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Aqua(azido)(μ-azido)bis{2-[(2-dimethylaminoethylimino)methyl]-6-methoxyphenolato}dicopper(II) monohydrate

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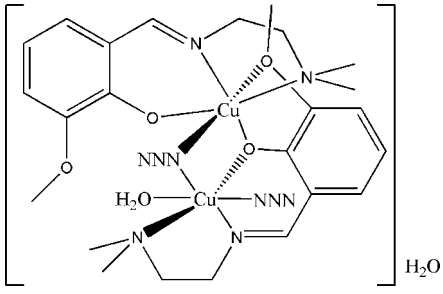
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.066; wR factor = 0.177; data-to-parameter ratio = 17.6.

The asymmetric unit of the title compound, $[Cu_2(C_{12}H_{17}N_2O_2)_2(N_3)(\mu\text{-}N_3)(H_2O)]\cdot H_2O$, consists of a dinuclear complex molecule and a solvent water molecule. One Cu atom is six-coordinated by the phenol O atom and by one imine and one amine N atoms from one Schiff base ligand, the phenol and ether O atoms of the second Schiff base, together with a terminal N atom of the bridging azide ligand, in an octahedral geometry. The coordination environment of the second Cu atom contains a phenol O and imine and amine N atoms from one Schiff base ligand, two further N atoms, one from the bridging and the other from a terminal azide ligand, and a coordinated water molecule, also in an octahedral geometry. The crystal structure involves O—H···N and O—H···O hydrogen bonds.

Related literature

For background on the chemistry of polynuclear complexes, see: Eshel *et al.* (2000); Jiang *et al.* (2005); Escuer *et al.* (2000); El-Behairy *et al.* (1997); Manhas *et al.* (2005). For their biological activity, see: Brückner *et al.* (2000); Harrop *et al.* (2003); Ren *et al.* (2002). For polynuclear complexes involving bridging ligands, see: Salem (2005); Dohlakiya & Patel (2005); Dey *et al.* (2004). For a related structure, see: Diao (2007).



Experimental

Crystal data

$[Cu_2(C_{12}H_{17}N_2O_2)_2(N_3)_2(H_2O)]\cdot H_2O$
M_r = 689.72
Monoclinic, $P2_1/c$
a = 16.232 (3) Å
b = 13.540 (2) Å
c = 13.997 (3) Å
β = 105.821 (2)°
V = 2959.7 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.49 mm^{-1}
T = 293 (2) K
0.45 × 0.40 × 0.38 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.553, T_{max} = 0.601
(expected range = 0.522–0.567)
25203 measured reflections
6982 independent reflections
4183 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.178
S = 1.02
6982 reflections
397 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5W—H5WB···N10^{i}	0.86 (6)	2.69 (4)	3.481 (8)	155 (8)
O5W—H5WA···O1	0.86 (6)	2.59 (6)	3.129 (5)	122 (6)
O5W—H5WA···O2	0.86 (6)	1.86 (6)	2.702 (4)	167 (8)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: SJ2351).

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supplementary materials

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Aqua(azido)(μ-azido)bis{2-[(2-dimethylaminoethylimino)methyl]-6-methoxyphenolato}dicopper(II) monohydrate

Y.-P. Diao and K. Li

Comment

Polynuclear complexes play an important role in the development of coordination chemistry (Eshel *et al.*, 2000; Jiang *et al.*, 2005; Escuer *et al.*, 2000; El-Behairy *et al.*, 1997; Manhas *et al.*, 2005). Some of the complexes have been found to have pharmacological and antitumor properties (Brückner *et al.*, 2000; Harrop *et al.*, 2003; Ren *et al.*, 2002). A prime strategy for designing these molecular materials is to use suitable bridging ligands (Salem, 2005; Dohlakiya & Patel, 2005; Dey *et al.*, 2004). The azide ligand displays a number of coordination modes and has become one of the most extensively studied building blocks in the field. We recently reported the structure of an azide-bridged polynuclear copper(II) complex (Diao, 2007) and we report herein the crystal structure of the related title complex (I), Fig 1.

