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An ionic organic–inorganic hybrid: tetrakis[bis(1,10-phenanthroline)- copper(I)] dodecatungstophosphate(V). Corrigendum

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The chemical name in the title of the paper by Meng, Liu & Chen [*Acta Cryst.* (2008), E64, m106] is corrected.

In the paper by Meng, Liu & Chen [*Acta Cryst.* (2008), E64, m106], the chemical name in the title is incorrect. The correct chemical name should be 'tetrakis[bis(1,10-phenanthroline)-copper(I)] dodecatungstosilicate'.

An ionic organic–inorganic hybrid: tetrakis[bis(1,10-phenanthroline)-copper(I)] dodecatungstophosphate(V)

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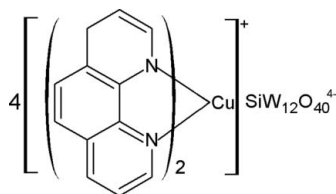
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.018$ Å; R factor = 0.041; wR factor = 0.072; data-to-parameter ratio = 16.4.

Single crystals of the title polyoxometallate-based organic–inorganic hybrid, $[\text{Cu}(\text{C}_{12}\text{H}_8\text{N}_2)_2]_4[\text{SiW}_{12}\text{O}_{40}]$, were grown under hydrothermal conditions. The discrete $[\text{SiW}_{12}\text{O}_{40}]^{4-}$ anions are of the Keggin type and are packed in a slightly distorted orthorhombic F -centred mode, with the complex $[\text{Cu}^{\text{I}}(\text{phen})_2]^+$ cations (phen is 1,10-phenanthroline) located in the voids of this arrangement. The four independent Cu^{I} cations are situated in the centres of more or less distorted tetrahedra made up of N atoms from the phen ligands. The anions and cations are linked together *via* weak hydrogen-bonding interactions, forming an extended three-dimensional network. Additional stabilization is achieved *via* π – π interactions between different phen molecules of adjacent $[\text{Cu}^{\text{I}}(\text{phen})_2]^+$ cations with shortest distances between 3.416 and 3.499 Å.

Related literature

The educt $\text{H}_4\text{SiW}_{12}\text{O}_{40} \cdot n\text{H}_2\text{O}$ was prepared according to literature procedures (Rocchiccioli-Deltcheff *et al.*, 1983). A review of polyoxometallates was given recently by Kurth *et al.* (2001). For the bond-valence model, see: Brown (2002).



Experimental

Crystal data

$[\text{Cu}(\text{C}_{12}\text{H}_8\text{N}_2)_2]_4[\text{SiW}_{12}\text{O}_{40}]$
 $M_r = 4570.08$
 Orthorhombic, $P2_12_12_1$
 $a = 18.332$ (3) Å
 $b = 21.173$ (3) Å
 $c = 27.901$ (4) Å

$V = 10830$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 13.55$ mm⁻¹
 $T = 293$ (2) K
 $0.23 \times 0.21 \times 0.20$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\text{min}} = 0.066$, $T_{\text{max}} = 0.072$
 (expected range = 0.061–0.066)

66617 measured reflections
 24930 independent reflections
 20506 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.065$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.072$
 $S = 0.99$
 24930 reflections
 1523 parameters
 2431 restraints

H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.37$ e Å⁻³
 Absolute structure: Flack (1983), with 11091 Friedel pairs
 Flack parameter: -0.006 (6)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C10—H10A···O17	0.93	2.64	3.503 (17)	154
C41—H41A···O26	0.93	2.74	3.131 (13)	106
C25—H25A···O10	0.93	2.43	3.329 (16)	162
C50—H50A···O35	0.93	2.62	3.477 (16)	153
C69—H69A···O34	0.93	2.59	3.322 (14)	136
C49—H49A···O5	0.93	2.36	3.276 (18)	169
C92—H92A···O15	0.93	3.04	3.491 (16)	111
C94—H94A···O24	0.93	2.62	3.326 (14)	134

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: Mercury (Version 1.4.2; Macrae *et al.*, 2006); software used to prepare material for publication: SHELXL97 (Sheldrick, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2165).

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supporting information

Acta Cryst. (2008). E64, m106 [https://doi.org/10.1107/S1600536807062903]

An ionic organic–inorganic hybrid: tetrakis[bis(1,10-phenanthroline)copper(I)] dodecatungstophosphate(V)

Fan-Xia Meng, Hong-Bo Liu and Ya-Guang Chen

S1. Comment

The structure of the title compound is built from four independent complex coordination cations $[\text{Cu}(\text{phen})_2]^+$ and one Keggin-type anion $[\text{SiW}_{12}\text{O}_{40}]^{4-}$. The Keggin anions are arranged in a slightly distorted orthorhombic F-centred packing mode (Fig. 1) with the $[\text{Cu}(\text{phen})_2]^+$ cations enclosing the Keggin anion, as shown in Fig. 2. In the Keggin anion, the Si—O and W—O distances as well as the corresponding angles are very similar to those of $\text{H}_4\text{SiW}_{12}\text{O}_{40}$ (Kurth *et al.*, 2001). The four Cu^+ centres are surrounded in a distorted tetrahedral manner by N atoms from two phen molecules each, with Cu—N distances ranging from 1.982 (10) Å to 2.097 (12) Å, and N—Cu—N bond angles ranging from 81.0 (4)° to 149.3 (4)°.

The structure is held together by weak hydrogen bonding interactions between the phen H atoms of the cations and the terminal and bridging O atoms of the anions (Table 2). Additional stabilization of the structure is reached *via* π – π interactions between adjacent phen molecules with shortest distances between 3.416 Å and 3.499 Å (Fig. 3).

Results of bond valence sum (BVS) calculations (Brown, 2002) are in accordance with expected values for hexavalent tungsten (average for the 12 W atoms 6.19 valence units) and monovalent copper (average for the 4 Cu atoms 0.99 valence units). The presence of Cu^+ was also confirmed by ESR experiments.

S2. Experimental

$\text{H}_4\text{SiW}_{12}\text{O}_{40}\cdot n\text{H}_2\text{O}$ was prepared according to the method given by Rocchiccioli-Deltcheff *et al.* (1983). The starting mixture of $\text{H}_4\text{SiW}_{12}\text{O}_{40}\cdot n\text{H}_2\text{O}$ (1.15 g), $\text{Cu}(\text{OAc})_2\cdot 2\text{H}_2\text{O}$ (0.16 g), phen (0.065 g), oxalic acid dihydrate (0.25 g) and H_2O (10 ml) was adjusted to pH = 2.5 by addition of HCl under stirring for 30 min. The final solution was transferred into a 25 ml Teflon lined autoclave and was heated at 443 K for 72 h. Then the autoclave was cooled with a rate of 10 K.h⁻¹ to room temperature. Deep-black block-like crystals were filtered off, washed with distilled water, and dried at ambient temperature (45% yield on W).

S3. Refinement

The U^{ij} parameters of all C atoms were restrained to be approximately equal by using the SIMU instruction in *SHELXL97*. Hydrogen atoms were placed geometrically and refined in the riding model with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ of the parent C atom. In the final Fourier map, the distance of the highest peak is 0.90 Å away from W2 and the distance of the deepest hole is 0.90 Å from W12.

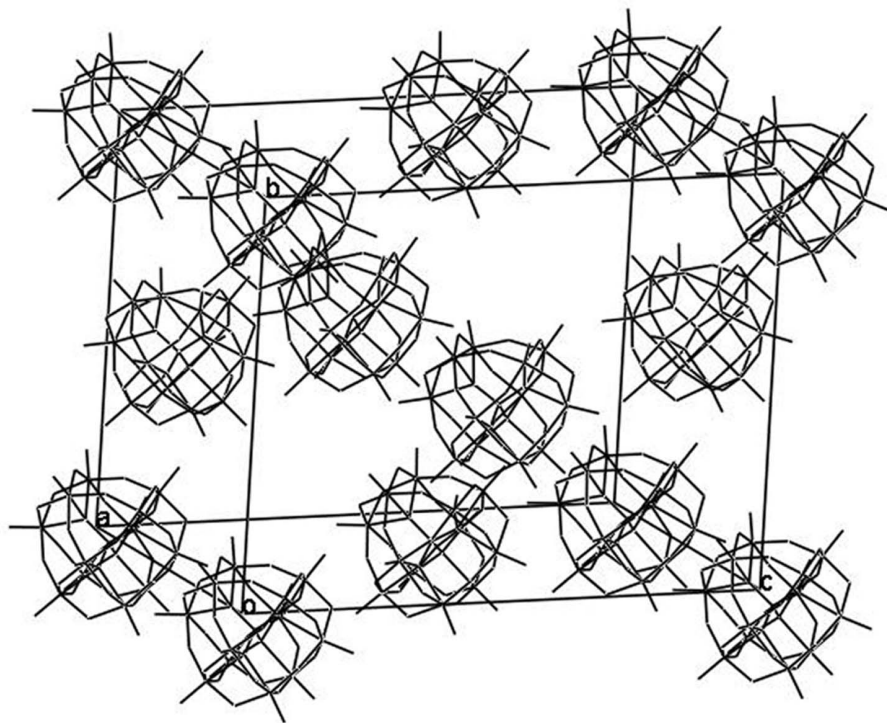


Figure 1

The packing of the $[\text{SiW}_{12}\text{O}_{40}]^{4-}$ heteropolyanions leading to a slightly distorted F-centred orthorhombic lattice. All other atoms are omitted for clarity.

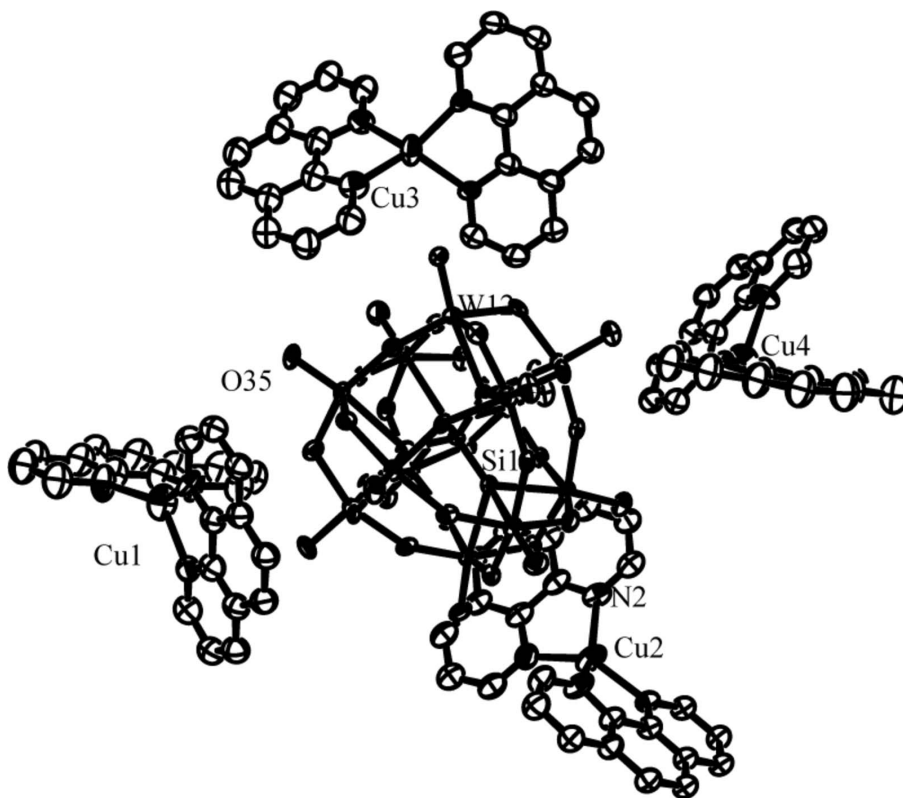


Figure 2

The Keggin-type $\text{SiW}_{12}\text{O}_{40}^{4-}$ anions with surrounding $[\text{Cu}(\text{phen})_2]^+$ cations displayed with anisotropic displacement parameters at the 30% probability level. H atoms are omitted for clarity.

