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Bis(3,5-dimethylpyrazole)[*N*-salicylidene-β-alaninato(2–)]copper(II) dihydrate

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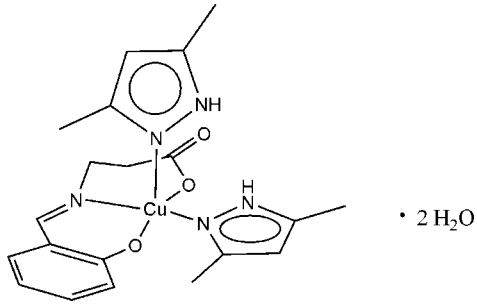
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.075; data-to-parameter ratio = 13.2.

In the title compound, $[Cu(C_{10}H_{10}NO_3)(C_5H_8N_2)_2]\cdot 2H_2O$, the Cu^{II} atom is coordinated by three N atoms and two O atoms in a distorted square-pyramidal geometry. The crystal packing is stabilized by intermolecular O—H···O and N—H···O hydrogen bonds.

Related literature

For related literature, see: Plesch *et al.* (1997); Raso *et al.* (1996, 1999); Warda (1997, 1998*a*,*b*,*c*).



· 2 H_2O

Experimental

Crystal data

$[Cu(C_{10}H_{10}NO_3)(C_5H_8N_2)_2]\cdot 2H_2O$
M_r = 483.02
Monoclinic, $P2_1/c$
a = 19.619 (4) Å
b = 8.2103 (15) Å
c = 13.890 (3) Å
β = 91.493 (2)°
V = 2236.7 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 298 (2) K
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.686, T_{max} = 0.905
11230 measured reflections
3965 independent reflections
3446 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.075
S = 1.05
3965 reflections
301 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.9191 (15)	Cu1—N2	2.0584 (16)
Cu1—N1	1.9634 (17)	Cu1—N4	2.2625 (18)
Cu1—O1	2.0211 (15)		
O3—Cu1—N1	90.03 (7)	O1—Cu1—N2	85.52 (6)
O3—Cu1—O1	166.22 (7)	O3—Cu1—N4	106.80 (7)
N1—Cu1—O1	89.65 (6)	N1—Cu1—N4	99.76 (7)
O3—Cu1—N2	91.13 (7)	O1—Cu1—N4	86.82 (6)
N1—Cu1—N2	164.27 (7)	N2—Cu1—N4	94.91 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1W	0.86	2.25	3.041 (3)	153
N5—H5A···O1W	0.86	2.09	2.911 (3)	159
O1W—H1WA···O2W^{i}	0.836 (10)	2.053 (14)	2.858 (3)	161 (3)
O2W—H2WB···O2^{ii}	0.840 (10)	1.902 (12)	2.729 (2)	168 (3)
O2W—H2WA···O2^{iii}	0.849 (10)	1.960 (13)	2.791 (2)	166 (3)
O1W—H1WB···O2W^{iv}	0.839 (10)	2.033 (11)	2.865 (3)	172 (3)

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2042).

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supporting information

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Bis(3,5-dimethylpyrazole)[*N*-salicylidene-*β*-alaninato(2–)]copper(II) dihydrate

Ji-Min Xie, Gan-Qing Zhao, Xiao-Jing Lu, Xiao-Meng Lü and Yuan-Zhi Song

S1. Comment

Copper (II) complexes of tridentate Schiff base ligands of the *N*-alkylidene or *N*-arylidene aminoacidato type have attracted considerable interest due to their richness in structural diversity, their electrochemical properties and also due to their use as potential models for a number of important biological systems (Raso *et al.*, 1999; Raso *et al.*, 1996). Several stuctural studies have been performed on Schiff base copper (II) complexes derived from salicylaldehyde and animo acids (Warda, 1997, 1998*a*,*b*,*c*). In this context we present here the crystal structure of the title Cu^{II} complex, (*N*-salicylidene-*β*-alanine)(3,5-dimethylprazole)$_2$]copper(II), in the form of its dihydrate.

