.13574 (16)	1.1428 (4)	0.3341 (2)	0.0422 (10)
C(18)	0.09927 (18)	1.1010 (6)	0.2988 (3)	0.0673 (16)

C(19)	0.0650 (2)	1.0730 (8)	0.3375 (6)	0.111 (3)
C(20)	0.0680 (3)	1.0858 (9)	0.4067 (6)	0.117 (3)
C(21)	0.1033 (3)	1.1243 (8)	0.4433 (4)	0.104 (3)
C(22)	0.1385 (2)	1.1537 (5)	0.4053 (3)	0.0569 (14)
C(23)	0.15930 (14)	1.2307 (4)	0.0704 (2)	0.0365 (9)
C(24)	0.21615 (14)	1.1184 (4)	0.0683 (2)	0.0328 (8)
C(25)	0.25409 (15)	1.0524 (4)	0.0820 (2)	0.0426 (10)
C(26)	0.27512 (18)	1.0159 (5)	0.0266 (3)	0.0545 (13)
C(27)	0.2601 (2)	1.0414 (5)	-0.0407 (2)	0.0577 (14)
C(28)	0.2242 (2)	1.1052 (5)	-0.0553 (2)	0.0526 (13)
C(29)	0.20135 (17)	1.1435 (4)	0.0004 (2)	0.0394 (10)
H(1)	0.025 (3)	0.784 (12)	0.233 (6)	0.20 (5)*
H(9)	0.0633	0.5677	0.3674	0.060*
H(10N)	0.0672	0.4809	0.4791	0.073*
H(11)	-0.0499	0.2671	0.3309	0.083*
H(12)	-0.0679	0.1336	0.4215	0.116*
H(12N)	0.1873	1.2136	0.4639	0.073*
H(13)	-0.0311	0.1475	0.5291	0.133*
H(14)	0.0215	0.2937	0.5494	0.103*
H(14N)	0.1489	1.2395	-0.0295	0.049*
H(16)	0.2264	1.2378	0.3643	0.054*
H(18)	0.0975	1.0918	0.2514	0.081*
H(19)	0.0399	1.0454	0.3155	0.133*
H(20)	0.0445	1.0671	0.4304	0.140*
H(21)	0.1045	1.1312	0.4908	0.124*
H(23)	0.1369	1.2775	0.0860	0.044*
H(25)	0.2644	1.0343	0.1265	0.051*
H(26)	0.3005	0.9722	0.0341	0.065*
H(27)	0.2756	1.0132	-0.0765	0.069*
H(28)	0.2147	1.1234	-0.1002	0.063*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
W(1)	0.02408 (10)	0.01523 (9)	0.01913 (9)	0.00006 (5)	-0.00245 (6)	-0.00061 (5)
Cu(2)	0.0216 (3)	0.0477 (4)	0.0322 (3)	0.0000	-0.0040 (2)	0.0000
Cu(1)	0.0300 (2)	0.0160 (2)	0.0255 (2)	0.00025 (17)	-0.0012 (2)	-0.00081 (16)
O(1)	0.105 (6)	0.069 (5)	0.200 (10)	0.0000	0.080 (6)	0.0000
N(2)	0.0287 (18)	0.044 (2)	0.0377 (19)	-0.0043 (15)	-0.0018 (15)	-0.0010 (15)
N(1)	0.048 (2)	0.0204 (17)	0.0353 (18)	-0.0029 (15)	0.0027 (16)	-0.0029 (13)
N(3)	0.045 (2)	0.0225 (18)	0.0347 (18)	0.0024 (15)	-0.0027 (15)	0.0004 (14)
N(4)	0.0310 (19)	0.033 (2)	0.037 (2)	-0.0025 (13)	-0.0035 (16)	0.0025 (13)
N(5)	0.070 (2)	0.050 (2)	0.035 (2)	-0.006 (2)	-0.017 (2)	-0.0103 (18)
N(6)	0.068 (3)	0.042 (2)	0.107 (4)	0.020 (2)	-0.031 (3)	-0.001 (2)
N(7)	0.055 (2)	0.079 (3)	0.0264 (19)	-0.017 (2)	0.0053 (18)	-0.0072 (18)
N(8)	0.069 (2)	0.052 (2)	0.0286 (18)	-0.014 (2)	0.0124 (19)	-0.0029 (17)
N(9)	0.0318 (19)	0.058 (2)	0.0361 (19)	-0.0047 (17)	-0.0057 (16)	0.0074 (17)
N(10)	0.058 (2)	0.083 (3)	0.040 (2)	0.004 (2)	-0.015 (2)	0.004 (2)

N(11)	0.042 (2)	0.0267 (18)	0.0315 (18)	0.0020 (14)	0.0016 (16)	-0.0003 (12)
