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

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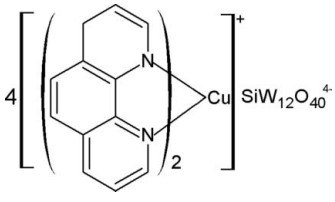
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.018 Å; $R$ factor = 0.041; $wR$ factor = 0.072; data-to-parameter ratio = 16.4.

Single crystals of the title polyoxometallate-based organic–inorganic hybrid, $[Cu(C_{12}H_8N_2)_2]_4[SiW_{12}O_{40}]$, were grown under hydrothermal conditions. The discrete $[SiW_{12}O_{40}]^{4-}$ anions are of the Keggin type and are packed in a slightly distorted orthorhombic $F$-centred mode, with the complex $[Cu^{I}(phen)_2]^+$ 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* $\pi$–$\pi$ interactions between different phen molecules of adjacent $[Cu^{I}(phen)_2]^+$ cations with shortest distances between 3.416 and 3.499 Å.

## Related literature

The educt $H_4SiW_{12}O_{40}\cdot nH_2O$ 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

$[Cu(C_{12}H_8N_2)_2]_4[SiW_{12}O_{40}]$
$M_r$ = 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) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 13.55 mm$^{-1}$
$T$ = 293 (2) K
0.23 × 0.21 × 0.20 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.066, $T_{max}$ = 0.072
(expected range = 0.061–0.066)
66617 measured reflections
24930 independent reflections
20506 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 1.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.37 e Å$^{-3}$
Absolute structure: Flack (1983), with 11091 Friedel pairs
Flack parameter: −0.006 (6)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10—H10$A$···O17 | 0.93 | 2.64 | 3.503 (17) | 154 |
| C41—H41$A$···O26 | 0.93 | 2.74 | 3.131 (13) | 106 |
| C25—H25$A$···O10 | 0.93 | 2.43 | 3.329 (16) | 162 |
| C50—H50$A$···O35 | 0.93 | 2.62 | 3.477 (16) | 153 |
| C69—H69$A$···O34 | 0.93 | 2.59 | 3.322 (14) | 136 |
| C49—H49$A$···O5 | 0.93 | 2.36 | 3.276 (18) | 169 |
| C92—H92$A$···O15 | 0.93 | 3.04 | 3.491 (16) | 111 |
| C94—H94$A$···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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# supplementary materials

*Acta Cryst.* (2008). E**64**, m106 [ **doi:10.1107/S1600536807062903** ]

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

**F.-X. Meng, H.-B. Liu and Y.-G. Chen**

## Comment

The structure of the title compound is built from four independent complex coordination cations $[Cu(phen)_2]^+$ and one Keggin-type anion $[SiW_{12}O_{40}]^{4-}$. The Keggin anions are arranged in a slightly distorted orthorhombic F-centred packing mode (Fig. 1) with the $[Cu(phen)_2]^+$ 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 $H_4SiW_{12}O_{40}$ (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.

## Experimental

$H_4SiW_{12}O_{40}.nH_2O$ was prepared according to the method given by Rocchiccioli-Deltcheff *et al.* (1983). The starting mixture of $H_4SiW_{12}O_{40}.nH_2O$ (1.15 g), $Cu(OAc)_2{\cdot}2H_2O$ (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).

## 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 $U_{iso}(H) = 1.2U_{eq}(C)$ 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.

**Figures**

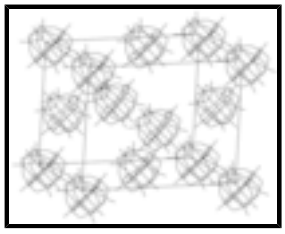

Fig. 1. The packing of the $[SiW_{12}O_{40}]^{4-}$ heteropolyanions leading to a slightly distorted F-centred orthorhombic lattice. All other atoms are omitted for clarity.

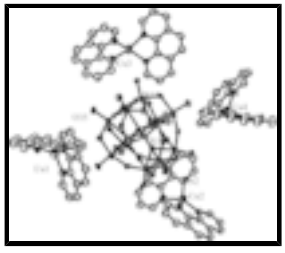

Fig. 2. The Keggin-type $SiW_{12}O_{40}^{4-}$ anions with surrounding $[Cu(phen)_2]^+$ cations displayed with aniostropic displacement parameters at the 30% probability level. H atoms are omitted for clarity.

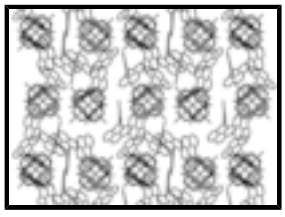

Fig. 3. Packing of the structure viewed down the *a* axis. H atoms are omitted for clarity.

