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catena-Poly[[[bis(4-aminobenzoato-κO)-copper(II)]-μ-1,1′-(pentane-1,5-diyl)-diimidazole] trihydrate]

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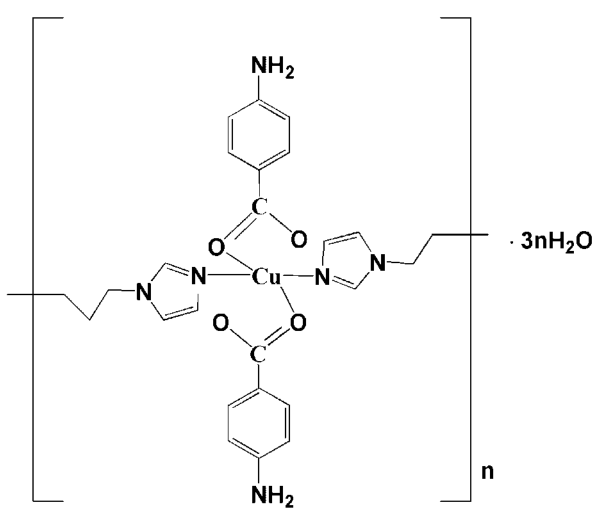
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.095; data-to-parameter ratio = 17.0.

In the title compound, $\{[Cu(C_7H_6NO_2)_2(C_{11}H_{16}N_4)]\cdot 3H_2O\}_n$, each Cu^{II} atom is coordinated by two O atoms from two 4-aminobenzoate anions, and two N atoms from two different 1,1′-(pentane-1,5-diyl)diimidazole (biim-5) ligands, to furnish a distorted square-planar geometry. The biim-5 ligand coordinates to two copper(II) cations, acting as a bridging ligand; as a result the copper(II) cations are connected to form an infinite chain structure. The polymeric chains are linked through a variety of hydrogen bonds to form a three-dimensional structure.

Related literature

For related literature, see: Batten & Robson (1998); Chen & Gao (2002); Ma *et al.* (2000); Moulton & Zaworotko (2001); Tong *et al.* (2002); Yang *et al.* (2005, 2006).



Experimental

Crystal data

$[Cu(C_7H_6NO_2)_2(C_{11}H_{16}N_4)]\cdot 3H_2O$
M_r = 594.12
Monoclinic, $P2_1/n$
a = 13.082 (9) Å
b = 11.151 (1) Å
c = 19.505 (2) Å
β = 93.725 (1)°
V = 2839.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.82 mm^{-1}
T = 293 (2) K
0.68 × 0.45 × 0.38 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.635, T_{max} = 0.746
16576 measured reflections
6488 independent reflections
4988 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.095
S = 1.03
6488 reflections
382 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2W—H2A···O4^{i}	0.86 (3)	2.09 (3)	2.954 (3)	174 (4)
N5—H5A···O1W^{ii}	0.79 (3)	2.32 (3)	3.100 (3)	172 (5)
N6—H6B···O1W^{iii}	0.88 (4)	2.18 (4)	3.046 (3)	170 (5)
O1W—H1A···O2W	0.86 (3)	1.95 (3)	2.805 (3)	172 (5)
O1W—H1B···O4	0.87 (3)	1.96 (3)	2.802 (2)	163 (4)
O2W—H2B···O1	0.94 (3)	2.01 (3)	2.889 (3)	155 (4)
O3W—H3A···O2	0.89 (3)	1.87 (3)	2.734 (3)	164 (4)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SF2009).

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supporting information

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catena-Poly[[[bis(4-aminobenzoato-*κO*)copper(II)]-*µ*-1,1′-(pentane-1,5-diyl)di-imidazole] trihydrate]

Wen-Li Zhang, Lai-Ping Zhang and Jian-Fang Ma

S1. Comment

In recent years, research into coordination polymers has been expanding rapidly because of their fascinating structural diversity and potential application as functional materials (Batten & Robson, 1998; Moulton & Zaworotko, 2001). To date, a number of one-, two- and three-dimensional infinite frameworks have been generated with linear N,*N*′-bidentate spacers (Tong *et al.*, 2002). Much of the work has been focused on coordination polymers with rigid ligands, such as 4,4′-bipyridine, pyrazine and their analogues. In our previous work, we have synthsis some compounds contaning 1,1′-(1,4-butanediyl)bis(imidazole) (Ma *et al.*, 2000; Yang *et al.*, 2006). However, flexible ligands such as 1,1′-(1,5-pentanediyl) bis(imidazole) have not been well explored to date. In the present paper, we report the preparation and crystal structure of three-dimensional supermolecule coordination polymer of compound, (I).