N(12)	0.097 (4)	0.059 (3)	0.028 (2)	0.015 (2)	0.009 (2)	-0.0020 (18)
N(13)	0.0363 (19)	0.0273 (18)	0.0283 (17)	0.0036 (13)	0.0021 (15)	0.0009 (12)
N(14)	0.046 (2)	0.046 (2)	0.0304 (18)	0.0035 (18)	-0.0019 (16)	0.0012 (16)
C(2)	0.030 (2)	0.032 (2)	0.0264 (18)	-0.0022 (16)	-0.0030 (16)	-0.0040 (15)
C(1)	0.034 (2)	0.0203 (19)	0.0285 (18)	-0.0010 (15)	0.0013 (16)	-0.0035 (14)
C(3)	0.0311 (19)	0.0179 (18)	0.0262 (17)	0.0002 (14)	-0.0043 (15)	0.0004 (13)
C(4)	0.032 (2)	0.023 (2)	0.0271 (19)	-0.0037 (14)	-0.0003 (17)	0.0012 (14)
C(5)	0.041 (2)	0.030 (2)	0.030 (2)	-0.0001 (17)	-0.0059 (18)	0.0013 (16)
C(6)	0.036 (2)	0.028 (2)	0.054 (2)	0.0076 (17)	-0.010 (2)	-0.0015 (18)
C(7)	0.030 (2)	0.038 (2)	0.033 (2)	-0.0081 (17)	0.0011 (17)	-0.0037 (17)
C(8)	0.042 (2)	0.033 (2)	0.0233 (18)	-0.0021 (18)	0.0009 (17)	-0.0063 (16)
C(9)	0.037 (2)	0.073 (3)	0.038 (2)	-0.007 (2)	-0.010 (2)	0.000 (2)
C(10)	0.039 (2)	0.054 (3)	0.051 (2)	0.009 (2)	0.007 (2)	0.013 (2)
C(11)	0.046 (3)	0.060 (3)	0.102 (4)	0.002 (2)	0.009 (3)	0.013 (3)
C(12)	0.075 (5)	0.057 (4)	0.163 (9)	0.003 (3)	0.038 (5)	0.037 (4)
C(13)	0.132 (8)	0.083 (6)	0.123 (7)	0.032 (5)	0.053 (6)	0.063 (5)
C(14)	0.112 (6)	0.084 (5)	0.065 (4)	0.031 (4)	0.033 (4)	0.035 (3)
C(15)	0.062 (3)	0.067 (3)	0.047 (2)	0.024 (3)	0.006 (2)	0.011 (2)
C(16)	0.059 (3)	0.044 (2)	0.032 (2)	0.003 (2)	-0.002 (2)	-0.0059 (19)
C(17)	0.051 (2)	0.026 (2)	0.052 (2)	0.0041 (19)	0.015 (2)	-0.0012 (19)
C(18)	0.050 (3)	0.056 (3)	0.096 (4)	-0.002 (2)	0.014 (3)	-0.016 (3)
C(19)	0.058 (4)	0.086 (6)	0.197 (10)	-0.015 (3)	0.059 (5)	-0.046 (6)
C(20)	0.099 (6)	0.081 (6)	0.181 (10)	-0.019 (5)	0.093 (7)	-0.022 (6)
C(21)	0.163 (9)	0.063 (4)	0.096 (5)	0.017 (5)	0.086 (6)	0.011 (4)
C(22)	0.076 (4)	0.042 (3)	0.056 (3)	0.005 (2)	0.031 (3)	0.003 (2)
C(23)	0.043 (2)	0.035 (2)	0.031 (2)	0.0034 (19)	0.0008 (18)	-0.0015 (17)
C(24)	0.043 (2)	0.021 (2)	0.034 (2)	-0.0031 (17)	0.0031 (18)	-0.0004 (15)
C(25)	0.049 (2)	0.032 (2)	0.046 (2)	0.005 (2)	0.003 (2)	-0.0017 (19)
C(26)	0.058 (3)	0.036 (2)	0.071 (3)	0.010 (2)	0.019 (2)	-0.005 (2)
C(27)	0.081 (4)	0.042 (3)	0.055 (3)	0.000 (2)	0.032 (2)	-0.009 (2)
C(28)	0.084 (4)	0.039 (2)	0.036 (2)	-0.002 (2)	0.015 (2)	-0.004 (2)
C(29)	0.060 (3)	0.027 (2)	0.032 (2)	-0.004 (2)	0.003 (2)	0.0008 (16)

Geometric parameters (Å, °)

W(1)—C(2)	2.165 (4)	C(10)—C(15)	1.388 (7)
W(1)—C(1)	2.176 (3)	C(11)—C(12)	1.390 (12)
W(1)—C(3)	2.163 (3)	C(12)—C(13)	1.436 (14)
W(1)—C(4)	2.166 (4)	C(13)—C(14)	1.329 (13)
W(1)—C(5)	2.166 (3)	C(14)—C(15)	1.383 (10)