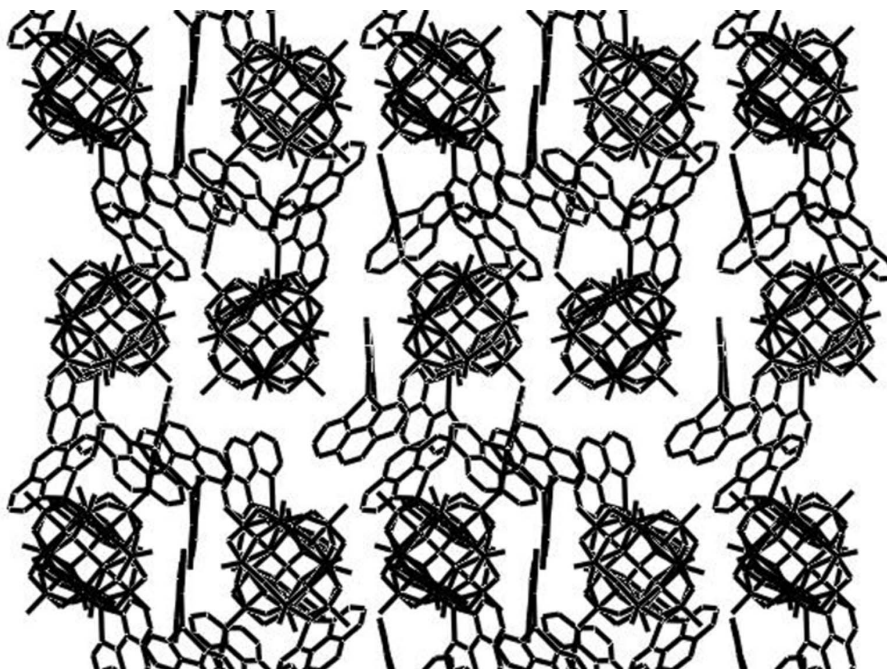


Figure 3

Packing of the structure viewed down the *a* axis. H atoms are omitted for clarity.

tetrakis[bis(1,10-phenanthroline)copper(I)] dodecatungstophosphate(V)

Crystal data

[Cu(C₁₂H₈N₂)₂]₄[SiW₁₂O₄₀]

M_r = 4570.08

Orthorhombic, *P*2₁2₁2₁

Hall symbol: P 2ac 2ab

a = 18.332 (3) Å

b = 21.173 (3) Å

c = 27.901 (4) Å

V = 10830 (3) Å³

Z = 4

F(000) = 8360

D_x = 2.803 Mg m⁻³

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 5100 reflections

θ = 1.5–28.4°

μ = 13.55 mm⁻¹

T = 293 K

Block, black

0.23 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

T_{min} = 0.066, *T_{max}* = 0.072

66617 measured reflections

24930 independent reflections

20506 reflections with *I* > 2σ(*I*)

R_{int} = 0.065

θ_{max} = 28.4°, θ_{min} = 1.5°

h = -24→19

k = -23→27

l = -37→37

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.041

wR(*F*²) = 0.072

S = 0.99

24930 reflections

1523 parameters

2431 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0109*P*)²]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.005

Δρ_{max} = 1.29 e Å⁻³

Δρ_{min} = -1.37 e Å⁻³

Extinction correction: *SHELXL97* (Sheldrick,
1997), *F_c** = *kF_c*[1 + 0.001 × *F_c*²λ³/sin(2θ)]^{-1/4}

Extinction coefficient: 0.000046 (2)

Absolute structure: Flack (1983), with 11091
Friedel pairs

Absolute structure parameter: -0.006 (6)

Special details

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

Refinement. Refinement of *F*² against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on *F*², conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative *F*². The threshold expression of *F*² > σ(*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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
W1	0.60792 (2)	0.469201 (19)	0.599936 (14)	0.02241 (9)
W2	0.32235 (2)	0.454247 (18)	0.430751 (14)	0.02309 (10)
W3	0.33999 (2)	0.462793 (18)	0.611797 (13)	0.02199 (9)
W4	0.59085 (3)	0.593174 (19)	0.506810 (14)	0.02581 (10)
W5	0.33766 (2)	0.342912 (17)	0.515962 (14)	0.02335 (9)
W6	0.49097 (2)	0.346761 (18)	0.601527 (14)	0.02234 (9)
W7	0.45059 (3)	0.588793 (19)	0.429200 (15)	0.02552 (10)
W8	0.58799 (3)	0.48431 (2)	0.419501 (14)	0.02656 (10)
W9	0.31693 (2)	0.573911 (17)	0.527752 (14)	0.02169 (9)
W10	0.61225 (2)	0.361745 (18)	0.512450 (14)	0.02279 (9)
W11	0.45668 (2)	0.584345 (18)	0.604974 (14)	0.02361 (10)
W12	0.45954 (3)	0.350016 (19)	0.426112 (14)	0.02600 (10)
O1	0.3909 (4)	0.3035 (3)	0.4642 (2)	0.0284 (17)
O2	0.2948 (4)	0.5093 (3)	0.4823 (2)	0.0216 (15)
O3	0.6255 (4)	0.4287 (3)	0.4668 (2)	0.0260 (16)
O4	0.3142 (4)	0.4051 (3)	0.5611 (2)	0.0225 (15)
O5	0.4766 (4)	0.2962 (3)	0.3830 (2)	0.040 (2)
O6	0.6245 (4)	0.5311 (3)	0.5497 (2)	0.0236 (16)
O7	0.5337 (4)	0.3340 (3)	0.4716 (2)	0.0260 (17)
O8	0.3881 (4)	0.5188 (3)	0.4142 (2)	0.0232 (16)
O9	0.3728 (4)	0.6203 (3)	0.5747 (2)	0.0238 (16)
O10	0.4750 (4)	0.6394 (3)	0.6467 (2)	0.0374 (19)
O11	0.2814 (5)	0.4414 (3)	0.6565 (2)	0.036 (2)
O12	0.5174 (4)	0.6098 (3)	0.5539 (2)	0.0268 (17)
O13	0.5669 (4)	0.3141 (3)	0.5628 (2)	0.0273 (17)
O14	0.6356 (4)	0.5528 (3)	0.4537 (2)	0.0280 (17)
O15	0.4233 (4)	0.6430 (3)	0.3883 (3)	0.042 (2)
O16	0.4196 (4)	0.4070 (3)	0.6228 (2)	0.0224 (16)
O17	0.6739 (4)	0.4887 (3)	0.6399 (2)	0.0332 (18)
O18	0.2796 (4)	0.5239 (3)	0.5787 (2)	0.0300 (17)
O19	0.4829 (4)	0.2906 (3)	0.6442 (2)	0.0355 (19)
O20	0.6509 (4)	0.6524 (3)	0.5164 (3)	0.0379 (19)
O21	0.5191 (4)	0.4207 (3)	0.4064 (2)	0.0250 (16)
O22	0.5636 (4)	0.4002 (3)	0.6315 (2)	0.0223 (16)
O23	0.5079 (4)	0.5168 (3)	0.4805 (2)	0.0234 (15)
O24	0.2464 (4)	0.6241 (3)	0.5203 (2)	0.0295 (17)
O25	0.4207 (4)	0.3244 (3)	0.5563 (2)	0.0217 (16)
O26	0.5269 (4)	0.6332 (3)	0.4602 (2)	0.0270 (17)
O27	0.2818 (4)	0.3853 (3)	0.4682 (2)	0.0267 (17)
O28	0.2804 (4)	0.2827 (3)	0.5299 (3)	0.037 (2)
O29	0.2543 (4)	0.4644 (3)	0.3904 (2)	0.0330 (17)
O30	0.6607 (4)	0.4099 (3)	0.5607 (2)	0.0292 (17)
O31	0.5301 (4)	0.5235 (3)	0.6190 (2)	0.0259 (17)
O32	0.3781 (4)	0.3922 (3)	0.3966 (2)	0.0276 (17)
O33	0.4139 (4)	0.4206 (3)	0.4838 (2)	0.0205 (14)

O34	0.5262 (4)	0.5471 (3)	0.3917 (2)	0.0321 (18)
O35	0.6791 (5)	0.3106 (3)	0.4969 (2)	0.040 (2)
O36	0.5229 (4)	0.4268 (3)	0.54623 (19)	0.0178 (15)
O37	0.3883 (4)	0.5316 (3)	0.6405 (2)	0.0273 (16)
O38	0.4131 (4)	0.5070 (3)	0.55134 (19)	0.0189 (15)
O39	0.6480 (5)	0.4753 (4)	0.3737 (2)	0.041 (2)
O40	0.3867 (4)	0.6033 (3)	0.4805 (2)	0.0236 (16)
Cu1	0.88189 (11)	0.40331 (9)	0.63125 (6)	0.0666 (5)
Cu2	0.30068 (11)	0.76365 (8)	0.64680 (6)	0.0582 (5)
Cu3	0.59060 (10)	0.34318 (8)	0.23805 (6)	0.0546 (4)
Cu4	0.05409 (10)	0.50611 (7)	0.39601 (5)	0.0526 (5)
C1	1.0407 (9)	0.3619 (7)	0.6296 (5)	0.072 (2)
H1B	1.0302	0.3288	0.6504	0.086*
C2	1.1133 (9)	0.3724 (7)	0.6121 (5)	0.071 (2)
H2A	1.1498	0.3442	0.6210	0.086*
C3	1.1301 (9)	0.4181 (7)	0.5850 (5)	0.069 (2)
H3A	1.1786	0.4232	0.5760	0.083*
C4	1.0785 (9)	0.4612 (7)	0.5681 (5)	0.065 (2)
C5	1.0918 (9)	0.5108 (6)	0.5383 (5)	0.066 (2)
H5A	1.1391	0.5162	0.5269	0.079*
C6	1.0412 (9)	0.5517 (6)	0.5246 (5)	0.066 (2)
H6A	1.0536	0.5862	0.5057	0.079*
C7	0.9673 (9)	0.5422 (6)	0.5394 (5)	0.062 (2)
C9	0.8384 (9)	0.5662 (6)	0.5374 (5)	0.068 (2)
H9A	0.7998	0.5913	0.5272	0.081*
C8	0.9082 (9)	0.5781 (6)	0.5241 (5)	0.066 (2)
H8A	0.9170	0.6120	0.5036	0.079*
C10	0.8276 (9)	0.5136 (6)	0.5677 (5)	0.063 (2)
H10A	0.7801	0.5041	0.5770	0.075*
C11	0.9506 (9)	0.4910 (6)	0.5695 (5)	0.0620 (19)
C12	1.0077 (9)	0.4502 (7)	0.5854 (5)	0.0626 (19)
C13	0.7946 (8)	0.2880 (6)	0.6035 (4)	0.049 (2)
H13A	0.8287	0.2810	0.5794	0.059*
C14	0.7347 (8)	0.2466 (5)	0.6062 (4)	0.045 (2)
H14B	0.7296	0.2131	0.5849	0.054*
C15	0.6849 (8)	0.2574 (5)	0.6408 (4)	0.0461 (19)
H15B	0.6445	0.2311	0.6435	0.055*
C16	0.6934 (8)	0.3087 (5)	0.6733 (4)	0.0439 (18)
C17	0.6425 (8)	0.3213 (6)	0.7102 (4)	0.0477 (18)
H17A	0.6014	0.2961	0.7142	0.057*
C18	0.6554 (8)	0.3721 (6)	0.7402 (4)	0.0481 (18)
H18A	0.6216	0.3816	0.7639	0.058*
C19	0.7189 (8)	0.4104 (6)	0.7358 (4)	0.0458 (18)
C20	0.7305 (8)	0.4614 (6)	0.7654 (4)	0.0514 (19)
H20A	0.6984	0.4708	0.7902	0.062*
C21	0.7909 (8)	0.4981 (6)	0.7570 (4)	0.052 (2)
H21A	0.8001	0.5332	0.7761	0.062*
C22	0.8385 (8)	0.4825 (6)	0.7197 (4)	0.053 (2)