The structure consists of monomeric units with a square pyramidal copper center (Fig. 1). The four basal positions are occupied by the tridentate, dianionic Schiff base ligand, which furnishes an ONO donor set, with the fourth position occupied by a 3, 5-dimethylprazole N. The coordination sphere is completed by the nitrogen atom of the remaining 3,5-dimethylprazole ligand at the apical position. The two nitrogen heterocycles are planar and exhibit an angle of 37.1° and 79.7° with the plane of the tridentate Schiff base, respectively.

Two solvate water molecules are present in the crystal lattice and hydrogen bonded with each other and the N—H groups of the 3,5-dimethylprazole ligands (see hydrogen bonding table). The interesting intermolecuelar hydrogen-bonding network also stabilizes the crystal structure as a whole. H atoms of O(2w) hydrogen bond to the neighboring carboxylate oxygen O2 and H atoms of O(1w) to form H-bonds to form a two dimensional sheet (Fig. 2). A network of oxygen atoms is formed by above H-bonds (Fig. 3). In addition, all the 3,5-dimethylprazole N—H protons are hydrogen bonded to adjacent water molecules O(1w).

S2. Experimental

The title compound was synthesized as described in the literature (Plesch *et al.*, 1997). To *β*-alanine (1.00 mmol) and lithium hydroxide monohydrate (1.00 mmol) in 10 ml of methanol was added salicylaldehyde (1.00 mmol in 10 ml of methanol). The yellow solution was stirred for 1.0 h at room temperature prior to cooling in an ice bath. The resultant mixture was added dropwise to copper (II) acetate monohydrate (1.00 mmol) and 3,5-dimethylpyrazole (2.00 mmol) in an aqueous methanolic solution (20 ml, 1;1 *v*/*v*), and heated with stirring for 2.0 h at 333 K. The dark green solution was filtered and left for several days, dark blue crystals had formed that were filtered off, washed with water, and dried under vacuum. Analysis found: C 50.12, H 6.04, N 14.93%; calculated: C 49.73, H 6.05, N 14.49%.

S3. Refinement

The positions of the H atoms of the water molecules were located in difference Fourier maps and refined freely along with an isotropic displacement parameter. Other H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (CH) and 0.97 Å (CH_2) and U_{iso}(H) = 1.2U_{eq}(C), with C—H = 0.96 Å (CH_3) and U_{iso}(H) = 1.5U_{eq}(C), and with N—H = 0.86 Å (NH) and U_{iso}(H) = 1.2U_{eq}(N).