W(1)—C(6)	2.145 (4)	C(17)—C(18)	1.384 (7)
W(1)—C(7)	2.165 (4)	C(17)—C(22)	1.394 (7)
W(1)—C(8)	2.146 (4)	C(18)—C(19)	1.403 (11)
Cu(2)—N(2)	1.980 (3)	C(19)—C(20)	1.356 (17)
Cu(2)—N(2) ⁱ	1.980 (3)	C(20)—C(21)	1.355 (14)
Cu(2)—N(9)	1.954 (3)	C(21)—C(22)	1.421 (12)
Cu(2)—N(9) ⁱ	1.954 (3)	C(24)—C(25)	1.400 (6)

Cu(1)—N(1)	2.001 (3)	C(24)—C(29)	1.403 (5)
Cu(1)—N(3) ⁱⁱ	2.022 (3)	C(25)—C(26)	1.364 (7)
Cu(1)—N(4) ⁱⁱⁱ	2.174 (3)	C(26)—C(27)	1.396 (7)
Cu(1)—N(11)	1.984 (3)	C(27)—C(28)	1.335 (8)
Cu(1)—N(13)	1.993 (3)	C(28)—C(29)	1.408 (7)
N(2)—C(2)	1.153 (5)	O(1)—H(1)	1.05 (12)
N(1)—C(1)	1.131 (5)	O(1)—H(1) ⁱ	1.05 (12)
N(3)—C(3)	1.137 (5)	N(10)—H(10N)	0.860
N(4)—C(4)	1.140 (5)	N(12)—H(12N)	0.860
N(5)—C(5)	1.136 (5)	N(14)—H(14N)	0.860
N(6)—C(6)	1.145 (6)	C(9)—H(9)	0.930
N(7)—C(7)	1.139 (5)	C(11)—H(11)	0.930
N(8)—C(8)	1.131 (5)	C(12)—H(12)	0.930
N(9)—C(9)	1.312 (6)	C(13)—H(13)	0.930
N(9)—C(10)	1.392 (6)	C(14)—H(14)	0.930
N(10)—C(9)	1.326 (6)	C(16)—H(16)	0.930
N(10)—C(15)	1.396 (8)	C(18)—H(18)	0.930
N(11)—C(16)	1.327 (5)	C(19)—H(19)	0.930
N(11)—C(17)	1.385 (6)	C(20)—H(20)	0.930
N(12)—C(16)	1.362 (7)	C(21)—H(21)	0.930
N(12)—C(22)	1.345 (8)	C(23)—H(23)	0.930
N(13)—C(23)	1.318 (5)	C(25)—H(25)	0.930
N(13)—C(24)	1.394 (5)	C(26)—H(26)	0.930
N(14)—C(23)	1.328 (5)	C(27)—H(27)	0.930
N(14)—C(29)	1.367 (6)	C(28)—H(28)	0.930
C(10)—C(11)	1.378 (8)		
N(5)⋯N(10) ^{iv}	2.802 (5)	C(27)⋯H(12N) ^{vi}	3.506
N(7)⋯N(14) ^v	2.973 (5)	C(27)⋯H(16) ^{vi}	3.538
N(8)⋯N(12) ^{vi}	2.889 (5)	C(28)⋯H(12N) ^{vi}	3.500
N(8)⋯C(26) ^{vii}	3.482 (6)	H(9)⋯H(14) ^{ix}	3.551
N(8)⋯C(27) ^{vii}	3.391 (7)	H(10N)⋯N(5) ^{viii}	1.968
N(10)⋯N(5) ^{viii}	2.802 (5)	H(10N)⋯C(5) ^{viii}	2.976
N(10)⋯C(14) ^{ix}	3.324 (10)	H(10N)⋯C(13) ^{ix}	3.580
N(10)⋯C(15) ^{ix}	3.485 (7)	H(10N)⋯C(14) ^{ix}	3.389
N(12)⋯N(8) ^v	2.889 (5)	H(10N)⋯C(15) ^{ix}	3.472
N(12)⋯C(28) ^v	3.451 (7)	H(11)⋯C(18) ^{xii}	3.360
N(14)⋯N(7) ^{vi}	2.973 (5)	H(11)⋯H(18) ^{xii}	2.795
N(14)⋯C(26) ^x	3.453 (6)	H(11)⋯H(23) ^{xii}	3.320
N(14)⋯C(27) ^x	3.515 (7)	H(12)⋯N(6) ^{xii}	3.152
C(9)⋯C(14) ^{ix}	3.531 (10)	H(12)⋯C(23) ^{xii}	3.104
C(14)⋯N(10) ^{ix}	3.324 (10)	H(12)⋯H(18) ^{xii}	3.476
C(14)⋯C(9) ^{ix}	3.531 (10)	H(12)⋯H(20) ^{ix}	3.589
C(15)⋯N(10) ^{ix}	3.485 (7)	H(12)⋯H(21) ^{ix}	3.453
C(15)⋯C(15) ^{ix}	3.539 (8)	H(12)⋯H(23) ^{xii}	2.652
C(23)⋯C(27) ^x	3.555 (7)	H(12N)⋯N(8) ^v	2.040
C(24)⋯C(28) ^x	3.433 (7)	H(12N)⋯C(8) ^v	2.971
C(26)⋯N(8) ^{vii}	3.482 (6)	H(12N)⋯C(27) ^v	3.506

C(26)···N(14) ^x	3.453 (6)	H(12N)···C(28) ^y	3.500