The complex is an azide-bridged dinuclear copper(II) complex. One Cu atom is six-coordinated by the phenolic O atom, one imine, and one amine N atoms from one Schiff base ligand, the phenolic and ether O atoms of the second Schiff base, together with a terminal N atom of the bridging azide ligand, in an octahedral geometry. The coordination sphere of the second Cu atom contains a phenolic O, imine and amine N atoms from one Schiff base ligand, two N atoms one from the bridging and the other from a terminal azide ligand, and a coordinated water molecule, also in an octahedral geometry.

Experimental

2-Hydroxy-3-methoxybenzaldehyde (0.2 mmol, 30.5 mg), *N*,*N*-dimethylethane-1,2-diamine (0.2 mmol, 17.5 mg), NaN_3 (0.2 mmol, 13.0 mg), and $Cu(CH_3COO)_2{\cdot}H_2O$ (0.2 mmol, 40.0 mg) were dissolved in an 95% ethanol solution (30 ml). The mixture was stirred at room temperature for 30 min to give a deep blue solution. After keeping the solution in air for a few days, deep blue crystals were formed.

Refinement

The crystals were very weakly diffracting and few high angle reflections were obtained. This explains the low measured fraction of data in this determination. Water H atoms were located from a difference Fourier map and refined isotropically. All other H atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, $U_{iso} = 1.2U_{eq}$ (C) for aromatic, 0.97 Å, $U_{iso} = 1.2U_{eq}$ (C) for CH_2 and 0.96 Å, $U_{iso} = 1.5U_{eq}$ (C) for CH_3 atoms.

Figures

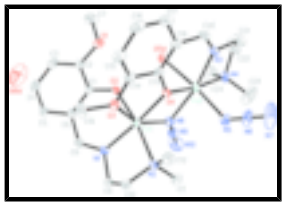


Fig. 1. The structure of the complex with displacement parameters drawn at the 30% probability level. Hydrogen atoms have been omitted for clarity.

Aqua(azido)(μ-azido)bis{2-[(2-dimethylaminoethylimino)methyl]- 6-methoxyphenolato}dicopper(II) monohydrate

Crystal data

$[Cu_2(C_{12}H_{17}N_2O_2)_2(N_3)_2(H_2O)]\cdot H_2O$	$F_{000} = 1432$
$M_r = 689.72$	$D_x = 1.548$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2127 reflections
$a = 16.232$ (3) Å	$\theta = 2.4$–$25.3°$
$b = 13.540$ (2) Å	$\mu = 1.49$ mm^{-1}
$c = 13.997$ (3) Å	$T = 293$ (2) K