H22A	0.8796	0.5074	0.7148	0.064*
C23	0.7675 (8)	0.3979 (6)	0.7000 (4)	0.0473 (17)
C24	0.7557 (8)	0.3461 (5)	0.6675 (4)	0.0426 (17)
C25	0.3226 (8)	0.6457 (6)	0.7115 (4)	0.0485 (19)
H25A	0.3621	0.6341	0.6925	0.058*
C26	0.3069 (8)	0.6103 (6)	0.7510 (4)	0.050 (2)
H26A	0.3374	0.5770	0.7594	0.060*
C27	0.2468 (7)	0.6232 (5)	0.7785 (4)	0.0433 (18)
H27A	0.2344	0.5973	0.8042	0.052*
C28	0.2046 (8)	0.6761 (5)	0.7673 (4)	0.0414 (17)
C29	0.1423 (7)	0.6931 (5)	0.7939 (4)	0.0403 (17)
H29A	0.1277	0.6684	0.8198	0.048*
C30	0.1029 (7)	0.7458 (5)	0.7817 (4)	0.0393 (17)
H30A	0.0622	0.7572	0.7996	0.047*
C31	0.1247 (7)	0.7838 (5)	0.7411 (4)	0.0366 (17)
C32	0.0865 (7)	0.8380 (5)	0.7277 (4)	0.0385 (18)
H14A	0.0458	0.8510	0.7449	0.046*
C33	0.1103 (7)	0.8714 (5)	0.6888 (4)	0.0400 (19)
H16A	0.0851	0.9072	0.6788	0.048*
C34	0.1701 (7)	0.8522 (5)	0.6651 (4)	0.0397 (18)
H34A	0.1849	0.8757	0.6387	0.048*
C35	0.1855 (7)	0.7669 (5)	0.7158 (4)	0.0368 (16)
C36	0.2252 (7)	0.7116 (5)	0.7270 (4)	0.0384 (16)
C37	0.2677 (8)	0.7625 (5)	0.5379 (4)	0.0476 (19)
H37A	0.2183	0.7617	0.5453	0.057*
C38	0.2869 (8)	0.7594 (5)	0.4894 (4)	0.0471 (18)
H38A	0.2515	0.7579	0.4656	0.057*
C39	0.3586 (8)	0.7588 (5)	0.4785 (5)	0.0448 (18)
H39A	0.3732	0.7555	0.4466	0.054*
C40	0.4112 (8)	0.7631 (5)	0.5146 (5)	0.0451 (18)
C41	0.4874 (8)	0.7642 (5)	0.5053 (4)	0.0459 (18)
H41A	0.5046	0.7599	0.4741	0.055*
C42	0.5339 (8)	0.7715 (5)	0.5412 (4)	0.0467 (18)
H42A	0.5833	0.7750	0.5341	0.056*
C43	0.5124 (8)	0.7743 (5)	0.5898 (4)	0.0456 (18)
C44	0.5599 (8)	0.7797 (5)	0.6280 (4)	0.0485 (19)
H44A	0.6099	0.7814	0.6226	0.058*
C45	0.5336 (8)	0.7825 (5)	0.6737 (5)	0.050 (2)
H45A	0.5653	0.7845	0.6997	0.060*
C46	0.4609 (8)	0.7822 (5)	0.6806 (5)	0.050 (2)
H46A	0.4437	0.7856	0.7118	0.059*
C47	0.4384 (8)	0.7741 (5)	0.6006 (4)	0.0435 (17)
C48	0.3863 (8)	0.7678 (5)	0.5622 (4)	0.0442 (17)
C49	0.6414 (9)	0.3090 (6)	0.3385 (5)	0.061 (2)
H49A	0.5928	0.3094	0.3480	0.073*
C50	0.6972 (9)	0.2964 (6)	0.3733 (5)	0.063 (2)
H50A	0.6842	0.2869	0.4047	0.075*
C51	0.7680 (9)	0.2981 (6)	0.3610 (5)	0.064 (2)

H51A	0.8033	0.2895	0.3840	0.077*
C52	0.7892 (9)	0.3123 (6)	0.3147 (5)	0.060 (2)
C53	0.8624 (9)	0.3151 (6)	0.2967 (5)	0.063 (2)
H53A	0.9011	0.3068	0.3173	0.076*
C54	0.8755 (9)	0.3289 (6)	0.2527 (5)	0.063 (2)
H54A	0.9242	0.3311	0.2435	0.076*
C55	0.8217 (9)	0.3411 (6)	0.2166 (5)	0.0580 (19)
C56	0.8319 (9)	0.3553 (6)	0.1692 (5)	0.061 (2)
H56A	0.8796	0.3580	0.1580	0.073*
C57	0.7777 (8)	0.3655 (6)	0.1375 (5)	0.061 (2)
H57A	0.7863	0.3748	0.1054	0.074*
C58	0.7073 (8)	0.3612 (6)	0.1566 (5)	0.058 (2)
H58A	0.6688	0.3679	0.1355	0.069*
C59	0.7477 (9)	0.3377 (6)	0.2328 (5)	0.0572 (18)
C60	0.7295 (9)	0.3230 (6)	0.2810 (5)	0.0576 (18)
C61	0.5135 (8)	0.2694 (6)	0.1586 (4)	0.048 (2)
H1A	0.5510	0.2400	0.1607	0.058*
C62	0.4621 (8)	0.2602 (6)	0.1238 (4)	0.046 (2)
H62A	0.4632	0.2246	0.1042	0.056*
C63	0.4092 (8)	0.3049 (5)	0.1186 (4)	0.0469 (19)
H63A	0.3748	0.3006	0.0943	0.056*
C64	0.4056 (7)	0.3564 (5)	0.1487 (4)	0.0444 (18)
C65	0.3516 (8)	0.4052 (6)	0.1482 (4)	0.0481 (18)
H65A	0.3168	0.4047	0.1240	0.058*
C66	0.3484 (8)	0.4517 (6)	0.1809 (4)	0.0500 (18)
H66A	0.3114	0.4817	0.1796	0.060*
C67	0.4031 (8)	0.4549 (6)	0.2184 (4)	0.0463 (18)
C68	0.4018 (8)	0.5016 (6)	0.2547 (4)	0.0519 (19)
H68A	0.3660	0.5327	0.2551	0.062*
C69	0.4542 (8)	0.4994 (6)	0.2886 (4)	0.053 (2)
H69A	0.4528	0.5280	0.3139	0.063*
C70	0.5103 (8)	0.4552 (6)	0.2865 (4)	0.052 (2)
H70A	0.5462	0.4556	0.3100	0.062*
C71	0.4595 (8)	0.4115 (6)	0.2193 (4)	0.0429 (17)
C72	0.4605 (8)	0.3609 (5)	0.1850 (4)	0.0434 (16)
C73	-0.1100 (9)	0.5450 (7)	0.4033 (5)	0.066 (2)
H73A	-0.0998	0.5820	0.3866	0.079*
C74	-0.1821 (9)	0.5298 (7)	0.4148 (5)	0.074 (2)
H74A	-0.2204	0.5560	0.4057	0.089*
C75	-0.1952 (9)	0.4752 (7)	0.4400 (5)	0.073 (2)
H75A	-0.2432	0.4660	0.4482	0.087*
C76	-0.1427 (8)	0.4338 (7)	0.4538 (5)	0.067 (2)
C77	-0.1518 (9)	0.3792 (6)	0.4788 (5)	0.068 (2)
H77A	-0.1989	0.3669	0.4867	0.081*
C78	-0.0988 (8)	0.3441 (6)	0.4921 (5)	0.064 (2)
H78A	-0.1087	0.3088	0.5108	0.077*
C79	-0.0279 (8)	0.3566 (6)	0.4796 (5)	0.0593 (19)
C80	0.0324 (8)	0.3194 (6)	0.4883 (5)	0.061 (2)