C(27)···N(8) ^{vii}	3.391 (7)	H(13)···C(20) ^{ix}	2.980
C(27)···N(14) ^x	3.515 (7)	H(13)···H(20) ^{ix}	2.384
C(27)···C(23) ^x	3.555 (7)	H(14)···N(5) ^{viii}	3.340
C(27)···C(29) ^x	3.524 (7)	H(14)···N(6) ^{viii}	2.890
C(28)···N(12) ^{vi}	3.451 (7)	H(14)···N(9) ^{ix}	3.538
C(28)···C(24) ^x	3.433 (7)	H(14)···N(10) ^{ix}	3.399
C(29)···C(27) ^x	3.524 (7)	H(14)···C(5) ^{viii}	3.525
N(3)···H(27) ^{vii}	3.329	H(14)···C(6) ^{viii}	3.310
N(4)···H(28) ^y	3.556	H(14)···C(9) ^{ix}	3.307
N(5)···H(10N) ^{iv}	1.968	H(14)···H(9) ^{ix}	3.551
N(5)···H(14) ^{iv}	3.340	H(14N)···N(7) ^{vi}	2.177
N(5)···H(26) ^{vii}	3.558	H(14N)···C(7) ^{vi}	3.267
N(6)···H(12) ^{xi}	3.152	H(14N)···C(26) ^x	3.489
N(6)···H(14) ^{iv}	2.890	H(14N)···H(26) ^x	3.371
N(6)···H(21) ^{vi}	3.534	H(16)···C(27) ^y	3.538
N(7)···H(14N) ^y	2.177	H(16)···H(27) ^y	3.190
N(7)···H(28) ^y	3.123	H(18)···C(11) ^{xi}	3.566
N(8)···H(12N) ^{vi}	2.040	H(18)···H(11) ^{xi}	2.795
N(8)···H(21) ^{vi}	3.475	H(18)···H(12) ^{xi}	3.476
N(8)···H(26) ^{vii}	3.080	H(20)···C(13) ^{ix}	3.222
N(8)···H(27) ^{vii}	2.904	H(20)···H(12) ^{ix}	3.589
N(9)···H(14) ^{ix}	3.538	H(20)···H(13) ^{ix}	2.384
N(10)···H(14) ^{ix}	3.399	H(21)···N(6) ^v	3.534
N(12)···H(28) ^y	3.531	H(21)···N(8) ^v	3.475
N(13)···H(27) ^x	3.472	H(21)···C(6) ^v	3.561
N(14)···H(26) ^x	3.508	H(21)···C(8) ^v	3.591
C(3)···H(27) ^{vii}	3.255	H(21)···H(12) ^{ix}	3.453
C(5)···H(10N) ^{iv}	2.976	H(23)···C(11) ^{xi}	3.374
C(5)···H(14) ^{iv}	3.525	H(23)···C(12) ^{xi}	3.024
C(5)···H(27) ^{vii}	3.555	H(23)···H(11) ^{xi}	3.320
C(6)···H(14) ^{iv}	3.310	H(23)···H(12) ^{xi}	2.652
C(6)···H(21) ^{vi}	3.561	H(23)···H(27) ^x	3.542
C(7)···H(14N) ^y	3.267	H(26)···N(5) ^{vii}	3.558
C(7)···H(28) ^y	3.453	H(26)···N(8) ^{vii}	3.080
C(8)···H(12N) ^{vi}	2.971	H(26)···N(14) ^x	3.508
C(8)···H(21) ^{vi}	3.591	H(26)···H(14N) ^x	3.371
C(8)···H(27) ^{vii}	2.947	H(27)···N(3) ^{vii}	3.329
C(9)···H(14) ^{ix}	3.307	H(27)···N(8) ^{vii}	2.904
C(11)···H(18) ^{xii}	3.566	H(27)···N(13) ^x	3.472
C(11)···H(23) ^{xii}	3.374	H(27)···C(3) ^{vii}	3.255
C(12)···H(23) ^{xii}	3.024	H(27)···C(5) ^{vii}	3.555
C(13)···H(10N) ^{ix}	3.580	H(27)···C(8) ^{vii}	2.947
C(13)···H(20) ^{ix}	3.222	H(27)···C(16) ^{vi}	3.493
C(14)···H(10N) ^{ix}	3.389	H(27)···C(23) ^x	3.348
C(15)···H(10N) ^{ix}	3.472	H(27)···H(16) ^{vi}	3.190
C(16)···H(27) ^y	3.493	H(27)···H(23) ^x	3.542
C(16)···H(28) ^y	3.513	H(28)···N(4) ^{vi}	3.556

C(18)···H(11) ^{xi}	3.360	H(28)···N(7) ^{vi}	3.123
C(20)···H(13) ^{ix}	2.980	H(28)···N(12) ^{vi}	3.531