As shown in Fig. 1, each Cu^{II} atom is primarily coordinated by two oxygen atoms from two *para*-aminobenzoate anions, and two nitrogen atoms from two different biim-5 ligands, to furnish a distorted square-planar geometry. The Cu—N distances range from 1.967 (2) to 1.975 (2) Å, which are similar to reported Cu—N distances. The Cu1—O distances of 1.970 (1) and 1.976 (1) Å are also similar to reported Cu—O distances (Yang *et al.*, 2006). The pendant carb-oxy oxygen atoms have weak bonding interactions with the Cu^{II} atom at the axial sites due to the Jahn-Teller effect. The Cu—O distances range from 2.712 to 2.727 Å, which indicated the weak bonding interactions. Each biim-5 ligand coordinates to two Cu^{II} atoms, acting as a bridging ligand and as a result, an one-dimensional chain structure is formed.

The hydrogen bonds in this study have been considered with liberal distance cut-off criteria of 2.5< D···A < 3.0 Å and 120 < D—H···A < 180 °. The selected hydrogen-bond distances and angles are listed in Table 2. It can be seen that there are three H atoms involved in hydrogen bonding in the asymmetric unit, two of which are from amino group and one of which from water molecules. The uncoordinated carboxylate O atoms are also involved in hydrogen bonds and play the role of acceptors. The polymeric chains are connected through various hydrogen bonds to form a three-dimensional structure (Fig. 2).

S2. Experimental

A mixture of $CuCl_2.2H_2O$ (0.171 g, 1 mmol), NaOH (0.08 g, 2 mmol) in water was stirring for 10 min at room temperature, then the $Cu(OH)_2$ solid was filtered. *P*-aminobenzoic acid was added to the $Cu(OH)_2$ suspension in water with stirring. Then biim-5 (0.204 g, 1 mmol) in ethanol was added with stirring for 1 h and blue precipitate was obtained. And then a minimum amount of ammonia (14 *M*) was added to get the blue solution. Suitable blue crystals were obtained from the filtrate after standing at room temperature for several days.

S3. Refinement

All H-atoms bound to carbon were refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C) for aromatic and 0.96 Å, U_{iso} = 1.2U_{eq} (C) for CH_2 group. The amino and aqua hydrogen atoms were located in a difference Fourier map and refined isotropically with U_{iso}(H) = 1.5 U_{eq}(N, O).

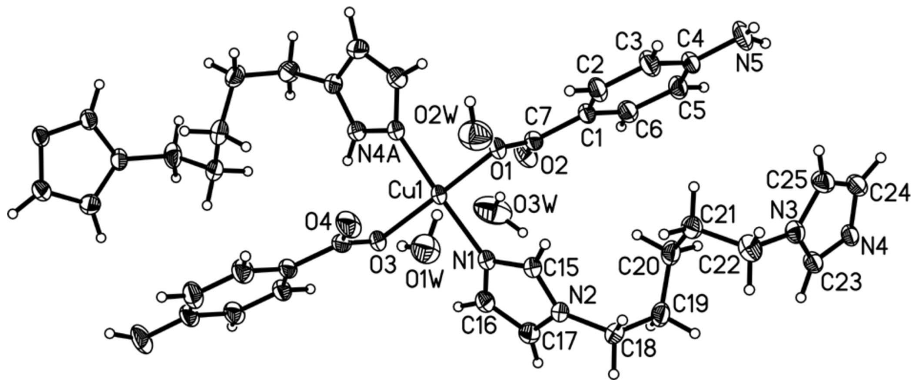

Figure 1

View of the compound (I). Displacement ellipsoids are drawn at the 30% probability level.