H80A	0.0263	0.2816	0.5047	0.074*
C81	0.0987 (8)	0.3358 (6)	0.4742 (5)	0.060 (2)
H81A	0.1385	0.3113	0.4832	0.072*
C82	0.1090 (8)	0.3875 (6)	0.4468 (4)	0.056 (2)
H82A	0.1557	0.3957	0.4353	0.067*
C83	-0.0138 (8)	0.4125 (6)	0.4504 (5)	0.0576 (18)
C84	-0.0728 (8)	0.4543 (6)	0.4398 (5)	0.0598 (18)
C85	-0.0082 (8)	0.4836 (6)	0.2937 (4)	0.0522 (19)
H85A	-0.0389	0.4530	0.3066	0.063*
C86	-0.0169 (8)	0.5001 (6)	0.2456 (4)	0.048 (2)
H86A	-0.0523	0.4810	0.2267	0.057*
C87	0.0278 (8)	0.5447 (6)	0.2275 (4)	0.0465 (19)
H15A	0.0216	0.5575	0.1959	0.056*
C88	0.0838 (7)	0.5724 (5)	0.2551 (4)	0.0419 (17)
C89	0.1332 (8)	0.6190 (6)	0.2394 (4)	0.0470 (18)
H18B	0.1282	0.6350	0.2085	0.056*
C90	0.1864 (8)	0.6408 (6)	0.2667 (4)	0.0454 (18)
H90A	0.2212	0.6677	0.2535	0.055*
C91	0.1912 (8)	0.6234 (5)	0.3175 (4)	0.0436 (18)
C92	0.2425 (7)	0.6472 (6)	0.3489 (4)	0.0458 (18)
H92A	0.2799	0.6733	0.3382	0.055*
C93	0.2366 (8)	0.6315 (5)	0.3962 (4)	0.0460 (18)
H93A	0.2705	0.6469	0.4181	0.055*
C94	0.1804 (7)	0.5925 (5)	0.4119 (4)	0.0446 (19)
H94A	0.1767	0.5835	0.4445	0.054*
C95	0.1379 (7)	0.5822 (6)	0.3349 (4)	0.0434 (16)
C96	0.0866 (8)	0.5533 (5)	0.3040 (4)	0.0431 (16)
N1	0.6898 (6)	0.3484 (5)	0.2020 (3)	0.044 (3)
N2	0.3141 (6)	0.7663 (4)	0.5743 (3)	0.043 (3)
N3	0.5138 (5)	0.4128 (4)	0.2520 (3)	0.036 (2)
N4	0.8272 (6)	0.4339 (4)	0.6915 (3)	0.043 (3)
N5	0.8061 (6)	0.3361 (4)	0.6328 (3)	0.039 (3)
N6	0.0418 (6)	0.5093 (4)	0.3219 (3)	0.044 (3)
N7	0.5144 (5)	0.3170 (4)	0.1898 (3)	0.035 (2)
N8	0.1326 (5)	0.5681 (4)	0.3827 (3)	0.035 (2)
N9	0.8820 (6)	0.4761 (5)	0.5842 (3)	0.049 (3)
N10	0.2100 (6)	0.8014 (4)	0.6771 (3)	0.035 (2)
N11	0.0552 (6)	0.4278 (4)	0.4352 (3)	0.039 (2)
N12	0.2834 (7)	0.6967 (4)	0.6987 (3)	0.051 (3)
N13	-0.0562 (7)	0.5068 (5)	0.4160 (3)	0.057 (3)
N14	0.9886 (6)	0.4021 (5)	0.6146 (4)	0.062 (3)
N15	0.4130 (6)	0.7775 (5)	0.6458 (3)	0.048 (3)
N16	0.6579 (7)	0.3203 (5)	0.2926 (3)	0.053 (3)
Si1	0.46447 (15)	0.46771 (11)	0.51552 (9)	0.0146 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
W1	0.0197 (2)	0.0235 (2)	0.0241 (2)	0.00063 (17)	-0.00485 (19)	-0.00050 (17)
W2	0.0207 (3)	0.0237 (2)	0.0249 (2)	0.00116 (17)	-0.00588 (19)	-0.00199 (17)
W3	0.0197 (2)	0.0234 (2)	0.0228 (2)	0.00076 (17)	0.00518 (18)	0.00090 (17)
W4	0.0210 (3)	0.0235 (2)	0.0330 (2)	-0.00702 (18)	-0.0007 (2)	0.00533 (17)
W5	0.0222 (3)	0.01697 (19)	0.0309 (2)	-0.00510 (17)	-0.0021 (2)	-0.00112 (17)
W6	0.0226 (3)	0.0199 (2)	0.0245 (2)	0.00215 (17)	-0.00037 (19)	0.00576 (17)
W7	0.0222 (3)	0.0258 (2)	0.0286 (2)	0.00014 (18)	0.0001 (2)	0.01133 (18)
W8	0.0213 (3)	0.0362 (2)	0.0221 (2)	0.00214 (19)	0.00498 (19)	0.00588 (18)
W9	0.0189 (2)	0.01701 (19)	0.0292 (2)	0.00386 (16)	0.00012 (19)	0.00018 (16)
W10	0.0198 (2)	0.0225 (2)	0.0260 (2)	0.00685 (17)	0.00054 (19)	-0.00064 (17)
W11	0.0233 (3)	0.0192 (2)	0.0283 (2)	0.00003 (17)	-0.00081 (19)	-0.00737 (17)
W12	0.0264 (3)	0.0262 (2)	0.0254 (2)	0.00377 (19)	-0.0027 (2)	-0.00968 (18)
O1	0.031 (5)	0.025 (4)	0.029 (4)	-0.003 (3)	-0.004 (4)	0.004 (3)
O2	0.014 (4)	0.019 (3)	0.031 (3)	0.002 (3)	0.002 (3)	0.004 (3)
O3	0.016 (4)	0.027 (4)	0.036 (4)	0.005 (3)	0.004 (3)	-0.005 (3)
O4	0.013 (4)	0.021 (3)	0.034 (4)	-0.003 (3)	-0.001 (3)	0.002 (3)
O5	0.026 (5)	0.054 (5)	0.039 (4)	0.012 (4)	-0.006 (4)	-0.023 (4)
O6	0.017 (4)	0.023 (4)	0.030 (4)	-0.002 (3)	0.005 (3)	0.001 (3)
O7	0.029 (5)	0.022 (4)	0.026 (4)	0.003 (3)	0.001 (3)	-0.003 (3)
O8	0.019 (4)	0.021 (3)	0.030 (3)	0.006 (3)	-0.002 (3)	0.004 (3)
O9	0.022 (4)	0.016 (3)	0.033 (4)	0.003 (3)	-0.005 (3)	0.003 (3)
O10	0.027 (5)	0.040 (5)	0.045 (4)	-0.002 (4)	0.008 (4)	-0.023 (4)
O11	0.039 (6)	0.043 (5)	0.026 (4)	0.003 (4)	0.009 (4)	0.006 (3)
O12	0.027 (5)	0.014 (3)	0.039 (4)	-0.003 (3)	0.004 (3)	0.005 (3)
O13	0.033 (5)	0.021 (4)	0.028 (4)	0.006 (3)	-0.006 (3)	-0.006 (3)
O14	0.019 (5)	0.035 (4)	0.030 (4)	0.003 (3)	0.006 (3)	0.009 (3)
O15	0.034 (5)	0.043 (5)	0.048 (5)	-0.007 (4)	0.000 (4)	0.022 (4)
O16	0.030 (5)	0.009 (3)	0.028 (3)	-0.008 (3)	0.003 (3)	0.000 (3)
O17	0.029 (5)	0.035 (4)	0.036 (4)	0.000 (3)	-0.017 (4)	-0.003 (3)
O18	0.023 (5)	0.032 (4)	0.035 (4)	0.007 (3)	0.002 (3)	-0.001 (3)
O19	0.034 (5)	0.032 (4)	0.041 (4)	0.005 (4)	-0.001 (4)	0.014 (3)
O20	0.032 (5)	0.030 (4)	0.052 (4)	-0.005 (3)	-0.003 (4)	0.004 (4)
O21	0.025 (5)	0.025 (4)	0.024 (3)	0.002 (3)	0.005 (3)	0.000 (3)
O22	0.014 (4)	0.023 (4)	0.030 (4)	0.006 (3)	-0.005 (3)	-0.007 (3)
O23	0.012 (4)	0.033 (4)	0.024 (3)	-0.003 (3)	-0.004 (3)	-0.002 (3)
O24	0.031 (5)	0.016 (3)	0.041 (4)	0.007 (3)	0.005 (4)	0.008 (3)
O25	0.020 (4)	0.015 (3)	0.030 (4)	0.006 (3)	0.001 (3)	-0.003 (3)
O26	0.030 (5)	0.022 (4)	0.028 (4)	-0.003 (3)	-0.002 (3)	0.008 (3)
O27	0.015 (4)	0.026 (4)	0.039 (4)	-0.002 (3)	-0.010 (3)	0.000 (3)
O28	0.032 (5)	0.016 (4)	0.064 (5)	-0.006 (3)	-0.015 (4)	0.004 (3)
O29	0.027 (5)	0.035 (4)	0.037 (4)	-0.002 (3)	-0.006 (4)	0.006 (3)
O30	0.028 (5)	0.031 (4)	0.029 (4)	0.005 (3)	0.007 (3)	-0.001 (3)
O31	0.030 (5)	0.018 (3)	0.030 (4)	0.000 (3)	0.005 (3)	-0.008 (3)
O32	0.026 (5)	0.034 (4)	0.023 (3)	0.000 (3)	-0.012 (3)	-0.008 (3)
O33	0.020 (4)	0.020 (3)	0.021 (3)	0.002 (3)	-0.001 (3)	0.004 (3)

O34	0.025 (5)	0.042 (4)	0.030 (4)	0.002 (3)	0.010 (3)	0.021 (3)
O35	0.031 (5)	0.035 (4)	0.053 (5)	0.020 (4)	-0.009 (4)	-0.007 (3)
O36	0.021 (4)	0.012 (3)	0.020 (3)	0.003 (3)	0.003 (3)	-0.005 (2)
O37	0.024 (5)	0.030 (4)	0.029 (4)	0.005 (3)	-0.003 (3)	0.001 (3)
O38	0.019 (4)	0.017 (3)	0.020 (3)	-0.001 (3)	0.000 (3)	0.007 (3)
O39	0.036 (6)	0.059 (5)	0.027 (4)	0.004 (4)	0.004 (4)	0.010 (4)
O40	0.023 (4)	0.015 (3)	0.033 (4)	0.002 (3)	-0.005 (3)	-0.001 (3)
Cu1	0.0489 (13)	0.0670 (12)	0.0838 (13)	-0.0113 (10)	0.0172 (10)	0.0242 (10)
Cu2	0.0609 (14)	0.0582 (11)	0.0555 (10)	0.0017 (9)	0.0334 (10)	0.0065 (8)
Cu3	0.0314 (11)	0.0685 (11)	0.0638 (10)	0.0077 (9)	-0.0003 (9)	0.0088 (9)
Cu4	0.0629 (13)	0.0515 (10)	0.0432 (8)	-0.0153 (8)	-0.0030 (9)	0.0243 (7)
C1	0.057 (5)	0.066 (5)	0.093 (5)	-0.007 (4)	0.003 (4)	0.011 (4)
C2	0.053 (5)	0.068 (5)	0.094 (5)	-0.002 (4)	0.002 (4)	0.008 (4)
C3	0.053 (4)	0.065 (4)	0.089 (4)	-0.007 (4)	0.005 (4)	0.008 (4)
C4	0.052 (4)	0.060 (4)	0.083 (4)	-0.009 (4)	0.006 (4)	0.007 (4)
C5	0.050 (4)	0.063 (4)	0.085 (4)	-0.014 (4)	0.010 (4)	0.003 (4)
C6	0.057 (4)	0.058 (4)	0.083 (4)	-0.013 (4)	0.009 (4)	0.008 (4)
C7	0.052 (4)	0.054 (4)	0.081 (4)	-0.009 (4)	0.011 (4)	0.005 (4)
C9	0.057 (5)	0.058 (4)	0.087 (5)	-0.001 (4)	0.010 (4)	0.010 (4)
C8	0.058 (4)	0.057 (4)	0.084 (4)	-0.007 (4)	0.008 (4)	0.011 (4)
C10	0.054 (4)	0.055 (4)	0.079 (4)	-0.003 (4)	0.010 (4)	0.008 (3)
C11	0.050 (4)	0.055 (4)	0.080 (4)	-0.010 (3)	0.009 (4)	0.006 (3)
C12	0.050 (4)	0.057 (4)	0.081 (4)	-0.011 (3)	0.008 (4)	0.006 (3)
C13	0.054 (5)	0.043 (4)	0.050 (4)	0.003 (4)	0.000 (4)	0.004 (4)
C14	0.054 (5)	0.036 (4)	0.045 (4)	-0.001 (4)	-0.002 (4)	0.001 (4)
C15	0.052 (4)	0.043 (4)	0.043 (4)	0.000 (3)	-0.004 (4)	0.004 (3)
C16	0.051 (4)	0.039 (3)	0.041 (3)	0.004 (3)	-0.003 (3)	0.005 (3)
C17	0.054 (4)	0.045 (4)	0.044 (3)	0.002 (3)	-0.003 (3)	0.002 (3)
C18	0.055 (4)	0.045 (4)	0.044 (3)	0.005 (3)	0.000 (3)	0.001 (3)
C19	0.055 (4)	0.040 (3)	0.042 (3)	0.001 (3)	-0.006 (3)	0.006 (3)
C20	0.059 (4)	0.048 (4)	0.047 (4)	0.003 (3)	-0.003 (4)	0.001 (3)
C21	0.062 (5)	0.041 (4)	0.051 (4)	0.001 (4)	-0.008 (4)	0.003 (4)
C22	0.059 (4)	0.044 (4)	0.056 (4)	-0.004 (4)	-0.004 (4)	0.006 (3)
C23	0.054 (4)	0.040 (3)	0.048 (3)	0.001 (3)	-0.004 (3)	0.006 (3)
C24	0.050 (4)	0.036 (3)	0.041 (3)	0.004 (3)	-0.004 (3)	0.008 (3)
C25	0.052 (4)	0.041 (4)	0.053 (4)	0.007 (4)	0.012 (4)	0.005 (3)
C26	0.055 (4)	0.044 (4)	0.052 (4)	0.007 (4)	0.007 (4)	0.007 (4)
C27	0.048 (4)	0.038 (3)	0.044 (4)	0.002 (3)	0.006 (3)	0.008 (3)
C28	0.046 (4)	0.036 (3)	0.042 (3)	0.006 (3)	0.007 (3)	0.004 (3)
C29	0.047 (4)	0.037 (3)	0.037 (3)	0.002 (3)	0.009 (3)	0.007 (3)
C30	0.044 (4)	0.035 (3)	0.038 (3)	0.004 (3)	0.007 (3)	0.001 (3)
C31	0.042 (4)	0.032 (3)	0.036 (3)	0.003 (3)	0.005 (3)	0.004 (3)
C32	0.042 (4)	0.036 (3)	0.037 (3)	0.004 (3)	0.009 (3)	0.000 (3)
C33	0.045 (4)	0.033 (4)	0.042 (4)	0.004 (4)	0.006 (4)	0.006 (3)
C34	0.046 (4)	0.033 (3)	0.040 (4)	-0.001 (3)	0.008 (3)	0.005 (3)
C35	0.044 (4)	0.030 (3)	0.036 (3)	0.000 (3)	0.005 (3)	0.004 (3)
C36	0.044 (4)	0.032 (3)	0.040 (3)	0.000 (3)	0.010 (3)	0.001 (3)
C37	0.052 (4)	0.033 (3)	0.057 (4)	0.000 (3)	0.014 (4)	0.002 (3)