C(23)···H(12) ^{xi}	3.104	H(28)···C(7) ^{vi}	3.453
C(23)···H(27) ^x	3.348	H(28)···C(16) ^{vi}	3.513
C(24)···H(28) ^x	3.476	H(28)···C(24) ^x	3.476
C(25)···H(28) ^x	3.477	H(28)···C(25) ^x	3.477
C(26)···H(14N) ^x	3.489		
C(2)—W(1)—C(1)	133.28 (14)	N(9)—C(10)—C(11)	131.1 (5)
C(2)—W(1)—C(3)	75.96 (14)	N(9)—C(10)—C(15)	107.9 (4)
C(2)—W(1)—C(4)	133.67 (14)	C(11)—C(10)—C(15)	120.9 (5)
C(2)—W(1)—C(5)	71.25 (15)	C(10)—C(11)—C(12)	116.2 (6)
C(2)—W(1)—C(6)	74.47 (16)	C(11)—C(12)—C(13)	121.0 (7)
C(2)—W(1)—C(7)	72.00 (15)	C(12)—C(13)—C(14)	122.0 (8)
C(2)—W(1)—C(8)	141.36 (14)	C(13)—C(14)—C(15)	116.5 (7)
C(1)—W(1)—C(3)	143.38 (14)	N(10)—C(15)—C(10)	105.7 (4)
C(1)—W(1)—C(4)	71.55 (13)	N(10)—C(15)—C(14)	130.9 (5)
C(1)—W(1)—C(5)	129.57 (14)	C(10)—C(15)—C(14)	123.3 (6)
C(1)—W(1)—C(6)	71.26 (15)	N(11)—C(16)—N(12)	109.7 (4)
C(1)—W(1)—C(7)	79.50 (15)	N(11)—C(17)—C(18)	130.5 (4)
C(1)—W(1)—C(8)	72.70 (15)	N(11)—C(17)—C(22)	108.2 (4)
C(3)—W(1)—C(4)	71.85 (13)	C(18)—C(17)—C(22)	121.2 (5)
C(3)—W(1)—C(5)	74.89 (14)	C(17)—C(18)—C(19)	117.2 (6)
C(3)—W(1)—C(6)	145.36 (15)	C(18)—C(19)—C(20)	120.8 (7)
C(3)—W(1)—C(7)	93.95 (14)	C(19)—C(20)—C(21)	123.8 (9)
C(3)—W(1)—C(8)	97.32 (15)	C(20)—C(21)—C(22)	116.5 (8)
C(4)—W(1)—C(5)	128.28 (15)	N(12)—C(22)—C(17)	106.0 (5)
C(4)—W(1)—C(6)	142.77 (15)	N(12)—C(22)—C(21)	133.6 (6)
C(4)—W(1)—C(7)	77.88 (15)	C(17)—C(22)—C(21)	120.4 (6)
C(4)—W(1)—C(8)	75.95 (15)	N(13)—C(23)—N(14)	113.3 (4)
C(5)—W(1)—C(6)	78.82 (17)	N(13)—C(24)—C(25)	131.7 (3)
C(5)—W(1)—C(7)	143.17 (16)	N(13)—C(24)—C(29)	108.0 (3)
C(5)—W(1)—C(8)	70.29 (15)	C(25)—C(24)—C(29)	120.1 (4)
C(6)—W(1)—C(7)	93.73 (17)	C(24)—C(25)—C(26)	116.7 (4)
C(6)—W(1)—C(8)	94.60 (17)	C(25)—C(26)—C(27)	122.7 (5)
C(7)—W(1)—C(8)	146.55 (16)	C(26)—C(27)—C(28)	122.0 (5)
N(2)—Cu(2)—N(2) ⁱ	163.78 (16)	C(27)—C(28)—C(29)	117.1 (4)
N(2)—Cu(2)—N(9)	91.10 (15)	N(14)—C(29)—C(24)	105.9 (3)
N(2)—Cu(2)—N(9) ⁱ	92.26 (15)	N(14)—C(29)—C(28)	132.6 (4)
N(2) ⁱ —Cu(2)—N(9)	92.26 (15)	C(24)—C(29)—C(28)	121.4 (4)
N(2) ⁱ —Cu(2)—N(9) ⁱ	91.10 (15)	H(1)—O(1)—H(1) ⁱ	116 (9)
N(9)—Cu(2)—N(9) ⁱ	156.03 (18)	C(9)—N(10)—H(10N)	126.4
N(1)—Cu(1)—N(3) ⁱⁱ	157.80 (15)	C(15)—N(10)—H(10N)	126.4
N(1)—Cu(1)—N(4) ⁱⁱⁱ	102.33 (14)	C(16)—N(12)—H(12N)	125.4
N(1)—Cu(1)—N(11)	87.14 (14)	C(22)—N(12)—H(12N)	125.4
N(1)—Cu(1)—N(13)	90.06 (13)	C(23)—N(14)—H(14N)	126.2
N(3) ⁱⁱ —Cu(1)—N(4) ⁱⁱⁱ	99.67 (14)	C(29)—N(14)—H(14N)	126.2
N(3) ⁱⁱ —Cu(1)—N(11)	88.48 (14)	N(9)—C(9)—H(9)	123.7

N(3) ⁱⁱ —Cu(1)—N(13)	89.08 (13)	N(10)—C(9)—H(9)	123.7
N(4) ⁱⁱⁱ —Cu(1)—N(11)	93.97 (14)	C(10)—C(11)—H(11)	121.9