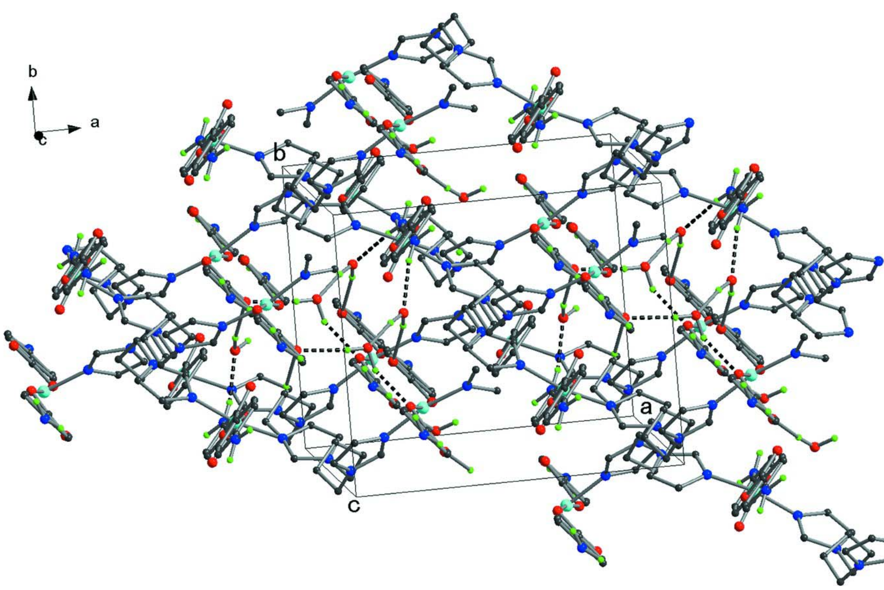

Figure 2

View of the three-dimensional superamolecular structure of (I). The hydrogen bonds are shown as dotted lines. H atoms on the C atoms have been omiited for clarity.

catena-poly[[[bis(4-aminobenzoato-κO)copper(II)]-μ- 1,1′-(pentane-1,5-diyl)diimidazole] trihydrate]

Crystal data

$[Cu(C_7H_6NO_2)_2(C_{11}H_{16}N_4)]\cdot 3H_2O$	β = 93.725 (1)°
M_r = 594.12	V = 2839.3 (4) Å^3
Monoclinic, $P2_1/n$	Z = 4
Hall symbol: -P 2yn	F(000) = 1244
a = 13.082 (9) Å	D_x = 1.390 Mg m^{-3}
b = 11.151 (1) Å	Mo $K\alpha$ radiation, λ = 0.71069 Å
c = 19.505 (2) Å	Cell parameters from 6488 reflections

$\theta = 1.8–28.5°$
$\mu = 0.82\ mm^{-1}$
$T = 293$ K
Block, blue
0.68 × 0.45 × 0.38 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.635$, $T_{max} = 0.746$
16576 measured reflections
6488 independent reflections
4988 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 28.5°$, $\theta_{min} = 1.8°$
$h = -17 \rightarrow 9$
$k = -14 \rightarrow 13$
$l = -25 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.095$
$S = 1.03$
6488 reflections
382 parameters
12 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
$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.6476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

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	0.724906 (17)	0.20985 (2)	0.494309 (9)	0.03977 (9)
C1	0.69874 (15)	0.25416 (18)	0.70179 (8)	0.0414 (4)
C2	0.63431 (17)	0.1687 (2)	0.72737 (9)	0.0515 (5)
H2	0.5989	0.1165	0.6971	0.062*
C3	0.62168 (18)	0.1595 (2)	0.79711 (10)	0.0578 (5)
H3	0.5772	0.1024	0.8131	0.069*
C4	0.67506 (17)	0.2352 (2)	0.84349 (9)	0.0503 (5)
C5	0.74098 (18)	0.32010 (19)	0.81822 (10)	0.0521 (5)
H5	0.7778	0.3708	0.8485	0.063*
C6	0.75202 (17)	0.32954 (18)	0.74842 (10)	0.0480 (4)
H6	0.7958	0.3873	0.7323	0.058*
C7	0.71394 (15)	0.26575 (18)	0.62690 (9)	0.0437 (4)