C38	0.053 (4)	0.037 (3)	0.052 (3)	0.000 (3)	0.006 (4)	-0.001 (3)
C39	0.053 (4)	0.030 (3)	0.051 (3)	0.003 (3)	0.015 (3)	0.001 (3)
C40	0.051 (4)	0.029 (3)	0.055 (3)	0.001 (3)	0.016 (3)	0.000 (3)
C41	0.054 (4)	0.031 (3)	0.052 (4)	0.003 (3)	0.017 (3)	-0.002 (3)
C42	0.052 (4)	0.030 (3)	0.058 (4)	0.003 (3)	0.020 (3)	0.000 (3)
C43	0.053 (4)	0.029 (3)	0.054 (4)	0.002 (3)	0.015 (3)	-0.001 (3)
C44	0.055 (4)	0.031 (3)	0.060 (4)	0.002 (3)	0.014 (4)	-0.001 (3)
C45	0.058 (5)	0.034 (4)	0.058 (4)	0.000 (4)	0.009 (4)	0.001 (4)
C46	0.058 (4)	0.035 (3)	0.057 (4)	0.002 (4)	0.014 (4)	-0.001 (3)
C47	0.052 (4)	0.026 (3)	0.052 (3)	0.000 (3)	0.017 (3)	0.000 (3)
C48	0.052 (4)	0.026 (3)	0.054 (3)	0.004 (3)	0.016 (3)	0.000 (3)
C49	0.055 (4)	0.064 (4)	0.063 (4)	0.001 (4)	0.002 (4)	0.000 (4)
C50	0.058 (5)	0.066 (4)	0.063 (4)	0.005 (4)	-0.001 (4)	0.006 (4)
C51	0.056 (4)	0.068 (4)	0.069 (4)	0.003 (4)	-0.002 (4)	0.003 (4)
C52	0.053 (4)	0.061 (4)	0.066 (4)	0.004 (4)	0.001 (4)	0.000 (4)
C53	0.053 (4)	0.067 (4)	0.070 (4)	0.002 (4)	-0.002 (4)	0.001 (4)
C54	0.052 (4)	0.065 (4)	0.073 (4)	0.001 (4)	0.005 (4)	-0.001 (4)
C55	0.048 (4)	0.058 (4)	0.068 (4)	-0.001 (4)	0.008 (4)	0.001 (4)
C56	0.051 (4)	0.061 (4)	0.070 (4)	-0.002 (4)	0.010 (4)	0.005 (4)
C57	0.052 (5)	0.064 (4)	0.068 (4)	0.000 (4)	0.012 (4)	0.002 (4)
C58	0.050 (4)	0.060 (4)	0.063 (4)	0.000 (4)	0.009 (4)	0.001 (4)
C59	0.049 (4)	0.058 (4)	0.065 (4)	0.001 (3)	0.005 (3)	0.001 (3)
C60	0.050 (4)	0.060 (4)	0.064 (4)	0.003 (3)	0.004 (3)	0.001 (3)
C61	0.049 (4)	0.048 (4)	0.048 (4)	0.000 (4)	0.002 (4)	-0.004 (3)
C62	0.051 (5)	0.048 (4)	0.041 (4)	-0.007 (4)	0.001 (4)	-0.011 (4)
C63	0.049 (4)	0.050 (4)	0.042 (3)	-0.008 (3)	-0.005 (3)	-0.005 (3)
C64	0.045 (4)	0.044 (4)	0.044 (3)	-0.003 (3)	-0.002 (3)	-0.003 (3)
C65	0.050 (4)	0.050 (4)	0.045 (3)	0.001 (3)	-0.009 (3)	-0.002 (3)
C66	0.049 (4)	0.049 (4)	0.053 (3)	0.000 (3)	-0.005 (3)	-0.005 (3)
C67	0.048 (4)	0.047 (4)	0.044 (3)	-0.006 (3)	-0.004 (3)	-0.007 (3)
C68	0.052 (4)	0.050 (4)	0.054 (4)	0.002 (3)	-0.001 (4)	-0.009 (3)
C69	0.052 (5)	0.052 (4)	0.053 (4)	-0.003 (4)	-0.002 (4)	-0.016 (4)
C70	0.050 (4)	0.054 (4)	0.051 (4)	-0.003 (4)	-0.005 (4)	-0.009 (3)
C71	0.046 (4)	0.043 (3)	0.040 (3)	-0.005 (3)	-0.003 (3)	-0.006 (3)
C72	0.044 (4)	0.044 (3)	0.042 (3)	-0.006 (3)	0.000 (3)	-0.005 (3)
C73	0.053 (4)	0.070 (4)	0.076 (4)	0.003 (4)	0.000 (4)	0.016 (4)
C74	0.055 (5)	0.078 (5)	0.089 (4)	0.007 (4)	-0.001 (4)	0.017 (4)
C75	0.055 (4)	0.073 (4)	0.090 (4)	0.002 (4)	0.003 (4)	0.015 (4)
C76	0.051 (4)	0.069 (4)	0.082 (4)	0.004 (4)	0.001 (4)	0.014 (4)
C77	0.051 (4)	0.069 (4)	0.084 (4)	-0.007 (4)	0.004 (4)	0.016 (4)
C78	0.052 (4)	0.059 (4)	0.081 (4)	-0.002 (4)	0.009 (4)	0.012 (3)
C79	0.048 (4)	0.056 (4)	0.074 (4)	-0.001 (3)	0.010 (4)	0.012 (3)
C80	0.050 (4)	0.057 (4)	0.077 (4)	0.004 (4)	0.008 (4)	0.017 (4)
C81	0.050 (5)	0.052 (4)	0.078 (4)	0.008 (4)	0.004 (4)	0.015 (4)
C82	0.045 (5)	0.054 (4)	0.068 (4)	0.003 (4)	0.006 (4)	0.016 (4)
C83	0.045 (4)	0.056 (4)	0.072 (4)	0.000 (3)	0.005 (4)	0.013 (3)
C84	0.047 (4)	0.059 (4)	0.073 (3)	0.000 (3)	0.003 (3)	0.013 (3)
C85	0.049 (4)	0.054 (4)	0.053 (4)	-0.003 (3)	0.002 (3)	0.006 (3)

C86	0.046 (4)	0.052 (4)	0.045 (4)	-0.003 (4)	0.003 (4)	0.004 (4)
C87	0.047 (4)	0.050 (4)	0.042 (3)	0.001 (3)	0.005 (3)	0.003 (3)
C88	0.043 (4)	0.046 (3)	0.036 (3)	-0.001 (3)	0.007 (3)	0.003 (3)
C89	0.048 (4)	0.050 (4)	0.043 (3)	-0.001 (3)	0.007 (3)	0.001 (3)
C90	0.045 (4)	0.048 (3)	0.044 (3)	-0.003 (3)	0.008 (3)	-0.001 (3)
C91	0.043 (4)	0.045 (3)	0.042 (3)	-0.001 (3)	0.005 (3)	0.003 (3)
C92	0.046 (4)	0.048 (4)	0.043 (3)	-0.002 (3)	0.006 (3)	0.003 (3)
C93	0.047 (4)	0.044 (3)	0.046 (3)	0.003 (3)	0.002 (3)	0.001 (3)
C94	0.044 (4)	0.045 (4)	0.044 (4)	0.001 (3)	0.001 (4)	0.004 (3)
C95	0.044 (4)	0.045 (3)	0.041 (3)	0.001 (3)	0.002 (3)	0.005 (3)
C96	0.043 (3)	0.045 (3)	0.041 (3)	0.000 (3)	0.002 (3)	0.004 (3)
N1	0.045 (8)	0.055 (7)	0.031 (5)	-0.008 (6)	0.010 (5)	0.005 (5)
N2	0.059 (8)	0.029 (5)	0.041 (6)	-0.004 (5)	0.017 (6)	0.007 (4)
N3	0.034 (7)	0.050 (6)	0.024 (4)	-0.001 (5)	0.009 (4)	-0.008 (4)
N4	0.044 (8)	0.031 (5)	0.055 (6)	0.002 (5)	-0.010 (6)	-0.006 (4)
N5	0.037 (7)	0.028 (5)	0.053 (6)	0.011 (4)	0.017 (5)	-0.001 (4)
N6	0.055 (8)	0.047 (6)	0.029 (5)	-0.019 (5)	-0.008 (5)	0.006 (4)
N7	0.028 (6)	0.041 (6)	0.035 (5)	0.005 (4)	0.011 (5)	-0.003 (4)
N8	0.038 (7)	0.024 (5)	0.044 (5)	0.008 (4)	-0.007 (5)	0.002 (4)
N9	0.033 (7)	0.042 (6)	0.071 (7)	0.010 (5)	0.013 (6)	0.016 (5)
N10	0.039 (7)	0.037 (5)	0.028 (5)	-0.005 (5)	0.013 (5)	0.006 (4)
N11	0.035 (7)	0.033 (5)	0.049 (6)	0.003 (4)	0.007 (5)	0.009 (4)
N12	0.064 (9)	0.034 (6)	0.056 (6)	0.010 (5)	0.021 (6)	-0.002 (5)
N13	0.055 (9)	0.066 (8)	0.050 (6)	0.027 (6)	-0.019 (6)	0.001 (5)
N14	0.037 (8)	0.050 (7)	0.099 (9)	-0.005 (5)	0.000 (7)	0.019 (6)
N15	0.045 (8)	0.053 (7)	0.046 (6)	0.012 (5)	0.003 (6)	0.005 (5)
N16	0.064 (9)	0.052 (7)	0.043 (6)	-0.003 (6)	0.005 (6)	0.011 (5)
Si1	0.0176 (15)	0.0133 (11)	0.0129 (11)	-0.0029 (10)	0.0014 (11)	0.0003 (10)