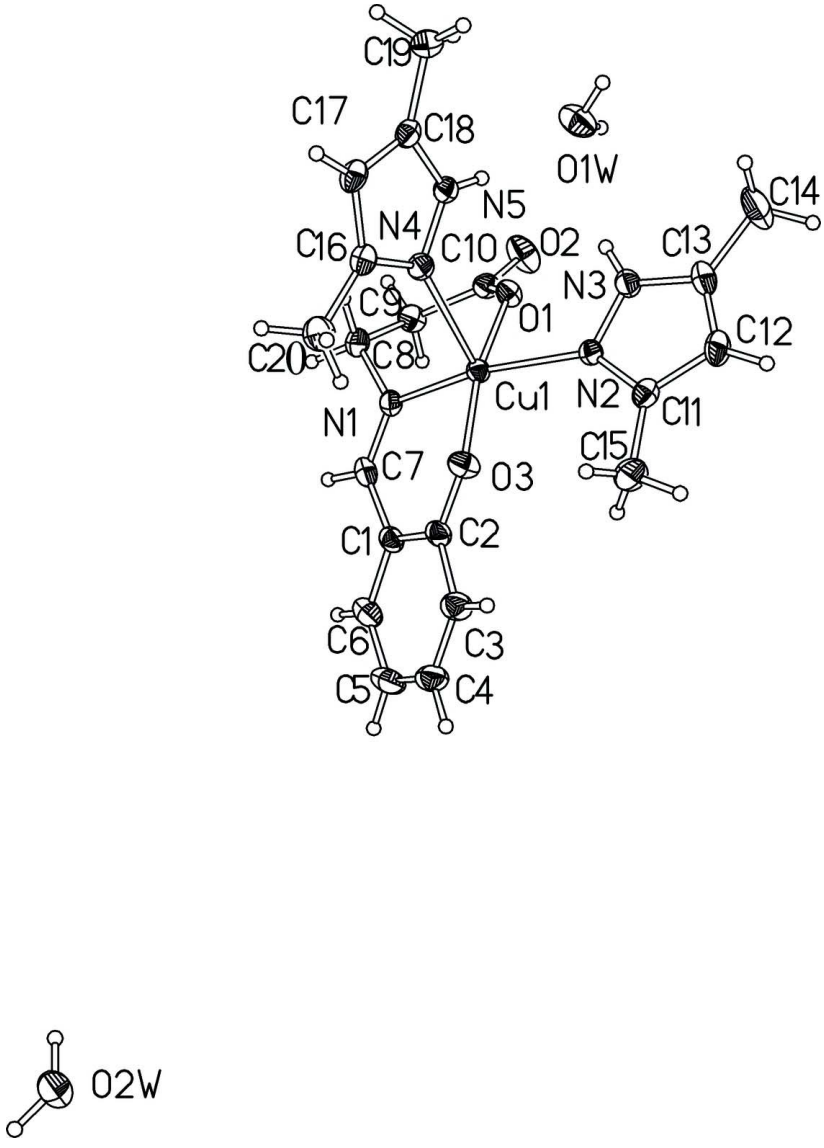

Figure 1

The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

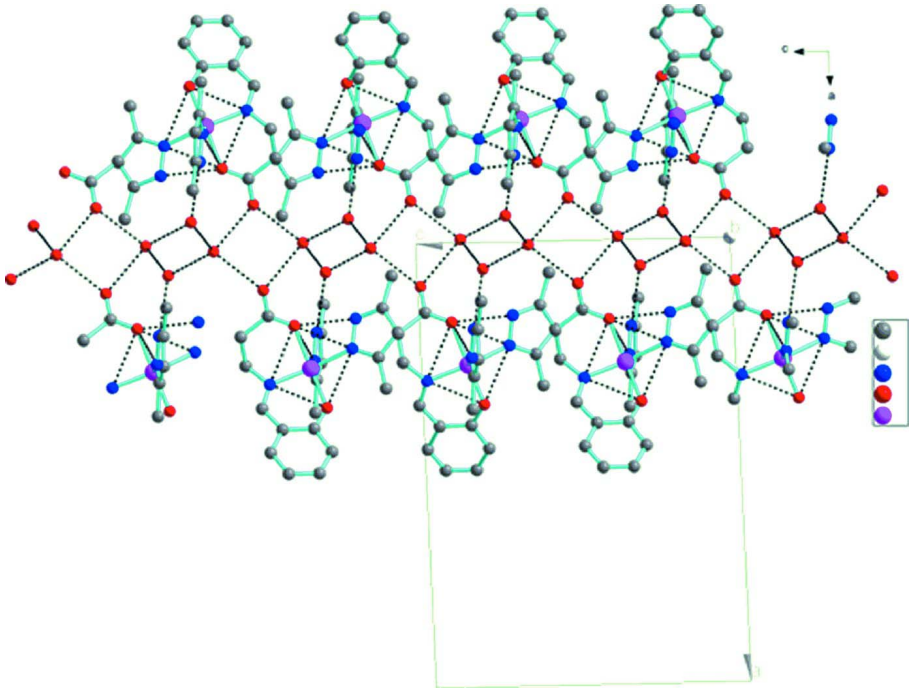

Figure 2

Two-dimensional network of the title compound formed by hydrogen bonds (dashed lines).