N(4) ⁱⁱⁱ —Cu(1)—N(13)	99.71 (14)	C(12)—C(11)—H(11)	121.9
N(11)—Cu(1)—N(13)	166.32 (15)	C(11)—C(12)—H(12)	119.5
Cu(2)—N(2)—C(2)	160.9 (3)	C(13)—C(12)—H(12)	119.5
Cu(1)—N(1)—C(1)	173.5 (3)	C(12)—C(13)—H(13)	119.0
Cu(1) ^{xiii} —N(3)—C(3)	175.4 (3)	C(14)—C(13)—H(13)	119.0
Cu(1) ^{xiv} —N(4)—C(4)	172.1 (3)	C(13)—C(14)—H(14)	121.7
Cu(2)—N(9)—C(9)	124.8 (3)	C(15)—C(14)—H(14)	121.8
Cu(2)—N(9)—C(10)	128.6 (3)	N(11)—C(16)—H(16)	125.2
C(9)—N(9)—C(10)	106.5 (3)	N(12)—C(16)—H(16)	125.2
C(9)—N(10)—C(15)	107.3 (4)	C(17)—C(18)—H(18)	121.4
Cu(1)—N(11)—C(16)	127.3 (3)	C(19)—C(18)—H(18)	121.4
Cu(1)—N(11)—C(17)	125.9 (2)	C(18)—C(19)—H(19)	119.6
C(16)—N(11)—C(17)	106.8 (3)	C(20)—C(19)—H(19)	119.6
C(16)—N(12)—C(22)	109.2 (4)	C(19)—C(20)—H(20)	118.1
Cu(1)—N(13)—C(23)	124.3 (3)	C(21)—C(20)—H(20)	118.1
Cu(1)—N(13)—C(24)	130.6 (2)	C(20)—C(21)—H(21)	121.7
C(23)—N(13)—C(24)	105.1 (3)	C(22)—C(21)—H(21)	121.7
C(23)—N(14)—C(29)	107.6 (3)	N(13)—C(23)—H(23)	123.3
W(1)—C(2)—N(2)	175.6 (3)	N(14)—C(23)—H(23)	123.4
W(1)—C(1)—N(1)	174.2 (3)	C(24)—C(25)—H(25)	121.7
W(1)—C(3)—N(3)	175.3 (3)	C(26)—C(25)—H(25)	121.7
W(1)—C(4)—N(4)	178.7 (3)	C(25)—C(26)—H(26)	118.7
W(1)—C(5)—N(5)	176.6 (3)	C(27)—C(26)—H(26)	118.7
W(1)—C(6)—N(6)	174.9 (4)	C(26)—C(27)—H(27)	119.0
W(1)—C(7)—N(7)	177.9 (4)	C(28)—C(27)—H(27)	119.0
W(1)—C(8)—N(8)	178.4 (4)	C(27)—C(28)—H(28)	121.4
N(9)—C(9)—N(10)	112.6 (4)	C(29)—C(28)—H(28)	121.4
C(2)—W(1)—C(1)—N(1)	-131 (3)	N(13)—Cu(1)—N(1)—C(1)	-82 (3)
C(1)—W(1)—C(2)—N(2)	53 (4)	N(3) ⁱⁱ —Cu(1)—N(4) ⁱⁱⁱ —C(4) ⁱⁱⁱ	100 (2)
C(2)—W(1)—C(3)—N(3)	64 (4)	N(4) ⁱⁱⁱ —Cu(1)—N(3) ⁱⁱ —C(3) ⁱⁱ	-165 (4)
C(3)—W(1)—C(2)—N(2)	-153 (4)	N(3) ⁱⁱ —Cu(1)—N(11)—C(16)	-82.6 (3)
C(2)—W(1)—C(4)—N(4)	115 (14)	N(3) ⁱⁱ —Cu(1)—N(11)—C(17)	98.0 (3)
C(4)—W(1)—C(2)—N(2)	160 (4)	N(11)—Cu(1)—N(3) ⁱⁱ —C(3) ⁱⁱ	-72 (4)
C(2)—W(1)—C(5)—N(5)	-89 (6)	N(3) ⁱⁱ —Cu(1)—N(13)—C(23)	-47.8 (3)
C(5)—W(1)—C(2)—N(2)	-74 (4)	N(3) ⁱⁱ —Cu(1)—N(13)—C(24)	133.9 (3)
C(2)—W(1)—C(6)—N(6)	22 (5)	N(13)—Cu(1)—N(3) ⁱⁱ —C(3) ⁱⁱ	95 (4)
C(6)—W(1)—C(2)—N(2)	9 (4)	N(4) ⁱⁱⁱ —Cu(1)—N(11)—C(16)	17.0 (3)
C(2)—W(1)—C(7)—N(7)	51 (11)	N(4) ⁱⁱⁱ —Cu(1)—N(11)—C(17)	-162.4 (3)
C(7)—W(1)—C(2)—N(2)	108 (4)	N(11)—Cu(1)—N(4) ⁱⁱⁱ —C(4) ⁱⁱⁱ	11 (2)
C(2)—W(1)—C(8)—N(8)	98 (13)	N(4) ⁱⁱⁱ —Cu(1)—N(13)—C(23)	-147.5 (3)
C(8)—W(1)—C(2)—N(2)	-68 (4)	N(4) ⁱⁱⁱ —Cu(1)—N(13)—C(24)	34.3 (3)
C(1)—W(1)—C(3)—N(3)	-148 (4)	N(13)—Cu(1)—N(4) ⁱⁱⁱ —C(4) ⁱⁱⁱ	-169 (2)
C(3)—W(1)—C(1)—N(1)	93 (3)	N(11)—Cu(1)—N(13)—C(23)	32.0 (7)