Geometric parameters (Å, °)

W1—O17	1.695 (7)	C25—H25A	0.9300
W1—O22	1.888 (6)	C26—C27	1.371 (17)
W1—O31	1.908 (7)	C26—H26A	0.9300
W1—O30	1.927 (6)	C27—C28	1.396 (16)
W1—O6	1.943 (6)	C27—H27A	0.9300
W1—O36	2.341 (6)	C28—C36	1.405 (15)
W2—O29	1.695 (7)	C28—C29	1.409 (17)
W2—O8	1.880 (7)	C29—C30	1.373 (15)
W2—O32	1.917 (7)	C29—H29A	0.9300
W2—O2	1.920 (6)	C30—C31	1.445 (14)
W2—O27	1.943 (6)	C30—H30A	0.9300
W2—O33	2.349 (6)	C31—C35	1.367 (16)
W3—O11	1.706 (7)	C31—C32	1.394 (15)
W3—O37	1.885 (7)	C32—C33	1.368 (14)
W3—O16	1.903 (7)	C32—H14A	0.9300
W3—O4	1.928 (6)	C33—C34	1.343 (16)
W3—O18	1.937 (7)	C33—H16A	0.9300

W3—O38	2.349 (6)	C34—N10	1.342 (14)
W4—O20	1.690 (7)	C34—H34A	0.9300
W4—O6	1.882 (6)	C35—N10	1.378 (12)
W4—O14	1.897 (6)	C35—C36	1.413 (15)
W4—O12	1.913 (7)	C36—N12	1.365 (15)
W4—O26	1.946 (6)	C37—N2	1.327 (16)
W4—O23	2.339 (6)	C37—C38	1.399 (16)
W5—O28	1.697 (7)	C37—H37A	0.9300
W5—O4	1.872 (6)	C38—C39	1.350 (17)
W5—O27	1.905 (6)	C38—H38A	0.9300
W5—O25	1.932 (7)	C39—C40	1.398 (18)
W5—O1	1.933 (7)	C39—H39A	0.9300
W5—O33	2.338 (6)	C40—C48	1.408 (16)
W6—O19	1.690 (6)	C40—C41	1.421 (18)
W6—O25	1.865 (7)	C41—C42	1.324 (17)
W6—O13	1.893 (7)	C41—H41A	0.9300
W6—O16	1.921 (7)	C42—C43	1.413 (15)
W6—O22	1.938 (6)	C42—H42A	0.9300
W6—O36	2.366 (6)	C43—C44	1.382 (17)
W7—O15	1.695 (7)	C43—C47	1.390 (18)
W7—O40	1.875 (7)	C44—C45	1.365 (15)
W7—O26	1.895 (7)	C44—H44A	0.9300
W7—O8	1.918 (7)	C45—C46	1.345 (19)
W7—O34	1.948 (7)	C45—H45A	0.9300
W7—O23	2.339 (6)	C46—N15	1.313 (16)
W8—O39	1.698 (7)	C46—H46A	0.9300
W8—O21	1.882 (7)	C47—N15	1.347 (13)
W8—O3	1.898 (6)	C47—C48	1.441 (18)
W8—O34	1.911 (7)	C48—N2	1.366 (16)
W8—O14	1.943 (7)	C49—N16	1.337 (14)
W8—O23	2.350 (6)	C49—C50	1.437 (19)
W9—O24	1.687 (7)	C49—H49A	0.9300
W9—O18	1.901 (7)	C50—C51	1.34 (2)
W9—O2	1.908 (6)	C50—H50A	0.9300
W9—O9	1.932 (6)	C51—C52	1.380 (18)
W9—O40	1.939 (7)	C51—H51A	0.9300
W9—O38	2.356 (6)	C52—C53	1.43 (2)
W10—O35	1.691 (7)	C52—C60	1.46 (2)
W10—O30	1.908 (7)	C53—C54	1.284 (16)
W10—O3	1.921 (6)	C53—H53A	0.9300
W10—O13	1.919 (7)	C54—C55	1.433 (19)
W10—O7	1.929 (7)	C54—H54A	0.9300
W10—O36	2.339 (6)	C55—C56	1.369 (16)
W11—O10	1.681 (6)	C55—C59	1.43 (2)
W11—O12	1.888 (6)	C56—C57	1.349 (19)
W11—O31	1.904 (7)	C56—H56A	0.9300
W11—O9	1.913 (6)	C57—C58	1.398 (19)
W11—O37	1.949 (7)	C57—H57A	0.9300

W11—O38	2.358 (6)	C58—N1	1.334 (14)
W12—O5	1.687 (6)	C58—H58A	0.9300
W12—O7	1.890 (7)	C59—N1	1.384 (17)
W12—O1	1.919 (7)	C59—C60	1.420 (17)
W12—O32	1.924 (7)	C60—N16	1.353 (18)
W12—O21	1.933 (7)	C61—N7	1.330 (13)
W12—O33	2.351 (6)	C61—C62	1.368 (17)
O23—Si1	1.634 (7)	C61—H1A	0.9300
O33—Si1	1.623 (6)	C62—C63	1.363 (17)
O36—Si1	1.621 (7)	C62—H62A	0.9300
O38—Si1	1.605 (7)	C63—C64	1.377 (15)
Cu1—N5	1.990 (10)	C63—H63A	0.9300
Cu1—N14	2.011 (12)	C64—C65	1.432 (17)
Cu1—N9	2.023 (9)	C64—C72	1.431 (16)
Cu1—N4	2.062 (10)	C65—C66	1.344 (15)
Cu2—N10	2.030 (10)	C65—H65A	0.9300
Cu2—N2	2.037 (9)	C66—C67	1.450 (17)
Cu2—N12	2.050 (10)	C66—H66A	0.9300
Cu2—N15	2.080 (12)	C67—C71	1.383 (18)
Cu3—N16	2.018 (11)	C67—C68	1.415 (15)
Cu3—N7	2.019 (10)	C68—C69	1.351 (17)
Cu3—N1	2.081 (10)	C68—H68A	0.9300
Cu3—N3	2.074 (10)	C69—C70	1.391 (18)
Cu4—N11	1.988 (8)	C69—H69A	0.9300
Cu4—N8	1.982 (10)	C70—N3	1.319 (13)
Cu4—N6	2.082 (8)	C70—H70A	0.9300
Cu4—N13	2.097 (12)	C71—N3	1.350 (14)
C1—N14	1.347 (17)	C71—C72	1.437 (14)
C1—C2	1.43 (2)	C72—N7	1.364 (15)
C1—H1B	0.9300	C73—N13	1.324 (17)
C2—C3	1.267 (17)	C73—C74	1.40 (2)
C2—H2A	0.9300	C73—H73A	0.9300
C3—C4	1.396 (19)	C74—C75	1.374 (18)
C3—H3A	0.9300	C74—H74A	0.9300
C4—C5	1.360 (17)	C75—C76	1.356 (19)
C4—C12	1.41 (2)	C75—H75A	0.9300
C5—C6	1.326 (18)	C76—C77	1.361 (17)
C5—H5A	0.9300	C76—C84	1.408 (14)
C6—C7	1.430 (19)	C77—C78	1.278 (18)
C6—H6A	0.9300	C77—H77A	0.9300
C7—C11	1.405 (17)	C78—C79	1.372 (19)
C7—C8	1.389 (19)	C78—H78A	0.9300
C9—C8	1.36 (2)	C79—C80	1.378 (18)
C9—C10	1.411 (16)	C79—C83	1.459 (17)
C9—H9A	0.9300	C80—C81	1.324 (18)
C8—H8A	0.9300	C80—H80A	0.9300
C10—N9	1.356 (16)	C81—C82	1.349 (15)
C10—H10A	0.9300	C81—H81A	0.9300

C11—N9	1.360 (17)	C82—N11	1.342 (15)
C11—C12	1.43 (2)	C82—H82A	0.9300
C12—N14	1.349 (15)	C83—N11	1.373 (16)
C13—N5	1.321 (14)	C83—C84	1.428 (18)
C13—C14	1.408 (17)	C84—N13	1.329 (15)
C13—H13A	0.9300	C85—N6	1.324 (15)
C14—C15	1.349 (17)	C85—C86	1.396 (14)
C14—H14B	0.9300	C85—H85A	0.9300
C15—C16	1.422 (15)	C86—C87	1.348 (16)
C15—H15B	0.9300	C86—H86A	0.9300
C16—C24	1.399 (17)	C87—C88	1.411 (17)
C16—C17	1.415 (17)	C87—H15A	0.9300
C17—C18	1.384 (15)	C88—C96	1.425 (14)
C17—H17A	0.9300	C88—C89	1.409 (16)
C18—C19	1.423 (18)	C89—C90	1.320 (17)
C18—H18A	0.9300	C89—H18B	0.9300
C19—C23	1.364 (17)	C90—C91	1.468 (15)
C19—C20	1.376 (16)	C90—H90A	0.9300
C20—C21	1.372 (18)	C91—C92	1.382 (17)
C20—H20A	0.9300	C91—C95	1.396 (17)
C21—C22	1.397 (17)	C92—C93	1.364 (15)
C21—H21A	0.9300	C92—H92A	0.9300
C22—N4	1.312 (13)	C93—C94	1.393 (16)
C22—H22A	0.9300	C93—H93A	0.9300
C23—N4	1.354 (16)	C94—N8	1.303 (14)
C23—C24	1.441 (16)	C94—H94A	0.9300
C24—N5	1.356 (14)	C95—N8	1.371 (13)
C25—N12	1.345 (15)	C95—C96	1.416 (17)
C25—C26	1.364 (15)	C96—N6	1.338 (14)
O17—W1—O22	100.9 (3)	C24—C16—C17	121.0 (12)
O17—W1—O31	101.7 (3)	C24—C16—C15	116.6 (12)
O22—W1—O31	90.8 (3)	C17—C16—C15	122.4 (13)
O17—W1—O30	100.0 (3)	C18—C17—C16	118.3 (13)
O22—W1—O30	88.7 (3)	C18—C17—H17A	120.9
O31—W1—O30	157.9 (3)	C16—C17—H17A	120.9
O17—W1—O6	101.4 (3)	C17—C18—C19	122.1 (13)
O22—W1—O6	157.7 (3)	C17—C18—H18A	118.9
O31—W1—O6	85.0 (3)	C19—C18—H18A	118.9
O30—W1—O6	87.2 (3)	C23—C19—C20	119.3 (13)
O17—W1—O36	171.5 (3)	C23—C19—C18	119.1 (12)
O22—W1—O36	73.5 (2)	C20—C19—C18	121.4 (13)
O31—W1—O36	84.9 (2)	C21—C20—C19	117.8 (13)
O30—W1—O36	73.8 (3)	C21—C20—H20A	121.1
O6—W1—O36	84.3 (2)	C19—C20—H20A	121.1
O29—W2—O8	102.5 (3)	C20—C21—C22	119.9 (13)
O29—W2—O32	98.6 (3)	C20—C21—H21A	120.1
O8—W2—O32	92.0 (3)	C22—C21—H21A	120.1

