

Bis[μ -2-methoxy-6-[(methylimino)methyl]phenolato]bis([2-methoxy-6-[(methylimino)methyl]phenolato]copper(II))

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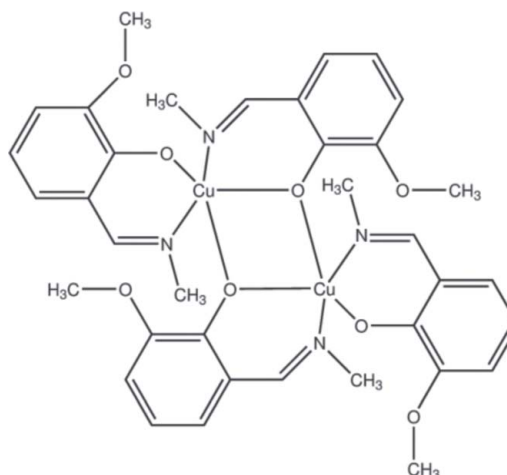
Received 3 September 2013; accepted 10 September 2013

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.031; wR factor = 0.084; data-to-parameter ratio = 37.5.

The title compound, $[\text{Cu}_2(\text{C}_9\text{H}_{10}\text{NO}_2)_4]$, is built of discrete centrosymmetric dimers. The Cu^{II} atoms are each five coordinated by two deprotonated Schiff base ligands that are bonded differently to the metal atoms. Of the two phenolate O atoms, one is coordinated to one Cu^{II} atom, whereas another bridges the two metal atoms. The basal plane of the square pyramid around Cu^{II} atoms is formed by the imino N and phenolate O atoms of the bidentate and the monodentate/bidentate Schiff base ligands. The bridging phenolate oxygen occupies the apical position of the coordination sphere with a considerably longer Cu—O bond length. In the crystal, the dimeric molecules pack relative to each other in such a way that the Cu_2O_2 planes of adjacent dimers are orthogonal.

Related literature

For direct synthesis using metal powders and Schiff base ligands, see: Chygorin *et al.* (2012*a,b*) and references therein. For the structure of the Schiff base ligand 2-methoxy-6-iminomethylphenol, see: Chatziefthimiou *et al.* (2006). For structures of metal complexes of this Schiff base ligand, see: Meally *et al.* (2010, 2012); Zhang & Feng (2010).



Experimental

Crystal data

$[\text{Cu}_2(\text{C}_9\text{H}_{10}\text{NO}_2)_4]$

$M_r = 783.8$

Orthorhombic, *Pbca*

$a = 10.1889$ (12) Å

$b = 15.2033$ (5) Å

$c = 21.6254$ (9) Å

$V = 3349.9$ (4) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 1.33$ mm⁻¹

$T = 100$ K

$0.59 \times 0.47 \times 0.10$ mm

Data collection

Oxford Diffraction Gemini diffractometer

Absorption correction: analytical

[*CrysAlis PRO* (Agilent, 2011)

based on Clark & Reid (1995)]

$T_{\text{min}} = 0.597$, $T_{\text{max}} = 0.88$

110425 measured reflections

8673 independent reflections

7021 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.084$

$S = 1.05$

8673 reflections

231 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.64$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.37$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cu1—O21	1.9044 (7)	Cu1—N17	2.0032 (8)
Cu1—O11	1.9243 (7)	Cu1—O11 ⁱ	2.4329 (8)
Cu1—N27	1.9925 (8)		

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

This work was partly supported by the State Fund for Fundamental Researches of Ukraine (project 54.3/005). The authors acknowledge the facilities, scientific and technical assistance of the Australian Microscopy & Microanalysis Research Facility at the Centre for Microscopy, Characterization & Analysis, the University of Western Australia, a

facility funded by the University, State and Commonwealth Governments.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5344).

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supplementary materials

Acta Cryst. (2013). E69, m551–m552 [doi:10.1107/S1600536813025105]

Bis{ μ -2-methoxy-6-[(methylimino)methyl]phenolato}bis({2-methoxy-6-[(methylimino)methyl]phenolato}copper(II))

Tetyana V. Sydoruk, Elena A. Buvaylo, Vladimir N. Kokozay, Olga Yu. Vassilyeva and Brian W. Skelton

1. Comment

The Schiff base ligand 2-methoxy-6-iminomethylphenol (HL) (Chatziefthimiou *et al.* 2006) with various connectivity fashions is usually used as a multidentate linker between several metal centres thus affording electronic and magnetic exchanges. [Ni₇], [Zn₇] (Meally *et al.*, 2010), [Co₇] (Meally *et al.*, 2012) and [Mn₇] (Zhang *et al.*, 2010) complexes of HL (singly deprotonated at the phenolate site) with planar hexagonal disc-like cores which possess double-bowl metallocalix[6]arene topologies have shown to act as host cavities accommodating numerous guest solvent molecules.