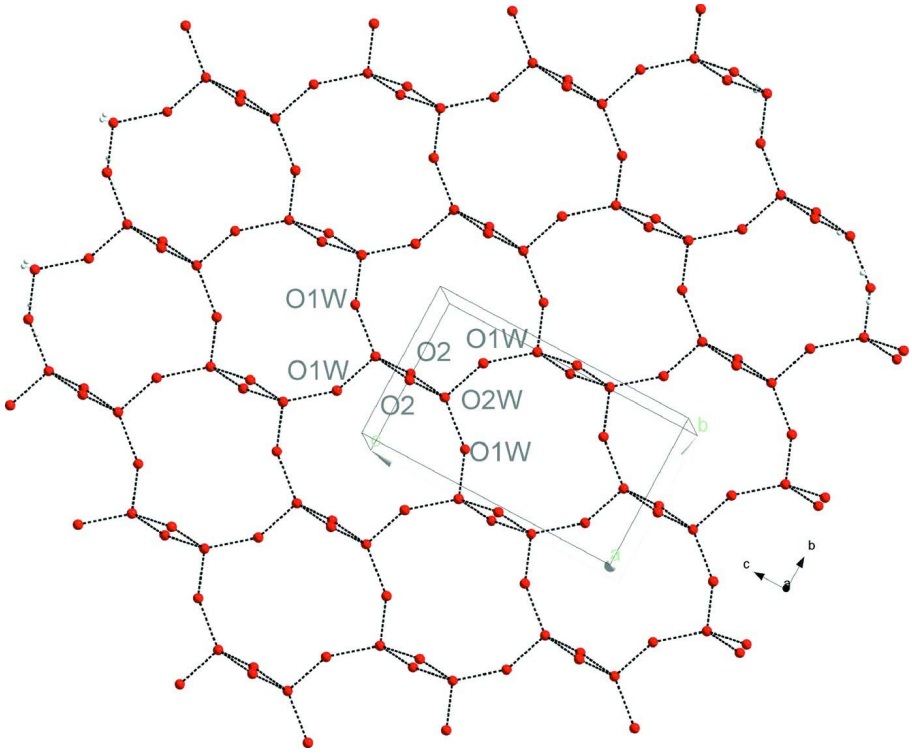

Figure 3

The Plot of oxygen cluster formed between the title compound and water by hydrogen bonds (dashed lines).

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Crystal data

$[Cu(C_{10}H_{10}NO_3)(C_5H_8N_2)_2]\cdot 2H_2O$
$M_r = 483.02$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 19.619$ (4) Å
$b = 8.2103$ (15) Å
$c = 13.890$ (3) Å
$\beta = 91.493$ (2)°
$V = 2236.7$ (7) Å^3
$Z = 4$
$F(000) = 1012$
$D_x = 1.434$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5668 reflections
$\theta = 2.7$–$27.5°$
$\mu = 1.02$ mm^{-1}
$T = 298$ K
Block, blue
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.686$, $T_{max} = 0.905$
11230 measured reflections
3965 independent reflections
3446 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.7°$
$h = -18\rightarrow23$
$k = -9\rightarrow9$
$l = -16\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.075$
$S = 1.05$
3965 reflections
301 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2 + 1.1315P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0056 (4)

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 $F^2 > \sigma(F^2)$ 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}
Cu1	0.274799 (12)	0.57312 (3)	0.850618 (16)	0.02768 (10)
C1	0.41151 (10)	0.4081 (3)	0.95032 (15)	0.0337 (5)
C2	0.41039 (10)	0.4380 (3)	0.84957 (16)	0.0344 (5)