C8	0.72368 (15)	0.13276 (17)	0.28845 (8)	0.0437 (4)
C9	0.66706 (18)	0.05414 (19)	0.24653 (10)	0.0543 (5)
H9	0.6230	0.0002	0.2659	0.065*
C10	0.6749 (2)	0.0543 (2)	0.17607 (10)	0.0605 (6)
H10	0.6364	0.0002	0.1488	0.073*
C11	0.73957 (18)	0.1343 (2)	0.14575 (9)	0.0531 (5)
C12	0.79721 (18)	0.21209 (19)	0.18774 (10)	0.0531 (5)
H12	0.8418	0.2653	0.1684	0.064*
C13	0.78948 (16)	0.21189 (18)	0.25818 (9)	0.0483 (5)
H13	0.8287	0.2652	0.2855	0.058*
C14	0.71565 (16)	0.1321 (2)	0.36461 (9)	0.0487 (5)
C15	0.88170 (14)	0.07802 (17)	0.58180 (9)	0.0418 (4)
H15	0.8333	0.0438	0.6087	0.050*
C16	0.95172 (16)	0.17479 (19)	0.50186 (10)	0.0484 (5)
H16	0.9602	0.2202	0.4626	0.058*
C17	1.02826 (16)	0.1299 (2)	0.54402 (10)	0.0536 (5)
H17	1.0982	0.1392	0.5396	0.064*
C18	1.03590 (17)	0.0044 (2)	0.65268 (10)	0.0568 (6)
H18A	1.0945	−0.0381	0.6367	0.068*
H18B	0.9898	−0.0544	0.6704	0.068*
C19	1.07186 (15)	0.0899 (2)	0.71027 (10)	0.0565 (5)
H19A	1.1139	0.0454	0.7443	0.068*
H19B	1.1148	0.1509	0.6914	0.068*
C20	0.98658 (16)	0.15138 (19)	0.74596 (10)	0.0529 (5)
H20A	1.0170	0.2083	0.7789	0.063*
H20B	0.9449	0.1964	0.7120	0.063*
C21	0.91748 (15)	0.0677 (2)	0.78300 (10)	0.0549 (5)
H21A	0.8871	0.0110	0.7499	0.066*
H21B	0.8622	0.1146	0.8003	0.066*
C22	0.96906 (17)	−0.00216 (19)	0.84230 (10)	0.0541 (5)
H22A	0.9211	−0.0603	0.8585	0.065*
H22B	1.0269	−0.0458	0.8261	0.065*
C23	1.09798 (15)	0.12327 (18)	0.90985 (9)	0.0438 (4)
H23	1.1518	0.1089	0.8820	0.053*
C24	1.00978 (16)	0.18889 (19)	0.99050 (10)	0.0501 (5)
H24	0.9912	0.2289	1.0296	0.060*
C25	0.94779 (16)	0.1173 (2)	0.95058 (10)	0.0546 (5)
H25	0.8794	0.0999	0.9566	0.065*
N1	0.85934 (12)	0.14264 (14)	0.52616 (7)	0.0413 (3)
N2	0.98308 (12)	0.06823 (15)	0.59449 (7)	0.0443 (4)
N3	1.00482 (12)	0.07559 (14)	0.89960 (7)	0.0429 (4)
N4	1.10431 (12)	0.19343 (14)	0.96448 (7)	0.0422 (4)
N5	0.6617 (2)	0.2274 (2)	0.91329 (9)	0.0714 (6)
N6	0.7484 (2)	0.1342 (2)	0.07524 (9)	0.0745 (7)
O1	0.67388 (10)	0.18549 (13)	0.58642 (6)	0.0461 (3)
O2	0.76375 (14)	0.35143 (14)	0.60610 (7)	0.0639 (4)
O1W	0.69005 (16)	−0.12845 (16)	0.48742 (9)	0.0730 (5)
O3	0.76716 (11)	0.21141 (14)	0.39921 (6)	0.0529 (4)