The Schiff base, a bright yellow crystalline solid, is usually obtained by the standard method of condensation of the substituted salicylaldehyde with aqueous solution of methylamine in methanol (Meally *et al.*, 2010). In the present work, we used a mixture of 2-hydroxy-3-methoxy-benzaldehyde and methylamine hydrochloride to react with copper powder and transition metal salt, NiCl₂·6H₂O, in an attempt to prepare a heterometallic complex with HL ligand. Details of the used synthetic approach as well as its applications were given by Chygorin *et al.* (2012*a*) and Chygorin *et al.* (2012*b*). However, the monometallic [Cu₂L₄] **1** was isolated instead. As there is no evidence of the influence of NiCl₂·6H₂O on the formation of **1** it can be presumed that the given copper complex may be synthesized starting from metallic copper or copper salt as well. To the best of our knowledge no copper complexes of HL have been structurally characterized.

The molecular structure of **1** consists of discrete centrosymmetric dimers [Cu₂L₄] (Fig. 1). The copper atoms are five coordinated each by two deprotonated Schiff base ligands that are bonded differently to the metal centres. Of the two phenolate oxygen atoms, O21 is coordinated to one copper atom, whereas O11 bridges the two metal centres. The basal plane of the square pyramid around copper atoms is formed by the coordination of the imino nitrogen, N27, and phenolate oxygen, O21, atoms of the bidentate Schiff base ligand and N17 and O11 donor atoms of the tridentate *L* with Cu–O/N distances in the range 1.9044 (7)–2.0032 (8) Å (Table 1). The bridging phenolate oxygen O11 { $-x + 1, -y + 1, -z + 1$ } occupies the apical position of the coordination sphere with the bond distance of 2.4329 (8) Å. The elongation of the apical contact is typical for copper (II) complexes. The *trans* angles at the metal atom are equal to 169.53 (3) and 175.12 (3)°, the *cis* angles vary from 79.17 (3) to 105.57 (3)°. The deviation of the copper(II) ion from the basal plane is 0.13 Å. The bridge angle Cu1–O11–Cu1 { $-x + 1, -y + 1, -z + 1$ } involving the phenolate oxygen is 100.8 (2)°, the separation between the metal centres is about 3.37 Å.

In the crystal lattice, the dimeric molecules pack relative to each other in such a way that Cu₂O₂ planes of the adjacent dimers are orthogonal (Fig. 2).

2. Experimental

2-Hydroxy-3-methoxy-benzaldehyde (0.30 g, 2 mmol), $\text{CH}_3\text{NH}_2\cdot\text{HCl}$ (0.14 g, 2 mmol), NEt_3 (0.3 ml, 2 mmol) were added to 20 ml of methanol and stirred magnetically for 30 min. After that copper powder (0.06 g, 1 mmol) and $\text{NiCl}_2\cdot 6\text{H}_2\text{O}$ (0.23 g, 1 mmol) were added to the yellow solution and the mixture was heated to 323 K under stirring for an hour. The resulting green solution was filtered and allowed to stand at room temperature. Dark-green rhombic plates of the title compound were formed next day. They were collected by filter-suction, washed with dry Pr^iOH and finally dried *in vacuo* (yield: 32%).

3. Refinement

Hydrogen atoms were placed at idealized positions ($\text{C-H} = 0.95 \text{ \AA}$, $U_{\text{isoH}} = 1.2U_{\text{eq C}}$ for CH, 0.98 \AA , $1.5U_{\text{eq C}}$ for CH_3) and refined as part of riding models.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP II* (Johnson, 1976); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