C(1)—W(1)—C(4)—N(4)	-112 (14)	N(11)—Cu(1)—N(13)—C(24)	-146.3 (5)
C(4)—W(1)—C(1)—N(1)	95 (3)	N(13)—Cu(1)—N(11)—C(16)	-162.4 (5)

C(1)—W(1)—C(5)—N(5)	140 (6)	N(13)—Cu(1)—N(11)—C(17)	18.1 (7)
C(5)—W(1)—C(1)—N(1)	-30 (3)	Cu(2)—N(2)—C(2)—W(1)	-28 (5)
C(1)—W(1)—C(6)—N(6)	-126 (5)	Cu(1)—N(1)—C(1)—W(1)	95 (4)
C(6)—W(1)—C(1)—N(1)	-87 (3)	Cu(1) ^{xiii} —N(3)—C(3)—W(1)	-53 (7)
C(1)—W(1)—C(7)—N(7)	-166 (11)	Cu(1) ^{xiv} —N(4)—C(4)—W(1)	11 (16)
C(7)—W(1)—C(1)—N(1)	176 (3)	Cu(2)—N(9)—C(9)—N(10)	-178.3 (3)
C(1)—W(1)—C(8)—N(8)	-42 (13)	Cu(2)—N(9)—C(10)—C(11)	2.3 (8)
C(8)—W(1)—C(1)—N(1)	15 (3)	Cu(2)—N(9)—C(10)—C(15)	178.3 (3)
C(3)—W(1)—C(4)—N(4)	66 (14)	C(9)—N(9)—C(10)—C(11)	-174.8 (6)
C(4)—W(1)—C(3)—N(3)	-150 (4)	C(9)—N(9)—C(10)—C(15)	1.2 (6)
C(3)—W(1)—C(5)—N(5)	-9 (6)	C(10)—N(9)—C(9)—N(10)	-1.1 (6)
C(5)—W(1)—C(3)—N(3)	-10 (4)	C(9)—N(10)—C(15)—C(10)	0.3 (6)
C(3)—W(1)—C(6)—N(6)	54 (5)	C(9)—N(10)—C(15)—C(14)	178.9 (7)
C(6)—W(1)—C(3)—N(3)	31 (4)	C(15)—N(10)—C(9)—N(9)	0.5 (6)
C(3)—W(1)—C(7)—N(7)	-22 (11)	Cu(1)—N(11)—C(16)—N(12)	-179.4 (3)
C(7)—W(1)—C(3)—N(3)	134 (4)	Cu(1)—N(11)—C(17)—C(18)	-0.3 (5)
C(3)—W(1)—C(8)—N(8)	174 (13)	Cu(1)—N(11)—C(17)—C(22)	178.7 (3)
C(8)—W(1)—C(3)—N(3)	-78 (4)	C(16)—N(11)—C(17)—C(18)	-179.8 (3)
C(4)—W(1)—C(5)—N(5)	42 (7)	C(16)—N(11)—C(17)—C(22)	-0.9 (5)
C(5)—W(1)—C(4)—N(4)	14 (14)	C(17)—N(11)—C(16)—N(12)	0.1 (4)
C(4)—W(1)—C(6)—N(6)	-123 (5)	C(16)—N(12)—C(22)—C(17)	-1.3 (6)
C(6)—W(1)—C(4)—N(4)	-115 (14)	C(16)—N(12)—C(22)—C(21)	-179.3 (7)
C(4)—W(1)—C(7)—N(7)	-93 (11)	C(22)—N(12)—C(16)—N(11)	0.7 (6)
C(7)—W(1)—C(4)—N(4)	165 (14)	Cu(1)—N(13)—C(23)—N(14)	-177.5 (3)
C(4)—W(1)—C(8)—N(8)	-117 (13)	Cu(1)—N(13)—C(24)—C(25)	-5.3 (6)
C(8)—W(1)—C(4)—N(4)	-36 (14)	Cu(1)—N(13)—C(24)—C(29)	178.5 (3)
C(5)—W(1)—C(6)—N(6)	95 (5)	C(23)—N(13)—C(24)—C(25)	176.2 (4)
C(6)—W(1)—C(5)—N(5)	-166 (6)	C(23)—N(13)—C(24)—C(29)	-0.0 (3)
C(5)—W(1)—C(7)—N(7)	48 (11)	C(24)—N(13)—C(23)—N(14)	1.1 (5)
C(7)—W(1)—C(5)—N(5)	-85 (6)	C(23)—N(14)—C(29)—C(24)	1.6 (5)
C(5)—W(1)—C(8)—N(8)	103 (13)	C(23)—N(14)—C(29)—C(28)	-174.7 (5)
C(8)—W(1)—C(5)—N(5)	95 (6)	C(29)—N(14)—C(23)—N(13)	-1.8 (5)
C(6)—W(1)—C(7)—N(7)	124 (11)	N(9)—C(10)—C(11)—C(12)	178.2 (6)
C(7)—W(1)—C(6)—N(6)	-48 (5)	N(9)—C(10)—C(15)—N(10)	-0.9 (6)
C(6)—W(1)—C(8)—N(8)	27 (13)	N(9)—C(10)—C(15)—C(14)	-179.6 (6)
C(8)—W(1)—C(6)—N(6)	164 (5)	C(11)—C(10)—C(15)—N(10)	175.5 (5)
C(7)—W(1)—C(8)—N(8)	-77 (13)	C(11)—C(10)—C(15)—C(14)	-3.2 (10)
C(8)—W(1)—C(7)—N(7)	-132 (11)	C(15)—C(10)—C(11)—C(12)	2.7 (9)
N(2)—Cu(2)—N(2) ⁱ —C(2) ⁱ	-7.9 (13)	C(10)—C(11)—C(12)—C(13)	-1.5 (11)