O29—W2—O2	103.1 (3)	N4—C22—C21	122.2 (13)
O8—W2—O2	84.8 (3)	N4—C22—H22A	118.9
O32—W2—O2	158.2 (3)	C21—C22—H22A	118.9
O29—W2—O27	99.9 (3)	N4—C23—C19	123.2 (12)
O8—W2—O27	157.4 (3)	N4—C23—C24	116.1 (12)
O32—W2—O27	87.5 (3)	C19—C23—C24	120.7 (13)
O2—W2—O27	87.3 (3)	N5—C24—C16	123.4 (11)
O29—W2—O33	169.7 (3)	N5—C24—C23	117.8 (12)
O8—W2—O33	85.2 (2)	C16—C24—C23	118.8 (12)
O32—W2—O33	74.0 (2)	N12—C25—C26	123.0 (13)
O2—W2—O33	84.3 (2)	N12—C25—H25A	118.5
O27—W2—O33	73.0 (2)	C26—C25—H25A	118.5
O11—W3—O37	101.0 (3)	C25—C26—C27	120.8 (13)
O11—W3—O16	101.6 (3)	C25—C26—H26A	119.6
O37—W3—O16	92.9 (3)	C27—C26—H26A	119.6
O11—W3—O4	102.3 (3)	C26—C27—C28	118.7 (11)
O37—W3—O4	156.6 (3)	C26—C27—H27A	120.7
O16—W3—O4	85.0 (3)	C28—C27—H27A	120.7
O11—W3—O18	99.5 (3)	C27—C28—C36	117.4 (12)
O37—W3—O18	87.4 (3)	C27—C28—C29	122.4 (11)
O16—W3—O18	158.4 (3)	C36—C28—C29	120.2 (11)
O4—W3—O18	86.2 (3)	C30—C29—C28	120.2 (11)
O11—W3—O38	171.7 (3)	C30—C29—H29A	119.9
O37—W3—O38	74.3 (2)	C28—C29—H29A	119.9
O16—W3—O38	85.7 (2)	C29—C30—C31	120.1 (12)
O4—W3—O38	82.3 (2)	C29—C30—H30A	119.9
O18—W3—O38	73.6 (3)	C31—C30—H30A	119.9
O20—W4—O6	101.8 (3)	C35—C31—C32	119.1 (10)
O20—W4—O14	100.2 (3)	C35—C31—C30	119.0 (11)
O6—W4—O14	92.3 (3)	C32—C31—C30	121.9 (11)
O20—W4—O12	102.3 (3)	C33—C32—C31	118.6 (11)
O6—W4—O12	85.6 (3)	C33—C32—H14A	120.7
O14—W4—O12	157.4 (3)	C31—C32—H14A	120.7
O20—W4—O26	100.0 (3)	C34—C33—C32	119.6 (11)
O6—W4—O26	158.0 (3)	C34—C33—H16A	120.2
O14—W4—O26	86.3 (3)	C32—C33—H16A	120.2
O12—W4—O26	87.4 (3)	N10—C34—C33	124.4 (10)
O20—W4—O23	170.6 (3)	N10—C34—H34A	117.8
O6—W4—O23	86.0 (3)	C33—C34—H34A	117.8
O14—W4—O23	74.0 (3)	N10—C35—C31	122.1 (11)
O12—W4—O23	83.4 (3)	N10—C35—C36	116.4 (11)
O26—W4—O23	72.5 (2)	C31—C35—C36	121.5 (10)
O28—W5—O4	103.3 (3)	N12—C36—C28	123.4 (11)
O28—W5—O27	100.5 (3)	N12—C36—C35	117.8 (10)
O4—W5—O27	90.9 (3)	C28—C36—C35	118.8 (11)
O28—W5—O25	101.6 (3)	N2—C37—C38	125.6 (14)
O4—W5—O25	86.1 (3)	N2—C37—H37A	117.2
O27—W5—O25	157.8 (3)	C38—C37—H37A	117.2

O28—W5—O1	99.2 (3)	C39—C38—C37	117.6 (14)
O4—W5—O1	157.3 (3)	C39—C38—H38A	121.2
O27—W5—O1	87.3 (3)	C37—C38—H38A	121.2
O25—W5—O1	87.1 (3)	C38—C39—C40	120.5 (12)
O28—W5—O33	170.7 (3)	C38—C39—H39A	119.8
O4—W5—O33	84.3 (2)	C40—C39—H39A	119.8
O27—W5—O33	73.8 (3)	C39—C40—C48	117.5 (13)
O25—W5—O33	83.9 (2)	C39—C40—C41	123.2 (12)
O1—W5—O33	73.5 (2)	C48—C40—C41	119.3 (13)
O19—W6—O25	103.8 (3)	C42—C41—C40	119.8 (12)
O19—W6—O13	102.1 (3)	C42—C41—H41A	120.1
O25—W6—O13	91.7 (3)	C40—C41—H41A	120.1
O19—W6—O16	101.0 (3)	C41—C42—C43	123.3 (14)
O25—W6—O16	84.7 (3)	C41—C42—H42A	118.3
O13—W6—O16	156.9 (3)	C43—C42—H42A	118.3
O19—W6—O22	99.7 (3)	C44—C43—C47	116.5 (12)
O25—W6—O22	156.2 (3)	C44—C43—C42	124.6 (14)
O13—W6—O22	87.4 (3)	C47—C43—C42	118.8 (13)
O16—W6—O22	87.0 (3)	C43—C44—C45	120.2 (14)
O19—W6—O36	170.4 (3)	C43—C44—H44A	119.9
O25—W6—O36	84.9 (2)	C45—C44—H44A	119.9
O13—W6—O36	73.0 (2)	C46—C45—C44	118.8 (14)
O16—W6—O36	83.9 (2)	C46—C45—H45A	120.6
O22—W6—O36	72.1 (2)	C44—C45—H45A	120.6
O15—W7—O40	102.6 (3)	N15—C46—C45	123.9 (13)
O15—W7—O26	100.9 (3)	N15—C46—H46A	118.1
O40—W7—O26	91.8 (3)	C45—C46—H46A	118.1
O15—W7—O8	101.6 (3)	N15—C47—C43	122.7 (13)
O40—W7—O8	85.4 (3)	N15—C47—C48	118.2 (12)
O26—W7—O8	157.5 (3)	C43—C47—C48	119.0 (12)
O15—W7—O34	98.9 (3)	N2—C48—C40	123.1 (13)
O40—W7—O34	158.3 (2)	N2—C48—C47	117.4 (11)
O26—W7—O34	86.9 (3)	C40—C48—C47	119.5 (13)
O8—W7—O34	87.6 (3)	N16—C49—C50	121.3 (15)
O15—W7—O23	170.4 (3)	N16—C49—H49A	119.3
O40—W7—O23	85.5 (2)	C50—C49—H49A	119.3
O26—W7—O23	73.3 (2)	C51—C50—C49	120.6 (14)
O8—W7—O23	84.1 (2)	C51—C50—H50A	119.7
O34—W7—O23	73.4 (2)	C49—C50—H50A	119.7
O39—W8—O21	102.0 (3)	C50—C51—C52	121.2 (15)
O39—W8—O3	102.7 (3)	C50—C51—H51A	119.4
O21—W8—O3	86.3 (3)	C52—C51—H51A	119.4
O39—W8—O34	99.1 (3)	C51—C52—C53	126.9 (15)
O21—W8—O34	91.2 (3)	C51—C52—C60	115.2 (15)
O3—W8—O34	158.2 (3)	C53—C52—C60	117.8 (13)
O39—W8—O14	99.4 (3)	C54—C53—C52	121.4 (16)
O21—W8—O14	158.6 (3)	C54—C53—H53A	119.3
O3—W8—O14	87.6 (3)	C52—C53—H53A	119.3

O34—W8—O14	87.0 (3)	C53—C54—C55	125.7 (16)
O39—W8—O23	169.5 (3)	C53—C54—H54A	117.1
O21—W8—O23	86.0 (2)	C55—C54—H54A	117.1
O3—W8—O23	84.5 (2)	C56—C55—C59	116.4 (15)
O34—W8—O23	73.7 (2)	C56—C55—C54	128.7 (15)
O14—W8—O23	72.9 (2)	C59—C55—C54	114.9 (13)
O24—W9—O18	99.6 (3)	C57—C56—C55	124.7 (15)
O24—W9—O2	101.9 (3)	C57—C56—H56A	117.6
O18—W9—O2	91.3 (3)	C55—C56—H56A	117.6
O24—W9—O9	99.8 (3)	C56—C57—C58	114.7 (14)
O18—W9—O9	88.1 (3)	C56—C57—H57A	122.7
O2—W9—O9	158.1 (3)	C58—C57—H57A	122.7
O24—W9—O40	102.7 (3)	N1—C58—C57	126.8 (14)
O18—W9—O40	157.7 (3)	N1—C58—H58A	116.6
O2—W9—O40	85.3 (3)	C57—C58—H58A	116.6
O9—W9—O40	87.1 (3)	N1—C59—C55	121.6 (12)
O24—W9—O38	170.8 (3)	N1—C59—C60	116.3 (13)
O18—W9—O38	74.1 (3)	C55—C59—C60	122.2 (14)
O2—W9—O38	85.1 (2)	N16—C60—C59	117.7 (14)
O9—W9—O38	73.7 (2)	N16—C60—C52	124.4 (13)
O40—W9—O38	83.7 (2)	C59—C60—C52	117.9 (15)
O35—W10—O30	100.7 (3)	N7—C61—C62	125.5 (13)
O35—W10—O3	102.2 (3)	N7—C61—H1A	117.2
O30—W10—O3	90.8 (3)	C62—C61—H1A	117.2
O35—W10—O13	99.5 (3)	C61—C62—C63	117.8 (12)
O30—W10—O13	88.0 (3)	C61—C62—H62A	121.1
O3—W10—O13	158.1 (3)	C63—C62—H62A	121.1
O35—W10—O7	101.2 (3)	C62—C63—C64	121.3 (12)
O30—W10—O7	158.1 (3)	C62—C63—H63A	119.4
O3—W10—O7	85.8 (3)	C64—C63—H63A	119.4
O13—W10—O7	87.1 (3)	C63—C64—C65	126.8 (12)
O35—W10—O36	171.0 (3)	C63—C64—C72	116.8 (12)
O30—W10—O36	74.2 (3)	C65—C64—C72	116.4 (11)
O3—W10—O36	85.4 (2)	C66—C65—C64	123.5 (12)
O13—W10—O36	73.2 (2)	C66—C65—H65A	118.2
O7—W10—O36	84.0 (2)	C64—C65—H65A	118.2
O10—W11—O12	102.0 (3)	C65—C66—C67	119.6 (13)
O10—W11—O31	100.7 (3)	C65—C66—H66A	120.2
O12—W11—O31	86.1 (3)	C67—C66—H66A	120.2
O10—W11—O9	100.9 (3)	C71—C67—C68	117.6 (12)
O12—W11—O9	91.5 (3)	C71—C67—C66	120.0 (11)
O31—W11—O9	158.2 (3)	C68—C67—C66	122.4 (13)
O10—W11—O37	100.0 (3)	C69—C68—C67	117.8 (13)
O12—W11—O37	158.0 (3)	C69—C68—H68A	121.1
O31—W11—O37	87.8 (3)	C67—C68—H68A	121.1
O9—W11—O37	86.3 (3)	C68—C69—C70	121.2 (12)
O10—W11—O38	171.3 (3)	C68—C69—H69A	119.4
O12—W11—O38	85.3 (2)	C70—C69—H69A	119.4