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

*Crystal data*

| | |
|---|---|
| $[Cu(C_{12}H_8N_2)_2]_4[SiW_{12}O_{40}]$ | $F_{000}$ = 8360 |
| $M_r$ = 4570.08 | $D_x$ = 2.803 Mg m$^{-3}$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 5100 reflections |
| *a* = 18.332 (3) Å | θ = 1.5–28.4º |
| *b* = 21.173 (3) Å | μ = 13.55 mm$^{-1}$ |
| *c* = 27.901 (4) Å | *T* = 293 (2) K |
| *V* = 10830 (3) Å$^3$ | Block, black |
| *Z* = 4 | 0.23 × 0.21 × 0.20 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD diffractometer | 24930 independent reflections |
| Radiation source: fine-focus sealed tube | 20506 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.065 |
| *T* = 293(2) K K | $\theta_{max}$ = 28.4º |
| φ and ω scans | $\theta_{min}$ = 1.5º |
| Absorption correction: multi-scan | *h* = −24→19 |

(SADABS; Bruker, 2001)
$T_{min}$ = 0.066, $T_{max}$ = 0.072
66617 measured reflections

$k$ = −23→27
$l$ = −37→37

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.041 | $w = 1/[\sigma^2(F_o^2) + (0.0109P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.072 | $(\Delta/\sigma)_{max}$ = 0.005 |
| $S$ = 0.99 | $\Delta\rho_{max}$ = 1.29 e Å$^{-3}$ |
| 24930 reflections | $\Delta\rho_{min}$ = −1.37 e Å$^{-3}$ |
| 1523 parameters | Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| 2431 restraints | Extinction coefficient: 0.000046 (2) |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), with 11091 Friedel pairs |
| Secondary atom site location: difference Fourier map | Flack 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 $F^2 > 2$sigma($F^2$) is used only for calculating R– factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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) |

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|---|---|---|---|---|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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) |

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|---|---|---|---|---|---|---|
| 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) |

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|---|---|---|---|---|---|---|
| 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 |

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|---|---|---|---|
| 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) |

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|---|---|---|---|
| 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) |

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| 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) |

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| 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) |

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| 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) |

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| 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 |

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| 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 (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*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 |