$\beta = 105.821$ (2)°	Block, deep blue
$V = 2959.7$ (9) Å^3	0.45 × 0.40 × 0.38 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	6982 independent reflections
Radiation source: fine-focus sealed tube	4183 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.083$
$T = 293(2)$ K	$\theta_{max} = 28.3°$
ω scans	$\theta_{min} = 1.3°$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -20\rightarrow20$
$T_{min} = 0.553$, $T_{max} = 0.601$	$k = -17\rightarrow18$
25203 measured reflections	$l = -18\rightarrow18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.066$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.178$	$w = 1/[\sigma^2(F_o^2) + (0.082P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
6982 reflections	$\Delta\rho_{max}$ = 0.85 e Å^{-3}
397 parameters	$\Delta\rho_{min}$ = −0.53 e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.22488 (4)	0.59328 (4)	0.30915 (4)	0.03150 (18)
Cu2	0.28782 (4)	0.41861 (4)	0.46588 (4)	0.03647 (19)
O1	0.3838 (2)	0.7739 (2)	0.5713 (2)	0.0438 (9)
O2	0.2983 (2)	0.6832 (2)	0.4120 (2)	0.0352 (8)
O3	0.1096 (2)	0.6710 (2)	0.3377 (2)	0.0392 (8)
O4	0.19356 (19)	0.5165 (2)	0.4158 (2)	0.0304 (7)
O5W	0.3560 (2)	0.5452 (2)	0.5539 (3)	0.0452 (9)
O6W	0.1580 (5)	0.9882 (5)	0.3801 (7)	0.138 (3)
N1	0.2379 (2)	0.6839 (3)	0.2025 (3)	0.0325 (9)
N2	0.1402 (2)	0.5160 (3)	0.1842 (3)	0.0353 (9)
N3	0.2400 (3)	0.3880 (3)	0.5808 (3)	0.0411 (10)
N4	0.3881 (3)	0.3180 (3)	0.5377 (3)	0.0473 (11)
N5	0.2209 (4)	0.3096 (4)	0.3707 (3)	0.0614 (14)
N6	0.1723 (3)	0.2499 (4)	0.3811 (4)	0.0616 (14)
N7	0.1258 (4)	0.1903 (5)	0.3929 (7)	0.134 (3)
N8	0.3252 (3)	0.4832 (3)	0.3445 (3)	0.0370 (9)
N9	0.3824 (3)	0.4609 (3)	0.3142 (3)	0.0497 (11)
N10	0.4393 (4)	0.4366 (5)	0.2847 (5)	0.094 (2)
C1	0.3224 (3)	0.7735 (3)	0.3996 (3)	0.0292 (10)
C2	0.3684 (3)	0.8273 (3)	0.4848 (4)	0.0358 (11)
C3	0.3930 (3)	0.9227 (4)	0.4769 (4)	0.0477 (13)
H3	0.4214	0.9571	0.5338	0.057*
C4	0.3763 (4)	0.9686 (4)	0.3858 (5)	0.0549 (15)
H4	0.3930	1.0338	0.3816	0.066*
C5	0.3355 (4)	0.9186 (3)	0.3019 (4)	0.0473 (13)
H5	0.3256	0.9496	0.2406	0.057*