O2W	0.55952 (17)	−0.03625 (18)	0.58310 (12)	0.0875 (6)
O4	0.65989 (14)	0.05708 (15)	0.39138 (7)	0.0671 (4)
O3W	0.8944 (2)	0.4784 (2)	0.52971 (15)	0.1152 (9)
H5A	0.704 (3)	0.261 (4)	0.937 (2)	0.173*
H5B	0.638 (4)	0.161 (3)	0.927 (2)	0.173*
H6A	0.698 (3)	0.091 (4)	0.051 (2)	0.173*
H6B	0.774 (4)	0.199 (4)	0.058 (2)	0.173*
H1A	0.645 (3)	−0.104 (4)	0.5145 (18)	0.173*
H1B	0.691 (3)	−0.078 (4)	0.4530 (17)	0.173*
H2A	0.496 (2)	−0.038 (4)	0.593 (2)	0.173*
H2B	0.577 (3)	0.045 (3)	0.584 (2)	0.173*
H3A	0.845 (2)	0.436 (4)	0.547 (2)	0.173*
H3B	0.952 (2)	0.449 (4)	0.558 (2)	0.173*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.04202 (14)	0.05555 (15)	0.02164 (11)	0.00707 (10)	0.00120 (8)	0.00176 (9)
C1	0.0499 (11)	0.0473 (10)	0.0272 (8)	0.0124 (9)	0.0031 (8)	0.0012 (7)
C2	0.0583 (12)	0.0659 (13)	0.0305 (9)	−0.0015 (10)	0.0036 (9)	−0.0037 (9)
C3	0.0654 (14)	0.0754 (14)	0.0333 (9)	−0.0059 (12)	0.0091 (9)	0.0021 (10)
C4	0.0611 (13)	0.0621 (13)	0.0282 (8)	0.0174 (10)	0.0062 (9)	−0.0008 (8)
C5	0.0675 (13)	0.0528 (12)	0.0353 (9)	0.0119 (10)	−0.0025 (9)	−0.0088 (8)
C6	0.0589 (12)	0.0454 (10)	0.0397 (9)	0.0064 (9)	0.0047 (9)	−0.0004 (8)
C7	0.0484 (11)	0.0519 (11)	0.0313 (9)	0.0139 (9)	0.0055 (8)	0.0052 (8)
C8	0.0519 (11)	0.0521 (11)	0.0274 (8)	0.0174 (9)	0.0044 (8)	0.0053 (8)
C9	0.0648 (13)	0.0584 (12)	0.0400 (10)	0.0036 (11)	0.0061 (10)	0.0058 (9)
C10	0.0808 (16)	0.0640 (14)	0.0361 (10)	0.0039 (12)	−0.0013 (10)	−0.0023 (10)
C11	0.0728 (14)	0.0586 (12)	0.0281 (8)	0.0209 (11)	0.0048 (9)	0.0041 (8)
C12	0.0677 (14)	0.0582 (12)	0.0346 (9)	0.0090 (10)	0.0111 (9)	0.0085 (9)
C13	0.0572 (12)	0.0550 (12)	0.0327 (9)	0.0100 (10)	0.0038 (8)	0.0013 (8)
C14	0.0523 (11)	0.0641 (13)	0.0302 (9)	0.0259 (10)	0.0063 (8)	0.0084 (9)
C15	0.0431 (10)	0.0515 (10)	0.0308 (8)	0.0052 (8)	0.0017 (7)	0.0023 (8)
C16	0.0497 (11)	0.0607 (12)	0.0354 (9)	0.0012 (10)	0.0068 (8)	0.0043 (9)
C17	0.0410 (10)	0.0758 (14)	0.0446 (10)	0.0005 (10)	0.0069 (9)	−0.0010 (10)
C18	0.0539 (12)	0.0754 (14)	0.0403 (10)	0.0257 (11)	−0.0038 (9)	0.0039 (10)
C19	0.0414 (10)	0.0871 (16)	0.0398 (10)	−0.0031 (11)	−0.0065 (8)	0.0059 (10)
C20	0.0565 (12)	0.0582 (12)	0.0419 (10)	0.0009 (10)	−0.0120 (9)	−0.0039 (9)
C21	0.0413 (10)	0.0783 (14)	0.0442 (10)	−0.0032 (10)	−0.0038 (9)	−0.0154 (10)
C22	0.0603 (13)	0.0522 (12)	0.0496 (11)	−0.0180 (10)	0.0012 (10)	−0.0102 (9)
C23	0.0428 (10)	0.0544 (11)	0.0343 (9)	−0.0051 (9)	0.0036 (8)	−0.0047 (8)
C24	0.0476 (11)	0.0656 (13)	0.0379 (10)	−0.0019 (10)	0.0077 (8)	−0.0067 (9)
C25	0.0414 (10)	0.0752 (14)	0.0479 (11)	−0.0067 (10)	0.0086 (9)	−0.0042 (10)
N1	0.0418 (8)	0.0544 (9)	0.0276 (7)	0.0055 (7)	0.0024 (6)	0.0011 (6)
N2	0.0422 (8)	0.0580 (10)	0.0321 (7)	0.0108 (7)	−0.0011 (6)	0.0000 (7)
N3	0.0445 (8)	0.0481 (9)	0.0358 (7)	−0.0073 (7)	0.0003 (7)	−0.0021 (7)
N4	0.0422 (8)	0.0558 (9)	0.0285 (7)	−0.0049 (7)	0.0018 (6)	−0.0013 (6)
N5	0.0936 (17)	0.0929 (17)	0.0282 (8)	0.0059 (13)	0.0091 (9)	−0.0018 (9)