N(2) ⁱ —Cu(2)—N(2)—C(2)	-7.9 (13)	C(11)—C(12)—C(13)—C(14)	0.6 (13)
N(2)—Cu(2)—N(9)—C(9)	33.0 (4)	C(12)—C(13)—C(14)—C(15)	-0.8 (14)
N(2)—Cu(2)—N(9)—C(10)	-143.5 (4)	C(13)—C(14)—C(15)—N(10)	-176.3 (7)
N(9)—Cu(2)—N(2)—C(2)	-109.8 (10)	C(13)—C(14)—C(15)—C(10)	2.1 (12)
N(2)—Cu(2)—N(9) ⁱ —C(9) ⁱ	-131.1 (4)	N(11)—C(17)—C(18)—C(19)	-179.7 (5)
N(2)—Cu(2)—N(9) ⁱ —C(10) ⁱ	52.3 (4)	N(11)—C(17)—C(22)—N(12)	1.3 (5)
N(9) ⁱ —Cu(2)—N(2)—C(2)	93.9 (10)	N(11)—C(17)—C(22)—C(21)	179.7 (5)
N(2) ⁱ —Cu(2)—N(9)—C(9)	-131.1 (4)	C(18)—C(17)—C(22)—N(12)	-179.6 (4)
N(2) ⁱ —Cu(2)—N(9)—C(10)	52.3 (4)	C(18)—C(17)—C(22)—C(21)	-1.3 (8)

N(9)—Cu(2)—N(2) ⁱ —C(2) ⁱ	93.9 (10)	C(22)—C(17)—C(18)—C(19)	1.4 (8)
N(2) ⁱ —Cu(2)—N(9) ⁱ —C(9) ⁱ	33.0 (4)	C(17)—C(18)—C(19)—C(20)	-0.5 (10)
N(2) ⁱ —Cu(2)—N(9) ⁱ —C(10) ⁱ	-143.5 (4)	C(18)—C(19)—C(20)—C(21)	-0.6 (11)
N(9) ⁱ —Cu(2)—N(2) ⁱ —C(2) ⁱ	-109.8 (10)	C(19)—C(20)—C(21)—C(22)	0.8 (13)
N(9)—Cu(2)—N(9) ⁱ —C(9) ⁱ	131.1 (4)	C(20)—C(21)—C(22)—N(12)	178.0 (7)
N(9)—Cu(2)—N(9) ⁱ —C(10) ⁱ	-45.5 (6)	C(20)—C(21)—C(22)—C(17)	0.1 (8)
N(9) ⁱ —Cu(2)—N(9)—C(9)	131.1 (4)	N(13)—C(24)—C(25)—C(26)	-175.5 (4)
N(9) ⁱ —Cu(2)—N(9)—C(10)	-45.5 (6)	N(13)—C(24)—C(29)—N(14)	-1.0 (4)
N(1)—Cu(1)—N(3) ⁱⁱ —C(3) ⁱⁱ	7 (4)	N(13)—C(24)—C(29)—C(28)	175.8 (4)
N(3) ⁱⁱ —Cu(1)—N(1)—C(1)	5 (3)	C(25)—C(24)—C(29)—N(14)	-177.8 (4)
N(1)—Cu(1)—N(4) ⁱⁱⁱ —C(4) ⁱⁱⁱ	-77 (2)	C(25)—C(24)—C(29)—C(28)	-0.9 (6)
N(4) ⁱⁱⁱ —Cu(1)—N(1)—C(1)	178 (2)	C(29)—C(24)—C(25)—C(26)	0.3 (6)
N(1)—Cu(1)—N(11)—C(16)	119.2 (3)	C(24)—C(25)—C(26)—C(27)	-0.3 (6)
N(1)—Cu(1)—N(11)—C(17)	-60.3 (3)	C(25)—C(26)—C(27)—C(28)	0.9 (8)
N(11)—Cu(1)—N(1)—C(1)	84 (2)	C(26)—C(27)—C(28)—C(29)	-1.4 (8)
N(1)—Cu(1)—N(13)—C(23)	110.0 (3)	C(27)—C(28)—C(29)—N(14)	177.3 (5)
N(1)—Cu(1)—N(13)—C(24)	-68.3 (3)	C(27)—C(28)—C(29)—C(24)	1.5 (7)

Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $x, y+1, z$; (iii) $-x+1/2, y+1/2, -z+1/2$; (iv) $x, -y+1, z-1/2$; (v) $x, -y+2, z+1/2$; (vi) $x, -y+2, z-1/2$; (vii) $-x+1/2, -y+3/2, -z$; (viii) $x, -y+1, z+1/2$; (ix) $-x, -y+1, -z+1$; (x) $-x+1/2, -y+5/2, -z$; (xi) $-x, y+1, -z+1/2$; (xii) $-x, y-1, -z+1/2$; (xiii) $x, y-1, z$; (xiv) $-x+1/2, y-1/2, -z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O(1)—H(1) \cdots N(6)	1.05 (12)	2.20 (12)	3.178 (7)	154 (10)
N(10)—H(10N) \cdots N(5) ^{viii}	0.86	1.97	2.802 (5)	163
N(12)—H(12N) \cdots N(8) ^v	0.86	2.04	2.888 (5)	169
N(14)—H(14N) \cdots N(7) ^{vi}	0.86	2.18	2.973 (5)	154

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