C6	0.3079 (3)	0.8201 (3)	0.3068 (4)	0.0345 (11)
C7	0.4359 (4)	0.8197 (5)	0.6593 (4)	0.0646 (18)
H7A	0.4902	0.8373	0.6493	0.097*
H7B	0.4446	0.7744	0.7139	0.097*
H7C	0.4078	0.8780	0.6736	0.097*
C8	0.2659 (3)	0.7731 (3)	0.2133 (3)	0.0351 (11)
H8	0.2585	0.8108	0.1560	0.042*
C9	0.1970 (3)	0.6477 (4)	0.1016 (3)	0.0418 (12)
H9A	0.2359	0.6047	0.0793	0.050*
H9B	0.1819	0.7027	0.0558	0.050*
C10	0.1179 (3)	0.5917 (4)	0.1052 (4)	0.0413 (12)
H10A	0.0760	0.6370	0.1184	0.050*
H10B	0.0929	0.5603	0.0416	0.050*
C11	0.1836 (4)	0.4311 (4)	0.1517 (4)	0.0564 (16)
H11A	0.1454	0.4007	0.0947	0.085*
H11B	0.1999	0.3838	0.2046	0.085*
H11C	0.2338	0.4540	0.1347	0.085*
C12	0.0606 (4)	0.4801 (4)	0.2041 (4)	0.0552 (15)
H12A	0.0330	0.5336	0.2282	0.083*
H12B	0.0740	0.4287	0.2531	0.083*
H12C	0.0229	0.4546	0.1439	0.083*
C13	0.1423 (3)	0.5545 (3)	0.4650 (3)	0.0301 (10)
C14	0.0934 (3)	0.6376 (3)	0.4233 (3)	0.0341 (11)
C15	0.0346 (3)	0.6781 (4)	0.4664 (4)	0.0455 (13)
H15	0.0013	0.7313	0.4363	0.055*
C16	0.0250 (3)	0.6399 (5)	0.5546 (4)	0.0545 (16)
H16	−0.0147	0.6676	0.5837	0.065*
C17	0.0733 (3)	0.5619 (5)	0.5986 (4)	0.0510 (14)
H17	0.0671	0.5379	0.6584	0.061*
C18	0.1334 (3)	0.5161 (4)	0.5550 (4)	0.0404 (12)
C19	0.0756 (4)	0.7652 (4)	0.2999 (5)	0.0628 (17)
H19A	0.0143	0.7616	0.2785	0.094*
H19B	0.0970	0.7830	0.2447	0.094*
H19C	0.0928	0.8140	0.3512	0.094*
C20	0.1824 (3)	0.4335 (4)	0.6068 (4)	0.0444 (13)
H20	0.1701	0.4122	0.6645	0.053*
C21	0.2859 (4)	0.3068 (5)	0.6420 (5)	0.0649 (18)
H21A	0.2825	0.3137	0.7098	0.078*
H21B	0.2604	0.2440	0.6163	0.078*
C22	0.3736 (5)	0.3103 (6)	0.6392 (6)	0.089 (2)
H22A	0.4022	0.2512	0.6711	0.107*
H22B	0.4009	0.3664	0.6783	0.107*
C23	0.4751 (4)	0.3570 (5)	0.5539 (6)	0.087 (2)
H23A	0.5143	0.3174	0.6027	0.130*
H23B	0.4769	0.4239	0.5770	0.130*
H23C	0.4909	0.3551	0.4927	0.130*
C24	0.3826 (6)	0.2214 (5)	0.4905 (7)	0.121 (4)
H24A	0.3864	0.2290	0.4237	0.182*
H24B	0.3289	0.1911	0.4896	0.182*