N6	0.1137 (19)	0.0827 (15)	0.0279 (8)	0.0114 (13)	0.0109 (10)	0.0024 (9)
O1	0.0482 (7)	0.0655 (9)	0.0245 (6)	0.0049 (6)	0.0022 (5)	0.0000 (6)
O2	0.0887 (12)	0.0600 (9)	0.0449 (8)	−0.0038 (9)	0.0186 (8)	0.0064 (7)
O1W	0.0865 (12)	0.0683 (11)	0.0655 (11)	0.0060 (9)	0.0135 (9)	0.0146 (9)
O3	0.0486 (8)	0.0851 (11)	0.0250 (6)	0.0149 (7)	0.0024 (6)	0.0009 (6)
O2W	0.0846 (13)	0.0803 (13)	0.0985 (15)	−0.0034 (11)	0.0133 (12)	−0.0157 (11)
O4	0.0865 (12)	0.0744 (10)	0.0425 (8)	0.0088 (9)	0.0203 (8)	0.0176 (7)
O3W	0.130 (2)	0.0837 (15)	0.140 (2)	0.0016 (14)	0.0703 (18)	0.0213 (14)

Geometric parameters (Å, º)

Cu1—N4^{i}	1.9677 (15)	C17—N2	1.367 (3)
Cu1—O3	1.9698 (12)	C17—H17	0.9300
Cu1—N1	1.9745 (15)	C18—N2	1.473 (2)
Cu1—O1	1.9757 (12)	C18—C19	1.524 (3)
C1—C2	1.387 (3)	C18—H18A	0.9700
C1—C6	1.392 (3)	C18—H18B	0.9700
C1—C7	1.493 (2)	C19—C20	1.517 (3)
C2—C3	1.385 (2)	C19—H19A	0.9700
C2—H2	0.9300	C19—H19B	0.9700
C3—C4	1.391 (3)	C20—C21	1.515 (3)
C3—H3	0.9300	C20—H20A	0.9700
C4—N5	1.387 (2)	C20—H20B	0.9700
C4—C5	1.392 (3)	C21—C22	1.516 (3)
C5—C6	1.382 (3)	C21—H21A	0.9700
C5—H5	0.9300	C21—H21B	0.9700
C6—H6	0.9300	C22—N3	1.467 (2)
C7—O2	1.239 (2)	C22—H22A	0.9700
C7—O1	1.283 (2)	C22—H22B	0.9700
C8—C9	1.381 (3)	C23—N4	1.320 (2)
C8—C13	1.391 (3)	C23—N3	1.333 (2)
C8—C14	1.496 (2)	C23—H23	0.9300
C9—C10	1.385 (3)	C24—C25	1.349 (3)
C9—H9	0.9300	C24—N4	1.368 (2)
C10—C11	1.389 (3)	C24—H24	0.9300
C10—H10	0.9300	C25—N3	1.363 (2)
C11—C12	1.383 (3)	C25—H25	0.9300
C11—N6	1.387 (2)	N4—Cu1^{ii}	1.9677 (15)
C12—C13	1.384 (3)	N5—H5A	0.79 (3)
C12—H12	0.9300	N5—H5B	0.86 (3)
C13—H13	0.9300	N6—H6A	0.92 (3)
C14—O4	1.247 (3)	N6—H6B	0.88 (4)
C14—O3	1.278 (3)	O1W—H1A	0.86 (3)
C15—N1	1.320 (2)	O1W—H1B	0.87 (3)
C15—N2	1.338 (2)	O2W—H2A	0.86 (3)
C15—H15	0.9300	O2W—H2B	0.94 (3)
C16—C17	1.350 (3)	O3W—H3A	0.89 (3)
C16—N1	1.374 (2)	O3W—H3B	0.97 (3)