C3	0.46327 (11)	0.3676 (3)	0.79666 (18)	0.0436 (5)
H3	0.4654	0.3886	0.7310	0.052*
C4	0.51165 (12)	0.2691 (3)	0.8394 (2)	0.0492 (6)
H4	0.5453	0.2232	0.8020	0.059*
C5	0.51139 (12)	0.2369 (3)	0.9370 (2)	0.0520 (6)
H5	0.5437	0.1675	0.9650	0.062*
C6	0.46268 (11)	0.3089 (3)	0.99167 (18)	0.0453 (6)
H6	0.4635	0.2917	1.0579	0.054*
C7	0.36357 (11)	0.4848 (3)	1.01174 (15)	0.0347 (5)
H7	0.3729	0.4800	1.0777	0.042*
C8	0.26606 (11)	0.6335 (3)	1.05720 (15)	0.0400 (5)
H8A	0.2552	0.7445	1.0385	0.048*
H8B	0.2909	0.6371	1.1185	0.048*
C9	0.20079 (12)	0.5386 (3)	1.06855 (15)	0.0408 (5)
H9A	0.1748	0.5898	1.1187	0.049*
H9B	0.2125	0.4297	1.0904	0.049*
C10	0.15528 (11)	0.5240 (3)	0.97922 (15)	0.0347 (5)
C11	0.25299 (12)	0.4552 (3)	0.63387 (14)	0.0351 (5)
C12	0.19798 (13)	0.4452 (3)	0.56921 (16)	0.0447 (6)
H12	0.1986	0.4032	0.5071	0.054*
C13	0.14291 (12)	0.5086 (3)	0.61390 (16)	0.0428 (6)
C14	0.07053 (15)	0.5313 (5)	0.5804 (2)	0.0755 (9)
H14A	0.0407	0.5058	0.6319	0.113*
H14B	0.0608	0.4603	0.5268	0.113*
H14C	0.0636	0.6423	0.5608	0.113*
C15	0.32401 (13)	0.4047 (4)	0.61519 (18)	0.0553 (7)
H15A	0.3537	0.4974	0.6211	0.083*
H15B	0.3263	0.3608	0.5513	0.083*
H15C	0.3381	0.3232	0.6611	0.083*
C16	0.30024 (11)	0.9729 (3)	0.83353 (15)	0.0348 (5)
C17	0.26279 (12)	1.1159 (3)	0.81797 (15)	0.0384 (5)
H17	0.2801	1.2206	0.8112	0.046*
C18	0.13169 (13)	1.1672 (3)	0.80069 (19)	0.0516 (6)
H18A	0.1246	1.1907	0.7335	0.077*
H18B	0.1353	1.2673	0.8361	0.077*
H18C	0.0939	1.1050	0.8234	0.077*
C19	0.37518 (13)	0.9516 (3)	0.8431 (2)	0.0542 (7)
H19A	0.3856	0.8382	0.8519	0.081*
H19B	0.3922	1.0121	0.8978	0.081*
H19C	0.3962	0.9906	0.7860	0.081*
C25	0.19588 (12)	1.0715 (2)	0.81468 (14)	0.0341 (5)
N1	0.30915 (9)	0.5592 (2)	0.98439 (12)	0.0309 (4)
N2	0.23273 (8)	0.5216 (2)	0.71677 (11)	0.0299 (4)
N3	0.16542 (9)	0.5538 (2)	0.70181 (13)	0.0365 (4)
H3A	0.1401	0.5982	0.7440	0.044*
N4	0.25830 (9)	0.8452 (2)	0.83905 (12)	0.0335 (4)
N5	0.19496 (9)	0.9095 (2)	0.82779 (12)	0.0328 (4)
H5A	0.1582	0.8527	0.8289	0.039*