H24C	0.4287	0.1805	0.5271	0.182*
H5WA	0.339 (5)	0.595 (4)	0.516 (5)	0.146*
H5WB	0.398 (4)	0.564 (5)	0.603 (4)	0.146*
H6WB	0.193 (5)	0.960 (5)	0.351 (7)	0.146*
H6WA	0.163 (6)	1.0516 (10)	0.377 (8)	0.146*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0369 (3)	0.0282 (3)	0.0286 (3)	−0.0004 (2)	0.0074 (2)	0.0004 (2)
Cu2	0.0433 (4)	0.0298 (3)	0.0350 (3)	0.0013 (3)	0.0084 (3)	0.0036 (2)
O1	0.047 (2)	0.045 (2)	0.0332 (19)	−0.0109 (16)	0.0007 (16)	−0.0076 (16)
O2	0.0448 (19)	0.0294 (17)	0.0280 (17)	−0.0084 (14)	0.0039 (15)	0.0026 (14)
O3	0.0408 (19)	0.0353 (18)	0.042 (2)	0.0120 (15)	0.0128 (16)	0.0020 (15)
O4	0.0332 (17)	0.0309 (17)	0.0282 (17)	0.0033 (13)	0.0104 (14)	0.0050 (13)
O5W	0.054 (2)	0.037 (2)	0.038 (2)	−0.0076 (17)	0.0005 (17)	0.0050 (16)
O6W	0.136 (6)	0.104 (5)	0.193 (8)	−0.007 (5)	0.078 (5)	−0.027 (6)
N1	0.035 (2)	0.031 (2)	0.029 (2)	0.0001 (17)	0.0049 (17)	0.0046 (16)
N2	0.044 (2)	0.033 (2)	0.026 (2)	−0.0020 (18)	0.0043 (18)	−0.0004 (17)
N3	0.054 (3)	0.036 (2)	0.033 (2)	−0.004 (2)	0.011 (2)	0.0099 (18)
N4	0.053 (3)	0.038 (2)	0.045 (3)	0.009 (2)	0.005 (2)	0.010 (2)
N5	0.088 (4)	0.041 (3)	0.044 (3)	−0.011 (3)	0.000 (3)	−0.003 (2)
N6	0.046 (3)	0.037 (3)	0.088 (4)	0.005 (2)	−0.004 (3)	0.001 (3)
N7	0.075 (5)	0.067 (5)	0.252 (10)	−0.018 (4)	0.034 (6)	0.017 (6)
N8	0.038 (2)	0.037 (2)	0.040 (2)	0.0066 (18)	0.017 (2)	0.0013 (18)
N9	0.059 (3)	0.040 (3)	0.055 (3)	0.005 (2)	0.023 (3)	0.003 (2)
N10	0.103 (5)	0.099 (5)	0.103 (5)	0.030 (4)	0.067 (4)	0.012 (4)
C1	0.026 (2)	0.025 (2)	0.036 (3)	0.0001 (18)	0.008 (2)	−0.0030 (19)
C2	0.039 (3)	0.032 (3)	0.037 (3)	0.000 (2)	0.011 (2)	−0.001 (2)
C3	0.049 (3)	0.038 (3)	0.053 (3)	−0.013 (2)	0.008 (3)	−0.014 (3)
C4	0.068 (4)	0.031 (3)	0.068 (4)	−0.016 (3)	0.022 (3)	−0.005 (3)
C5	0.064 (4)	0.032 (3)	0.051 (3)	−0.005 (2)	0.024 (3)	0.007 (2)
C6	0.036 (3)	0.026 (2)	0.041 (3)	−0.002 (2)	0.011 (2)	0.002 (2)
C7	0.057 (4)	0.087 (5)	0.041 (3)	−0.030 (3)	−0.003 (3)	−0.006 (3)
C8	0.038 (3)	0.036 (3)	0.034 (3)	0.002 (2)	0.014 (2)	0.006 (2)
C9	0.058 (3)	0.039 (3)	0.028 (3)	−0.006 (2)	0.011 (2)	0.003 (2)
C10	0.044 (3)	0.048 (3)	0.029 (2)	0.000 (2)	0.003 (2)	−0.002 (2)
C11	0.083 (5)	0.040 (3)	0.039 (3)	0.004 (3)	0.005 (3)	−0.008 (2)
C12	0.052 (3)	0.058 (4)	0.050 (3)	−0.024 (3)	0.006 (3)	−0.003 (3)
C13	0.024 (2)	0.036 (3)	0.029 (2)	−0.0091 (19)	0.0049 (19)	−0.009 (2)
C14	0.030 (2)	0.038 (3)	0.033 (3)	−0.005 (2)	0.005 (2)	−0.010 (2)
C15	0.032 (3)	0.050 (3)	0.056 (4)	−0.002 (2)	0.014 (3)	−0.016 (3)
C16	0.043 (3)	0.070 (4)	0.057 (4)	−0.006 (3)	0.024 (3)	−0.025 (3)
C17	0.044 (3)	0.075 (4)	0.038 (3)	−0.015 (3)	0.018 (3)	−0.015 (3)
C18	0.036 (3)	0.050 (3)	0.039 (3)	−0.015 (2)	0.016 (2)	−0.011 (2)
C19	0.073 (4)	0.049 (4)	0.065 (4)	0.027 (3)	0.016 (3)	0.015 (3)
C20	0.047 (3)	0.056 (3)	0.031 (3)	−0.018 (3)	0.012 (2)	0.004 (2)
C21	0.080 (5)	0.062 (4)	0.057 (4)	0.004 (3)	0.025 (4)	0.028 (3)