C16—H16	0.9300

N4^{i}—Cu1—O3	89.16 (6)	N2—C18—H18B	109.2
N4^{i}—Cu1—N1	169.04 (7)	C19—C18—H18B	109.2
O3—Cu1—N1	90.06 (6)	H18A—C18—H18B	107.9
N4^{i}—Cu1—O1	91.86 (6)	C20—C19—C18	114.84 (17)
O3—Cu1—O1	171.77 (6)	C20—C19—H19A	108.6
N1—Cu1—O1	90.48 (6)	C18—C19—H19A	108.6
C2—C1—C6	118.06 (16)	C20—C19—H19B	108.6
C2—C1—C7	122.31 (17)	C18—C19—H19B	108.6
C6—C1—C7	119.62 (18)	H19A—C19—H19B	107.5
C3—C2—C1	121.22 (19)	C21—C20—C19	114.83 (18)
C3—C2—H2	119.4	C21—C20—H20A	108.6
C1—C2—H2	119.4	C19—C20—H20A	108.6
C2—C3—C4	120.5 (2)	C21—C20—H20B	108.6
C2—C3—H3	119.8	C19—C20—H20B	108.6
C4—C3—H3	119.8	H20A—C20—H20B	107.5
N5—C4—C3	120.7 (2)	C20—C21—C22	115.50 (17)
N5—C4—C5	120.7 (2)	C20—C21—H21A	108.4
C3—C4—C5	118.60 (17)	C22—C21—H21A	108.4
C6—C5—C4	120.47 (19)	C20—C21—H21B	108.4
C6—C5—H5	119.8	C22—C21—H21B	108.4
C4—C5—H5	119.8	H21A—C21—H21B	107.5
C5—C6—C1	121.2 (2)	N3—C22—C21	112.43 (17)
C5—C6—H6	119.4	N3—C22—H22A	109.1
C1—C6—H6	119.4	C21—C22—H22A	109.1
O2—C7—O1	122.61 (16)	N3—C22—H22B	109.1
O2—C7—C1	119.56 (18)	C21—C22—H22B	109.1
O1—C7—C1	117.83 (17)	H22A—C22—H22B	107.8
C9—C8—C13	118.32 (17)	N4—C23—N3	111.48 (16)
C9—C8—C14	121.02 (19)	N4—C23—H23	124.3
C13—C8—C14	120.66 (19)	N3—C23—H23	124.3
C8—C9—C10	121.0 (2)	C25—C24—N4	109.38 (17)
C8—C9—H9	119.5	C25—C24—H24	125.3
C10—C9—H9	119.5	N4—C24—H24	125.3
C9—C10—C11	120.6 (2)	C24—C25—N3	106.62 (17)
C9—C10—H10	119.7	C24—C25—H25	126.7
C11—C10—H10	119.7	N3—C25—H25	126.7
C12—C11—N6	120.7 (2)	C15—N1—C16	105.85 (16)
C12—C11—C10	118.36 (17)	C15—N1—Cu1	127.69 (13)
N6—C11—C10	120.9 (2)	C16—N1—Cu1	125.30 (13)
C11—C12—C13	121.0 (2)	C15—N2—C17	107.20 (15)
C11—C12—H12	119.5	C15—N2—C18	126.28 (17)
C13—C12—H12	119.5	C17—N2—C18	126.52 (17)
C12—C13—C8	120.6 (2)	C23—N3—C25	107.03 (16)
C12—C13—H13	119.7	C23—N3—C22	126.39 (16)
C8—C13—H13	119.7	C25—N3—C22	126.51 (17)
O4—C14—O3	123.10 (17)	C23—N4—C24	105.47 (16)

O4—C14—C8	120.0 (2)	C23—N4—Cu1^{ii}	124.79 (13)
O3—C14—C8	116.91 (18)	C24—N4—Cu1^{ii}	129.60 (13)
N1—C15—N2	111.15 (16)	C4—N5—H5A	114 (4)
N1—C15—H15	124.4	C4—N5—H5B	116 (3)
N2—C15—H15	124.4	H5A—N5—H5B	119 (4)
C17—C16—N1	109.12 (17)	C11—N6—H6A	114 (3)
C17—C16—H16	125.4	C11—N6—H6B	116 (3)
N1—C16—H16	125.4	H6A—N6—H6B	122 (4)
C16—C17—N2	106.67 (17)	C7—O1—Cu1	108.37 (12)
C16—C17—H17	126.7	H1A—O1W—H1B	108 (3)
N2—C17—H17	126.7	C14—O3—Cu1	108.70 (12)
N2—C18—C19	111.85 (18)	H2A—O2W—H2B	105 (3)
N2—C18—H18A	109.2	H3A—O3W—H3B	99 (3)
C19—C18—H18A	109.2		