O1	0.17828 (7)	0.55934 (18)	0.89740 (10)	0.0343 (3)
O2	0.09666 (8)	0.4747 (3)	0.99071 (12)	0.0606 (5)
O3	0.36475 (7)	0.5303 (2)	0.80579 (10)	0.0399 (4)
O1W	0.05960 (9)	0.7752 (3)	0.79001 (15)	0.0595 (5)
O2W	0.99231 (9)	0.4897 (3)	0.85715 (12)	0.0528 (4)
H2WA	0.9600 (11)	0.500 (4)	0.8961 (17)	0.067 (9)*
H1WA	0.0321 (12)	0.706 (3)	0.810 (2)	0.072 (10)*
H2WB	1.0271 (9)	0.476 (4)	0.8928 (16)	0.058 (9)*
H1WB	0.0404 (14)	0.833 (3)	0.7478 (17)	0.076 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02796 (15)	0.02971 (15)	0.02528 (14)	0.00149 (10)	−0.00086 (10)	0.00056 (10)
C1	0.0271 (10)	0.0321 (11)	0.0416 (12)	−0.0041 (9)	−0.0038 (9)	0.0014 (9)
C2	0.0248 (10)	0.0335 (12)	0.0449 (12)	−0.0045 (9)	−0.0013 (9)	0.0002 (9)
C3	0.0332 (12)	0.0468 (14)	0.0512 (13)	0.0005 (10)	0.0059 (10)	−0.0008 (11)
C4	0.0309 (12)	0.0410 (14)	0.0759 (18)	0.0018 (10)	0.0055 (12)	−0.0046 (12)
C5	0.0307 (12)	0.0446 (15)	0.0803 (19)	0.0048 (10)	−0.0062 (12)	0.0098 (13)
C6	0.0359 (12)	0.0456 (14)	0.0537 (14)	−0.0031 (11)	−0.0097 (11)	0.0095 (11)
C7	0.0357 (12)	0.0363 (12)	0.0317 (11)	−0.0081 (10)	−0.0078 (9)	0.0032 (9)
C8	0.0468 (13)	0.0445 (13)	0.0286 (10)	0.0028 (11)	−0.0035 (10)	−0.0091 (10)
C9	0.0422 (13)	0.0541 (15)	0.0263 (11)	0.0059 (11)	0.0041 (9)	0.0004 (10)
C10	0.0330 (12)	0.0415 (13)	0.0300 (11)	0.0045 (10)	0.0059 (9)	−0.0005 (9)
C11	0.0477 (13)	0.0314 (11)	0.0263 (10)	−0.0006 (9)	0.0025 (9)	0.0011 (8)
C12	0.0604 (16)	0.0487 (14)	0.0247 (11)	−0.0051 (12)	−0.0035 (11)	−0.0023 (10)
C13	0.0454 (14)	0.0493 (14)	0.0330 (11)	−0.0087 (11)	−0.0105 (10)	0.0027 (10)
C14	0.0520 (17)	0.113 (3)	0.0606 (18)	−0.0044 (17)	−0.0240 (14)	−0.0052 (18)
C15	0.0554 (16)	0.0716 (19)	0.0392 (13)	0.0129 (14)	0.0088 (12)	−0.0129 (12)
C16	0.0413 (12)	0.0326 (12)	0.0308 (11)	−0.0064 (10)	0.0041 (9)	−0.0008 (9)
C17	0.0527 (14)	0.0254 (11)	0.0372 (11)	−0.0079 (10)	0.0015 (10)	0.0021 (9)
C18	0.0555 (16)	0.0375 (14)	0.0612 (15)	0.0095 (11)	−0.0110 (12)	−0.0007 (12)
C19	0.0431 (14)	0.0492 (16)	0.0703 (18)	−0.0084 (12)	0.0010 (13)	−0.0038 (13)
C25	0.0485 (13)	0.0274 (11)	0.0262 (10)	0.0008 (9)	−0.0030 (9)	0.0004 (8)
N1	0.0312 (9)	0.0327 (10)	0.0285 (9)	−0.0025 (7)	−0.0023 (7)	−0.0033 (7)
N2	0.0317 (9)	0.0307 (9)	0.0271 (8)	0.0010 (7)	−0.0015 (7)	−0.0007 (7)
N3	0.0330 (10)	0.0436 (11)	0.0328 (9)	0.0002 (8)	−0.0015 (8)	−0.0035 (8)
N4	0.0357 (10)	0.0283 (9)	0.0364 (9)	−0.0011 (8)	−0.0008 (8)	0.0014 (7)
N5	0.0347 (10)	0.0272 (9)	0.0363 (9)	−0.0022 (7)	−0.0032 (8)	−0.0008 (7)
O1	0.0303 (8)	0.0470 (9)	0.0256 (7)	−0.0002 (6)	0.0016 (6)	0.0016 (6)
O2	0.0342 (9)	0.1061 (16)	0.0418 (9)	−0.0092 (10)	0.0075 (7)	0.0070 (10)
O3	0.0344 (8)	0.0507 (10)	0.0346 (8)	0.0080 (7)	0.0022 (6)	0.0064 (7)
O1W	0.0404 (10)	0.0616 (13)	0.0760 (13)	−0.0042 (9)	−0.0066 (10)	0.0187 (11)
O2W	0.0421 (10)	0.0761 (13)	0.0402 (10)	−0.0044 (10)	0.0021 (8)	−0.0014 (9)