C22	0.087 (6)	0.089 (6)	0.086 (6)	0.028 (4)	0.013 (4)	0.050 (4)
C23	0.047 (4)	0.071 (5)	0.139 (7)	0.019 (3)	0.018 (4)	0.016 (5)
C24	0.122 (7)	0.062 (5)	0.142 (8)	0.048 (5)	−0.027 (6)	−0.029 (5)

Geometric parameters (Å, °)

Cu1—N1	1.987 (4)	C5—C6	1.414 (6)
Cu1—O4	1.995 (3)	C5—H5	0.9300
Cu1—O2	2.010 (3)	C6—C8	1.448 (6)
Cu1—N8	2.163 (4)	C7—H7A	0.9600
Cu1—N2	2.176 (4)	C7—H7B	0.9600
Cu1—O3	2.275 (3)	C7—H7C	0.9600
Cu2—O4	2.001 (3)	C8—H8	0.9300
Cu2—N3	2.010 (4)	C9—C10	1.503 (7)
Cu2—N5	2.085 (5)	C9—H9A	0.9700
Cu2—N8	2.140 (4)	C9—H9B	0.9700
Cu2—N4	2.150 (4)	C10—H10A	0.9700
Cu2—O5W	2.222 (3)	C10—H10B	0.9700
O1—C2	1.373 (6)	C11—H11A	0.9600
O1—C7	1.431 (6)	C11—H11B	0.9600
O2—C1	1.310 (5)	C11—H11C	0.9600
O3—C14	1.372 (6)	C12—H12A	0.9600
O3—C19	1.432 (6)	C12—H12B	0.9600
O4—C13	1.319 (5)	C12—H12C	0.9600
O5W—H5WA	0.86 (6)	C13—C18	1.407 (6)
O5W—H5WB	0.86 (6)	C13—C14	1.409 (7)
O6W—H6WB	0.87 (8)	C14—C15	1.373 (6)
O6W—H6WA	0.866 (10)	C15—C16	1.387 (7)
N1—C8	1.285 (6)	C15—H15	0.9300
N1—C9	1.472 (6)	C16—C17	1.358 (8)
N2—C12	1.476 (6)	C16—H16	0.9300
N2—C10	1.478 (6)	C17—C18	1.425 (7)
N2—C11	1.483 (6)	C17—H17	0.9300
N3—C20	1.253 (7)	C18—C20	1.448 (7)
N3—C21	1.467 (7)	C19—H19A	0.9600
N4—C24	1.456 (8)	C19—H19B	0.9600
N4—C23	1.466 (7)	C19—H19C	0.9600
N4—C22	1.506 (8)	C20—H20	0.9300
N5—N6	1.166 (7)	C21—C22	1.437 (9)
N6—N7	1.146 (7)	C21—H21A	0.9700
N8—N9	1.161 (6)	C21—H21B	0.9700
N9—N10	1.157 (7)	C22—H22A	0.9700
C1—C6	1.405 (6)	C22—H22B	0.9700
C1—C2	1.422 (6)	C23—H23A	0.9600
C2—C3	1.366 (6)	C23—H23B	0.9600
C3—C4	1.377 (8)	C23—H23C	0.9600
C3—H3	0.9300	C24—H24A	0.9600
C4—C5	1.360 (7)	C24—H24B	0.9600
C4—H4	0.9300	C24—H24C	0.9600