C6—C1—C2—C3	1.1 (3)	N2—C15—N1—C16	0.5 (2)
C7—C1—C2—C3	179.84 (19)	N2—C15—N1—Cu1	−167.55 (13)
C1—C2—C3—C4	−1.1 (3)	C17—C16—N1—C15	−0.8 (2)
C2—C3—C4—N5	179.2 (2)	C17—C16—N1—Cu1	167.69 (14)
C2—C3—C4—C5	0.2 (3)	N4^{i}—Cu1—N1—C15	119.0 (3)
N5—C4—C5—C6	−178.3 (2)	O3—Cu1—N1—C15	−155.13 (17)
C3—C4—C5—C6	0.7 (3)	O1—Cu1—N1—C15	16.65 (17)
C4—C5—C6—C1	−0.6 (3)	N4^{i}—Cu1—N1—C16	−46.9 (4)
C2—C1—C6—C5	−0.2 (3)	O3—Cu1—N1—C16	38.96 (16)
C7—C1—C6—C5	−179.02 (18)	O1—Cu1—N1—C16	−149.25 (16)
C2—C1—C7—O2	172.4 (2)	N1—C15—N2—C17	−0.1 (2)
C6—C1—C7—O2	−8.8 (3)	N1—C15—N2—C18	179.02 (18)
C2—C1—C7—O1	−7.3 (3)	C16—C17—N2—C15	−0.4 (2)
C6—C1—C7—O1	171.39 (18)	C16—C17—N2—C18	−179.49 (19)
C13—C8—C9—C10	−0.4 (3)	C19—C18—N2—C15	−99.2 (2)
C14—C8—C9—C10	−179.67 (19)	C19—C18—N2—C17	79.8 (2)
C8—C9—C10—C11	−0.4 (3)	N4—C23—N3—C25	0.0 (2)
C9—C10—C11—C12	1.2 (3)	N4—C23—N3—C22	177.13 (18)
C9—C10—C11—N6	179.4 (2)	C24—C25—N3—C23	−0.5 (2)
N6—C11—C12—C13	−179.4 (2)	C24—C25—N3—C22	−177.63 (19)
C10—C11—C12—C13	−1.1 (3)	C21—C22—N3—C23	−93.1 (2)
C11—C12—C13—C8	0.3 (3)	C21—C22—N3—C25	83.5 (2)
C9—C8—C13—C12	0.5 (3)	N3—C23—N4—C24	0.5 (2)
C14—C8—C13—C12	179.72 (17)	N3—C23—N4—Cu1^{ii}	−175.54 (12)
C9—C8—C14—O4	2.5 (3)	C25—C24—N4—C23	−0.8 (2)
C13—C8—C14—O4	−176.73 (18)	C25—C24—N4—Cu1^{ii}	174.99 (15)
C9—C8—C14—O3	−176.92 (18)	O2—C7—O1—Cu1	9.2 (2)
C13—C8—C14—O3	3.8 (3)	C1—C7—O1—Cu1	−171.10 (13)
N1—C16—C17—N2	0.7 (2)	N4^{i}—Cu1—O1—C7	−94.66 (13)
N2—C18—C19—C20	65.9 (2)	N1—Cu1—O1—C7	74.64 (13)
C18—C19—C20—C21	62.9 (2)	O4—C14—O3—Cu1	−9.3 (2)
C19—C20—C21—C22	63.4 (2)	C8—C14—O3—Cu1	170.13 (12)

C20—C21—C22—N3	66.3 (2)	N4^{i}—Cu1—O3—C14	−80.43 (13)
N4—C24—C25—N3	0.8 (2)	N1—Cu1—O3—C14	110.50 (13)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*W*—H2*A*···O4^{iii}	0.86 (3)	2.09 (3)	2.954 (3)	174 (4)
N5—H5*A*···O1*W*^{iv}	0.79 (3)	2.32 (3)	3.100 (3)	172 (5)
N6—H6*B*···O1*W*^{v}	0.88 (4)	2.18 (4)	3.046 (3)	170 (5)
O1*W*—H1*A*···O2*W*	0.86 (3)	1.95 (3)	2.805 (3)	172 (5)
O1*W*—H1*B*···O4	0.87 (3)	1.96 (3)	2.802 (2)	163 (4)
O2*W*—H2*B*···O1	0.94 (3)	2.01 (3)	2.889 (3)	155 (4)
O3*W*—H3*A*···O2	0.89 (3)	1.87 (3)	2.734 (3)	164 (4)

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