Geometric parameters (Å, º)

Cu1—O3	1.9191 (15)	C12—C13	1.363 (3)
Cu1—N1	1.9634 (17)	C12—H12	0.9300
Cu1—O1	2.0211 (15)	C13—N3	1.340 (3)
Cu1—N2	2.0584 (16)	C13—C14	1.495 (4)
Cu1—N4	2.2625 (18)	C14—H14A	0.9600
C1—C6	1.404 (3)	C14—H14B	0.9600
C1—C2	1.420 (3)	C14—H14C	0.9600
C1—C7	1.432 (3)	C15—H15A	0.9600
C2—O3	1.310 (2)	C15—H15B	0.9600
C2—C3	1.411 (3)	C15—H15C	0.9600
C3—C4	1.370 (3)	C16—N4	1.336 (3)
C3—H3	0.9300	C16—C17	1.399 (3)
C4—C5	1.381 (4)	C16—C19	1.483 (3)
C4—H4	0.9300	C17—C25	1.362 (3)
C5—C6	1.371 (4)	C17—H17	0.9300
C5—H5	0.9300	C18—C25	1.493 (3)
C6—H6	0.9300	C18—H18A	0.9600
C7—N1	1.279 (3)	C18—H18B	0.9600
C7—H7	0.9300	C18—H18C	0.9600
C8—N1	1.468 (3)	C19—H19A	0.9600
C8—C9	1.511 (3)	C19—H19B	0.9600
C8—H8A	0.9700	C19—H19C	0.9600
C8—H8B	0.9700	C25—N5	1.343 (3)
C9—C10	1.514 (3)	N2—N3	1.357 (2)
C9—H9A	0.9700	N3—H3A	0.8600
C9—H9B	0.9700	N4—N5	1.355 (2)
C10—O2	1.234 (3)	N5—H5A	0.8600
C10—O1	1.267 (2)	O1W—H1WA	0.836 (10)
C11—N2	1.343 (3)	O1W—H1WB	0.839 (10)
C11—C12	1.389 (3)	O2W—H2WA	0.849 (10)
C11—C15	1.483 (3)	O2W—H2WB	0.840 (10)
O3—Cu1—N1	90.03 (7)	C12—C13—C14	131.6 (2)
O3—Cu1—O1	166.22 (7)	C13—C14—H14A	109.5
N1—Cu1—O1	89.65 (6)	C13—C14—H14B	109.5
O3—Cu1—N2	91.13 (7)	H14A—C14—H14B	109.5
N1—Cu1—N2	164.27 (7)	C13—C14—H14C	109.5
O1—Cu1—N2	85.52 (6)	H14A—C14—H14C	109.5
O3—Cu1—N4	106.80 (7)	H14B—C14—H14C	109.5
N1—Cu1—N4	99.76 (7)	C11—C15—H15A	109.5
O1—Cu1—N4	86.82 (6)	C11—C15—H15B	109.5
N2—Cu1—N4	94.91 (6)	H15A—C15—H15B	109.5
C6—C1—C2	119.7 (2)	C11—C15—H15C	109.5
C6—C1—C7	119.0 (2)	H15A—C15—H15C	109.5
C2—C1—C7	121.18 (19)	H15B—C15—H15C	109.5
O3—C2—C3	119.9 (2)	N4—C16—C17	110.2 (2)