N1—Cu1—O4	169.90 (14)	O1—C7—H7A	109.5
N1—Cu1—O2	90.00 (14)	O1—C7—H7B	109.5
O4—Cu1—O2	90.10 (12)	H7A—C7—H7B	109.5
N1—Cu1—N8	111.68 (15)	O1—C7—H7C	109.5
O4—Cu1—N8	78.43 (14)	H7A—C7—H7C	109.5
O2—Cu1—N8	89.51 (14)	H7B—C7—H7C	109.5
N1—Cu1—N2	82.33 (15)	N1—C8—C6	125.7 (4)
O4—Cu1—N2	96.73 (13)	N1—C8—H8	117.1
O2—Cu1—N2	171.31 (13)	C6—C8—H8	117.1
N8—Cu1—N2	97.11 (15)	N1—C9—C10	107.5 (4)
N1—Cu1—O3	96.18 (14)	N1—C9—H9A	110.2
O4—Cu1—O3	73.73 (12)	C10—C9—H9A	110.2
O2—Cu1—O3	87.11 (13)	N1—C9—H9B	110.2
N8—Cu1—O3	151.94 (14)	C10—C9—H9B	110.2
N2—Cu1—O3	89.64 (14)	H9A—C9—H9B	108.5
O4—Cu2—N3	89.51 (15)	N2—C10—C9	109.8 (4)
O4—Cu2—N5	91.72 (17)	N2—C10—H10A	109.7
N3—Cu2—N5	96.77 (19)	C9—C10—H10A	109.7
O4—Cu2—N8	78.84 (13)	N2—C10—H10B	109.7
N3—Cu2—N8	166.90 (16)	C9—C10—H10B	109.7
N5—Cu2—N8	89.60 (18)	H10A—C10—H10B	108.2
O4—Cu2—N4	172.95 (15)	N2—C11—H11A	109.5
N3—Cu2—N4	84.47 (17)	N2—C11—H11B	109.5
N5—Cu2—N4	92.64 (19)	H11A—C11—H11B	109.5
N8—Cu2—N4	106.72 (16)	N2—C11—H11C	109.5
O4—Cu2—O5W	84.30 (13)	H11A—C11—H11C	109.5
N3—Cu2—O5W	87.57 (15)	H11B—C11—H11C	109.5
N5—Cu2—O5W	174.10 (16)	N2—C12—H12A	109.5
N8—Cu2—O5W	85.36 (14)	N2—C12—H12B	109.5
N4—Cu2—O5W	91.76 (15)	H12A—C12—H12B	109.5
C2—O1—C7	117.0 (4)	N2—C12—H12C	109.5
C1—O2—Cu1	127.7 (3)	H12A—C12—H12C	109.5
C14—O3—C19	118.0 (4)	H12B—C12—H12C	109.5
C14—O3—Cu1	111.4 (3)	O4—C13—C18	123.9 (4)
C19—O3—Cu1	126.8 (3)	O4—C13—C14	117.4 (4)
C13—O4—Cu1	120.9 (3)	C18—C13—C14	118.8 (4)
C13—O4—Cu2	127.3 (3)	O3—C14—C15	125.0 (5)
Cu1—O4—Cu2	106.29 (14)	O3—C14—C13	113.8 (4)
Cu2—O5W—H5WA	104 (5)	C15—C14—C13	121.2 (5)
Cu2—O5W—H5WB	146 (5)	C14—C15—C16	120.1 (5)
H5WA—O5W—H5WB	109 (8)	C14—C15—H15	119.9
H6WB—O6W—H6WA	109 (8)	C16—C15—H15	119.9
C8—N1—C9	118.6 (4)	C17—C16—C15	120.2 (5)
C8—N1—Cu1	126.8 (3)	C17—C16—H16	119.9
C9—N1—Cu1	113.8 (3)	C15—C16—H16	119.9
C12—N2—C10	108.8 (4)	C16—C17—C18	121.5 (5)
C12—N2—C11	108.5 (4)	C16—C17—H17	119.3
C10—N2—C11	110.4 (4)	C18—C17—H17	119.3
C12—N2—Cu1	113.6 (3)	C13—C18—C17	118.2 (5)