**Fig. 1**

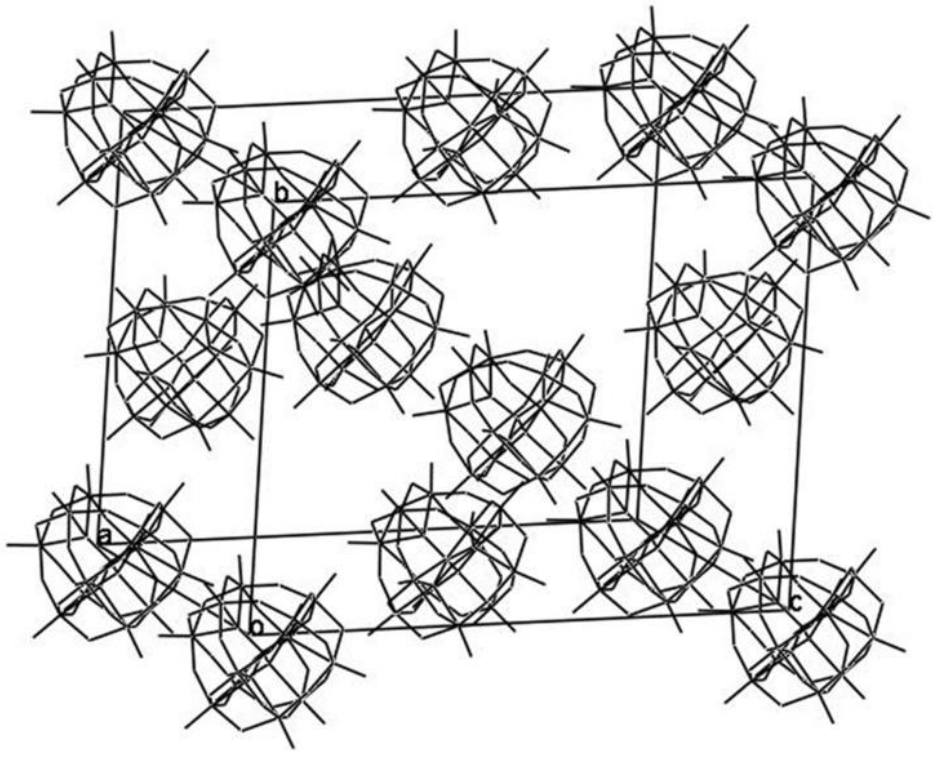


**Fig. 2**

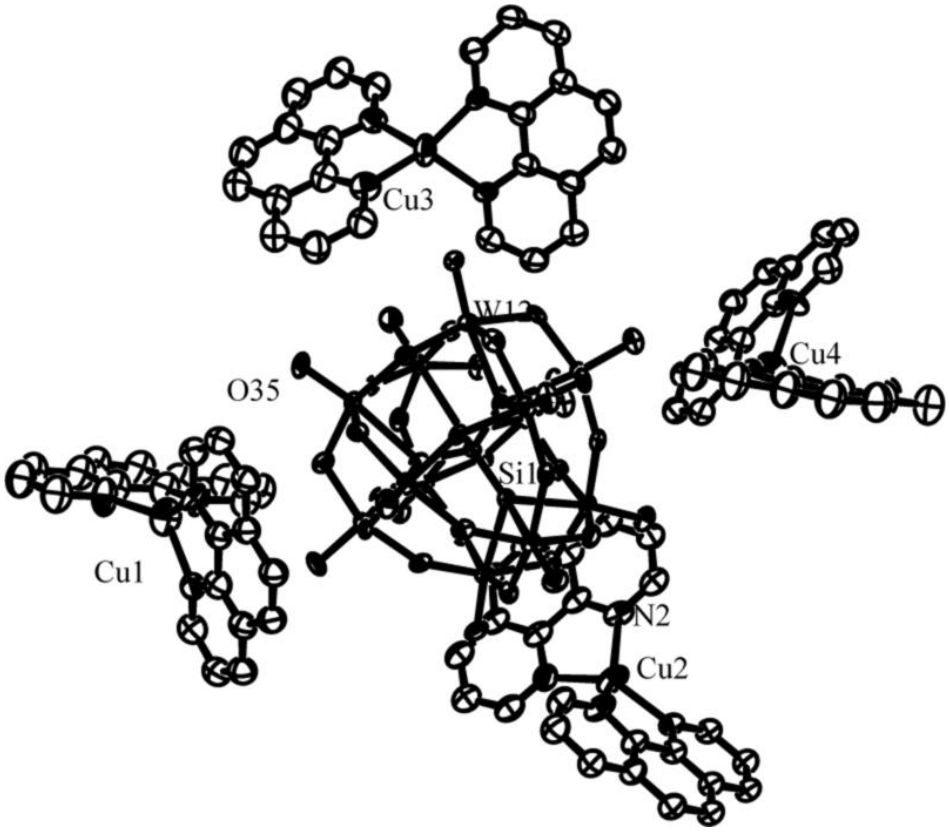
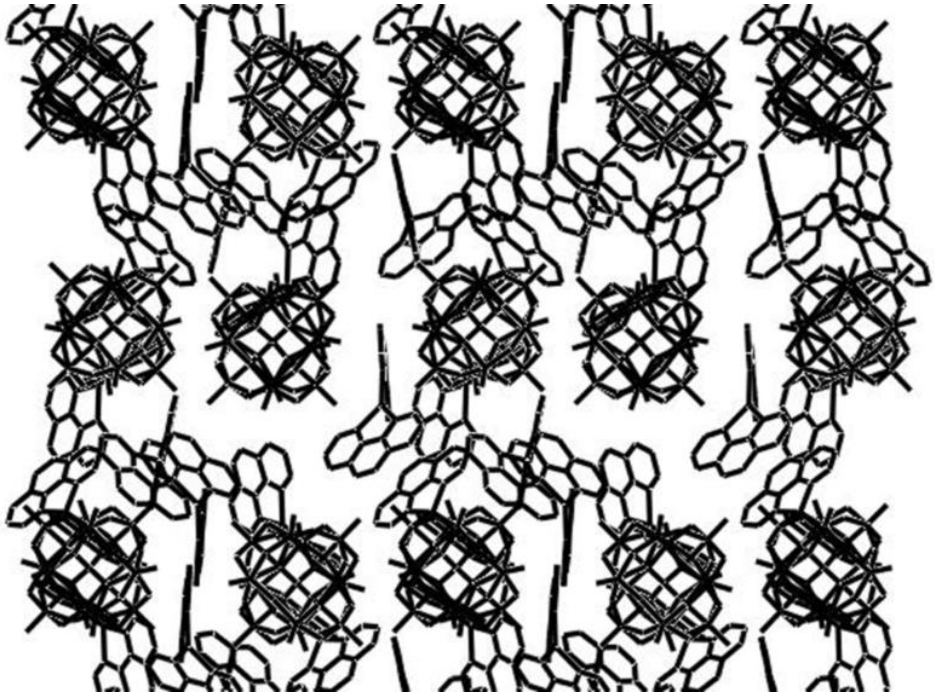


**Fig. 3**



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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), E**64**, m106] is corrected.

In the paper by Meng, Liu & Chen [*Acta Cryst.* (2008), E**64**, m106], the chemical name in the title is incorrect. The correct chemical name should be 'tetrakis[bis(1,10-phenanthroline)-copper(I)] dodecatungstosilicate'.