O3—C2—C1	123.36 (19)	N4—C16—C19	120.9 (2)
C3—C2—C1	116.7 (2)	C17—C16—C19	128.9 (2)
C4—C3—C2	121.8 (2)	C25—C17—C16	106.40 (19)
C4—C3—H3	119.1	C25—C17—H17	126.8
C2—C3—H3	119.1	C16—C17—H17	126.8
C3—C4—C5	121.2 (2)	C25—C18—H18A	109.5
C3—C4—H4	119.4	C25—C18—H18B	109.5
C5—C4—H4	119.4	H18A—C18—H18B	109.5
C6—C5—C4	118.8 (2)	C25—C18—H18C	109.5
C6—C5—H5	120.6	H18A—C18—H18C	109.5
C4—C5—H5	120.6	H18B—C18—H18C	109.5
C5—C6—C1	121.7 (2)	C16—C19—H19A	109.5
C5—C6—H6	119.2	C16—C19—H19B	109.5
C1—C6—H6	119.2	H19A—C19—H19B	109.5
N1—C7—C1	126.09 (19)	C16—C19—H19C	109.5
N1—C7—H7	117.0	H19A—C19—H19C	109.5
C1—C7—H7	117.0	H19B—C19—H19C	109.5
N1—C8—C9	111.26 (18)	N5—C25—C17	106.07 (19)
N1—C8—H8A	109.4	N5—C25—C18	121.7 (2)
C9—C8—H8A	109.4	C17—C25—C18	132.3 (2)
N1—C8—H8B	109.4	C7—N1—C8	119.03 (17)
C9—C8—H8B	109.4	C7—N1—Cu1	124.89 (15)
H8A—C8—H8B	108.0	C8—N1—Cu1	116.00 (13)
C8—C9—C10	116.01 (18)	C11—N2—N3	104.85 (16)
C8—C9—H9A	108.3	C11—N2—Cu1	137.47 (15)
C10—C9—H9A	108.3	N3—N2—Cu1	117.63 (13)
C8—C9—H9B	108.3	C13—N3—N2	112.44 (18)
C10—C9—H9B	108.3	C13—N3—H3A	123.8
H9A—C9—H9B	107.4	N2—N3—H3A	123.8
O2—C10—O1	123.1 (2)	C16—N4—N5	104.60 (17)
O2—C10—C9	116.86 (19)	C16—N4—Cu1	133.74 (15)
O1—C10—C9	120.03 (19)	N5—N4—Cu1	121.46 (13)
N2—C11—C12	109.6 (2)	C25—N5—N4	112.71 (18)
N2—C11—C15	124.32 (19)	C25—N5—H5A	123.6
C12—C11—C15	126.0 (2)	N4—N5—H5A	123.6
C13—C12—C11	107.2 (2)	C10—O1—Cu1	131.28 (13)
C13—C12—H12	126.4	C2—O3—Cu1	125.34 (14)
C11—C12—H12	126.4	H1WA—O1W—H1WB	110 (3)
N3—C13—C12	105.9 (2)	H2WA—O2W—H2WB	104 (3)
N3—C13—C14	122.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1*W*	0.86	2.25	3.041 (3)	153
N5—H5*A*···O1*W*	0.86	2.09	2.911 (3)	159
O1*W*—H1*WA*···O2*W*^{i}	0.84 (1)	2.05 (1)	2.858 (3)	161 (3)
O2*W*—H2*WB*···O2^{ii}	0.84 (1)	1.90 (1)	2.729 (2)	168 (3)

O2*W*—H2*WA*···O2^{iii}	0.85 (1)	1.96 (1)	2.791 (2)	166 (3)
O1*W*—H1*WB*···O2*W*^{iv}	0.84 (1)	2.03 (1)	2.865 (3)	172 (3)

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+1, y+1/2, -z+3/2$.