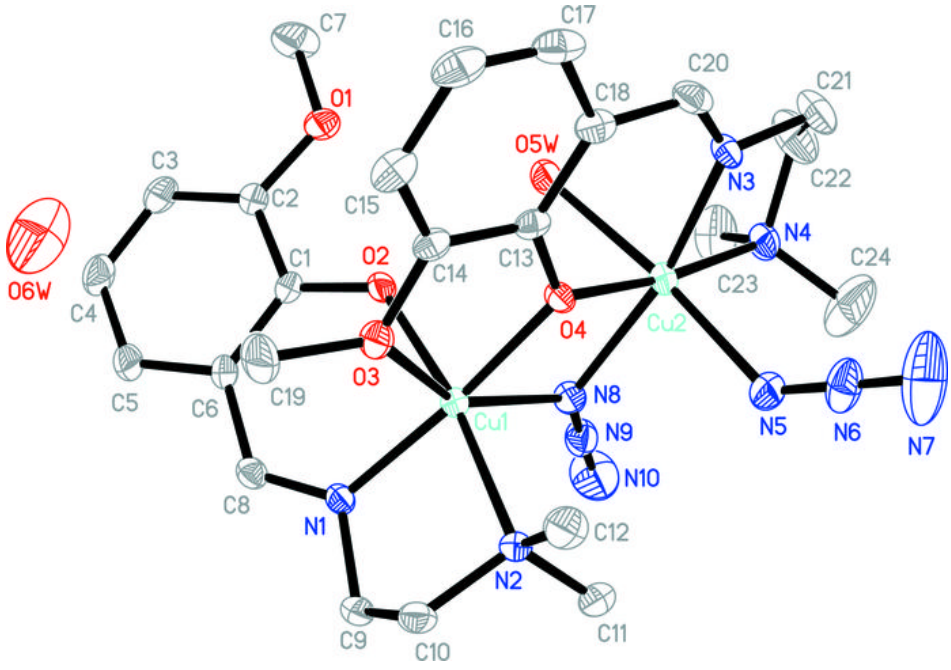
C10—N2—Cu1	103.8 (3)	C13—C18—C20	123.8 (5)
C11—N2—Cu1	111.7 (3)	C17—C18—C20	118.0 (5)
C20—N3—C21	119.9 (5)	O3—C19—H19A	109.5
C20—N3—Cu2	127.8 (4)	O3—C19—H19B	109.5
C21—N3—Cu2	112.1 (4)	H19A—C19—H19B	109.5
C24—N4—C23	109.3 (6)	O3—C19—H19C	109.5
C24—N4—C22	111.1 (6)	H19A—C19—H19C	109.5
C23—N4—C22	105.6 (5)	H19B—C19—H19C	109.5
C24—N4—Cu2	114.3 (4)	N3—C20—C18	125.9 (5)
C23—N4—Cu2	114.7 (4)	N3—C20—H20	117.1
C22—N4—Cu2	101.1 (3)	C18—C20—H20	117.1
N6—N5—Cu2	131.6 (5)	C22—C21—N3	108.0 (5)
N7—N6—N5	178.5 (7)	C22—C21—H21A	110.1
N9—N8—Cu2	127.7 (4)	N3—C21—H21A	110.1
N9—N8—Cu1	136.3 (4)	C22—C21—H21B	110.1
Cu2—N8—Cu1	96.01 (16)	N3—C21—H21B	110.1
N10—N9—N8	178.5 (6)	H21A—C21—H21B	108.4
O2—C1—C6	124.1 (4)	C21—C22—N4	116.0 (6)
O2—C1—C2	118.3 (4)	C21—C22—H22A	108.3
C6—C1—C2	117.6 (4)	N4—C22—H22A	108.3
C3—C2—O1	125.6 (4)	C21—C22—H22B	108.3
C3—C2—C1	121.0 (5)	N4—C22—H22B	108.3
O1—C2—C1	113.4 (4)	H22A—C22—H22B	107.4
C2—C3—C4	120.9 (5)	N4—C23—H23A	109.5
C2—C3—H3	119.5	N4—C23—H23B	109.5
C4—C3—H3	119.5	H23A—C23—H23B	109.5
C5—C4—C3	120.0 (5)	N4—C23—H23C	109.5
C5—C4—H4	120.0	H23A—C23—H23C	109.5
C3—C4—H4	120.0	H23B—C23—H23C	109.5
C4—C5—C6	120.9 (5)	N4—C24—H24A	109.5
C4—C5—H5	119.5	N4—C24—H24B	109.5
C6—C5—H5	119.5	H24A—C24—H24B	109.5
C1—C6—C5	119.5 (4)	N4—C24—H24C	109.5
C1—C6—C8	123.9 (4)	H24A—C24—H24C	109.5
C5—C6—C8	116.6 (4)	H24B—C24—H24C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5W—H5WB···N10^{i}	0.86 (6)	2.69 (4)	3.481 (8)	155 (8)
O5W—H5WA···O1	0.86 (6)	2.59 (6)	3.129 (5)	122 (6)
O5W—H5WA···O2	0.86 (6)	1.86 (6)	2.702 (4)	167 (8)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


C7
C16
C17
O1
C20
C21
C18
O5W
C3
N3
C22
C15
C2
N4
C24
C1
O2
C14
C13
C23
O6W
C4
O4
Cu2
O3
C5
C6
C19
N8
Cu1
N5
N6
N7
N9
N10
C8
N1
C12
N2
C9
C10
C11