O31—W11—O38	84.2 (2)	N3—C70—C69	121.8 (12)
O9—W11—O38	74.0 (2)	N3—C70—H70A	119.1
O37—W11—O38	73.0 (2)	C69—C70—H70A	119.1
O5—W12—O7	103.0 (3)	N3—C71—C67	123.4 (10)
O5—W12—O1	99.8 (3)	N3—C71—C72	117.0 (12)
O7—W12—O1	90.5 (3)	C67—C71—C72	119.5 (12)
O5—W12—O32	98.8 (3)	N7—C72—C71	116.9 (11)
O7—W12—O32	158.2 (3)	N7—C72—C64	122.2 (10)
O1—W12—O32	88.1 (3)	C71—C72—C64	120.8 (12)
O5—W12—O21	102.4 (3)	N13—C73—C74	120.1 (14)
O7—W12—O21	85.6 (3)	N13—C73—H73A	120.0
O1—W12—O21	157.8 (3)	C74—C73—H73A	120.0
O32—W12—O21	87.5 (3)	C73—C74—C75	118.4 (15)
O5—W12—O33	169.9 (3)	C73—C74—H74A	120.8
O7—W12—O33	84.9 (2)	C75—C74—H74A	120.8
O1—W12—O33	73.4 (2)	C76—C75—C74	124.4 (16)
O32—W12—O33	73.8 (2)	C76—C75—H75A	117.8
O21—W12—O33	84.4 (2)	C74—C75—H75A	117.8
W12—O1—W5	121.5 (3)	C75—C76—C77	127.4 (15)
W9—O2—W2	151.3 (4)	C75—C76—C84	111.6 (14)
W8—O3—W10	150.8 (4)	C77—C76—C84	121.0 (14)
W5—O4—W3	152.0 (4)	C78—C77—C76	123.3 (16)
W4—O6—W1	151.5 (4)	C78—C77—H77A	118.3
W12—O7—W10	151.6 (3)	C76—C77—H77A	118.3
W2—O8—W7	153.0 (3)	C77—C78—C79	122.3 (15)
W11—O9—W9	121.5 (3)	C77—C78—H78A	118.8
W11—O12—W4	151.7 (3)	C79—C78—H78A	118.8
W6—O13—W10	123.0 (3)	C80—C79—C78	127.2 (14)
W4—O14—W8	121.7 (4)	C80—C79—C83	114.8 (14)
W3—O16—W6	152.3 (3)	C78—C79—C83	117.7 (13)
W9—O18—W3	121.5 (4)	C81—C80—C79	122.3 (13)
W8—O21—W12	151.3 (3)	C81—C80—H80A	118.9
W1—O22—W6	123.1 (3)	C79—C80—H80A	118.9
Si1—O23—W7	124.2 (4)	C80—C81—C82	120.7 (14)
Si1—O23—W4	124.6 (3)	C80—C81—H81A	119.7
W7—O23—W4	91.9 (2)	C82—C81—H81A	119.7
Si1—O23—W8	123.5 (3)	N11—C82—C81	123.3 (14)
W7—O23—W8	91.6 (2)	N11—C82—H82A	118.4
W4—O23—W8	91.3 (2)	C81—C82—H82A	118.4
W6—O25—W5	152.5 (3)	N11—C83—C84	119.2 (12)
W7—O26—W4	122.2 (3)	N11—C83—C79	121.7 (12)
W5—O27—W2	121.6 (3)	C84—C83—C79	119.0 (14)
W10—O30—W1	121.0 (4)	N13—C84—C76	127.2 (14)
W1—O31—W11	151.5 (3)	N13—C84—C83	116.6 (13)
W2—O32—W12	121.3 (3)	C76—C84—C83	116.2 (13)
Si1—O33—W5	124.4 (3)	N6—C85—C86	123.1 (12)
Si1—O33—W2	124.4 (3)	N6—C85—H85A	118.4
W5—O33—W2	91.6 (2)	C86—C85—H85A	118.4

Si1—O33—W12	124.1 (4)	C87—C86—C85	117.8 (13)
W5—O33—W12	91.6 (2)	C87—C86—H86A	121.1
W2—O33—W12	90.9 (2)	C85—C86—H86A	121.1
W8—O34—W7	121.3 (3)	C86—C87—C88	121.9 (11)
Si1—O36—W1	125.0 (3)	C86—C87—H15A	119.0
Si1—O36—W10	124.3 (3)	C88—C87—H15A	119.0
W1—O36—W10	91.0 (2)	C87—C88—C96	115.5 (11)
Si1—O36—W6	124.3 (4)	C87—C88—C89	126.1 (11)
W1—O36—W6	91.2 (2)	C96—C88—C89	118.3 (12)
W10—O36—W6	90.8 (2)	C90—C89—C88	122.8 (12)
W3—O37—W11	121.9 (3)	C90—C89—H18B	118.6
Si1—O38—W3	125.1 (3)	C88—C89—H18B	118.6
Si1—O38—W9	125.2 (3)	C89—C90—C91	120.8 (12)
W3—O38—W9	90.7 (2)	C89—C90—H90A	119.6
Si1—O38—W11	123.8 (4)	C91—C90—H90A	119.6
W3—O38—W11	90.82 (19)	C92—C91—C95	118.8 (11)
W9—O38—W11	90.7 (2)	C92—C91—C90	124.2 (12)
W7—O40—W9	151.4 (3)	C95—C91—C90	116.9 (12)
N5—Cu1—N14	132.5 (4)	C93—C92—C91	118.1 (12)
N5—Cu1—N9	124.0 (4)	C93—C92—H92A	120.9
N14—Cu1—N9	81.9 (4)	C91—C92—H92A	120.9
N5—Cu1—N4	82.4 (4)	C92—C93—C94	120.5 (13)
N14—Cu1—N4	131.7 (5)	C92—C93—H93A	119.7
N9—Cu1—N4	106.9 (4)	C94—C93—H93A	119.7
N10—Cu2—N2	120.1 (4)	N8—C94—C93	122.4 (11)
N10—Cu2—N12	81.5 (4)	N8—C94—H94A	118.8
N2—Cu2—N12	137.6 (4)	C93—C94—H94A	118.8
N10—Cu2—N15	139.5 (4)	N8—C95—C91	121.7 (11)
N2—Cu2—N15	82.2 (4)	N8—C95—C96	116.8 (11)
N12—Cu2—N15	105.1 (4)	C91—C95—C96	121.5 (11)
N16—Cu3—N7	149.3 (4)	N6—C96—C88	122.2 (11)
N16—Cu3—N1	81.0 (4)	N6—C96—C95	118.9 (10)
N7—Cu3—N1	107.3 (4)	C88—C96—C95	119.0 (11)
N16—Cu3—N3	116.4 (4)	C58—N1—C59	115.9 (12)
N7—Cu3—N3	81.4 (4)	C58—N1—Cu3	132.9 (10)
N1—Cu3—N3	130.2 (4)	C59—N1—Cu3	111.2 (8)
N11—Cu4—N8	130.4 (4)	C37—N2—C48	115.6 (11)
N11—Cu4—N6	125.1 (4)	C37—N2—Cu2	132.9 (10)
N8—Cu4—N6	82.6 (4)	C48—N2—Cu2	111.3 (9)
N11—Cu4—N13	82.5 (4)	C70—N3—C71	118.0 (11)
N8—Cu4—N13	138.2 (4)	C70—N3—Cu3	130.9 (9)
N6—Cu4—N13	99.2 (4)	C71—N3—Cu3	111.1 (7)
N14—C1—C2	117.0 (14)	C22—N4—C23	117.6 (12)
N14—C1—H1B	121.5	C22—N4—Cu1	131.2 (9)
C2—C1—H1B	121.5	C23—N4—Cu1	111.0 (8)
C3—C2—C1	123.1 (16)	C13—N5—C24	117.0 (11)
C3—C2—H2A	118.4	C13—N5—Cu1	130.5 (9)
C1—C2—H2A	118.4	C24—N5—Cu1	112.3 (8)

C2—C3—C4	122.5 (17)	C85—N6—C96	119.3 (10)
C2—C3—H3A	118.8	C85—N6—Cu4	130.7 (9)
C4—C3—H3A	118.8	C96—N6—Cu4	109.0 (8)
C5—C4—C12	120.3 (15)	C61—N7—C72	116.3 (11)
C5—C4—C3	126.1 (16)	C61—N7—Cu3	130.8 (9)
C12—C4—C3	113.7 (14)	C72—N7—Cu3	112.2 (7)
C4—C5—C6	123.7 (16)	C94—N8—C95	118.3 (11)
C4—C5—H5A	118.2	C94—N8—Cu4	129.3 (8)
C6—C5—H5A	118.2	C95—N8—Cu4	112.2 (8)
C5—C6—C7	119.2 (14)	C11—N9—C10	116.1 (12)
C5—C6—H6A	120.4	C11—N9—Cu1	112.0 (9)
C7—C6—H6A	120.4	C10—N9—Cu1	131.8 (10)
C11—C7—C8	115.8 (15)	C34—N10—C35	116.2 (10)
C11—C7—C6	119.1 (14)	C34—N10—Cu2	131.2 (7)
C8—C7—C6	125.0 (14)	C35—N10—Cu2	112.6 (8)
C8—C9—C10	116.3 (15)	C82—N11—C83	117.0 (11)
C8—C9—H9A	121.9	C82—N11—Cu4	132.1 (9)
C10—C9—H9A	121.9	C83—N11—Cu4	110.9 (8)
C9—C8—C7	123.3 (14)	C25—N12—C36	116.7 (10)
C9—C8—H8A	118.3	C25—N12—Cu2	131.3 (9)
C7—C8—H8A	118.3	C36—N12—Cu2	111.7 (8)
N9—C10—C9	124.3 (14)	C73—N13—C84	118.3 (14)
N9—C10—H10A	117.9	C73—N13—Cu4	130.5 (11)
C9—C10—H10A	117.9	C84—N13—Cu4	110.4 (9)
N9—C11—C7	124.2 (14)	C1—N14—C12	118.7 (14)
N9—C11—C12	116.2 (12)	C1—N14—Cu1	128.8 (10)
C7—C11—C12	119.6 (15)	C12—N14—Cu1	112.5 (10)
N14—C12—C4	125.0 (15)	C46—N15—C47	117.7 (13)
N14—C12—C11	117.0 (14)	C46—N15—Cu2	131.6 (9)
C4—C12—C11	118.0 (13)	C47—N15—Cu2	110.3 (9)
N5—C13—C14	124.9 (13)	C49—N16—C60	117.2 (13)
N5—C13—H13A	117.6	C49—N16—Cu3	128.8 (11)
C14—C13—H13A	117.6	C60—N16—Cu3	113.7 (9)
C15—C14—C13	117.4 (12)	O38—Si1—O33	108.8 (4)
C15—C14—H14B	121.3	O38—Si1—O36	109.5 (3)
C13—C14—H14B	121.3	O33—Si1—O36	109.7 (3)
C14—C15—C16	120.8 (13)	O38—Si1—O23	109.2 (3)
C14—C15—H15B	119.6	O33—Si1—O23	110.0 (3)
C16—C15—H15B	119.6	O36—Si1—O23	109.5 (4)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C10—H10A \cdots O17	0.93	2.64	3.503 (17)	154
C41—H41A \cdots O26	0.93	2.74	3.131 (13)	106
C25—H25A \cdots O10	0.93	2.43	3.329 (16)	162
C50—H50A \cdots O35	0.93	2.62	3.477 (16)	153
C69—H69A \cdots O34	0.93	2.59	3.322 (14)	136

C49—H49A···O5	0.93	2.36	3.276 (18)	169
C92—H92A···O15	0.93	3.04	3.491 (16)	111
C94—H94A···O24	0.93	2.62	3.326 (14)	134