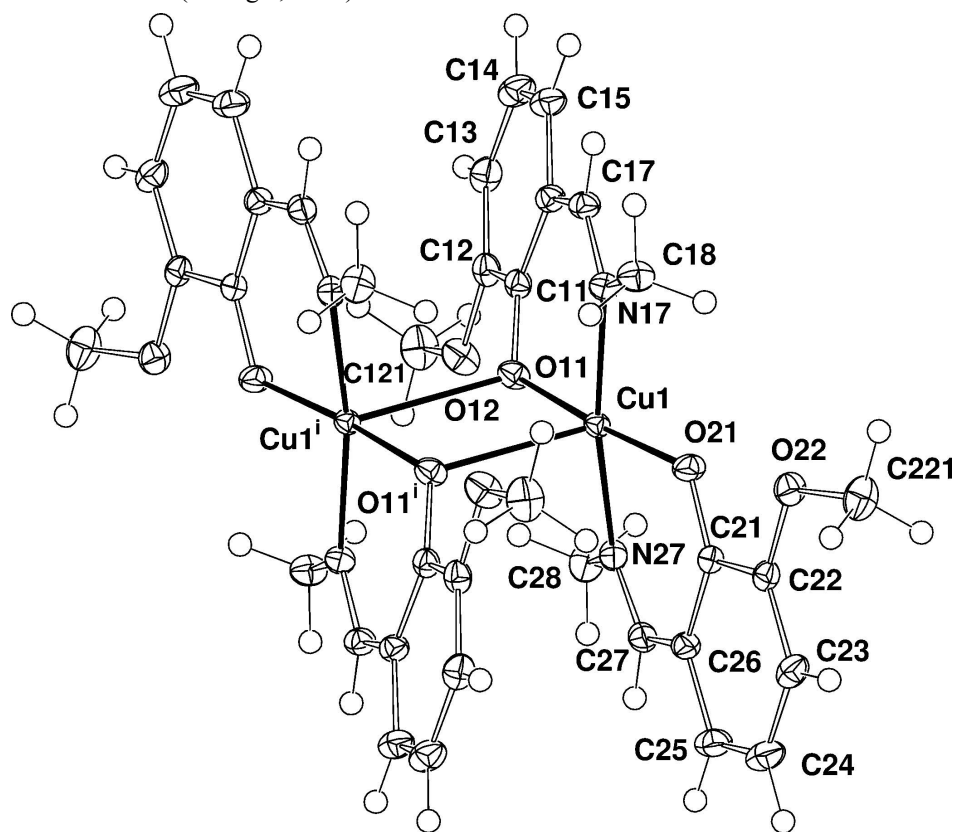
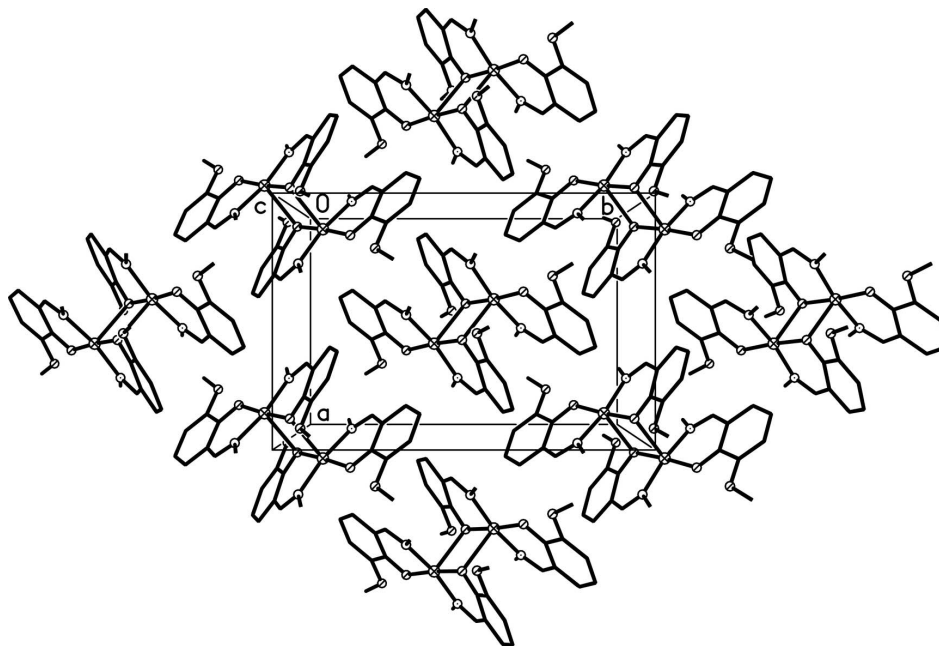


Figure 1

Molecular structure of the complex with the numbering scheme (the non-hydrogen atoms shown as 30% thermal ellipsoids). Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

**Figure 2**

Packing diagram viewed down the *c* axis (CH and CH₃ hydrogen atoms were omitted for clarity).

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Crystal data

[Cu₂(C₉H₁₀NO₂)₄]

M_r = 783.8

Orthorhombic, *Pbca*

Hall symbol: -p 2ac 2ab

a = 10.1889 (12) Å

b = 15.2033 (5) Å

c = 21.6254 (9) Å

V = 3349.9 (4) Å³

Z = 4

F(000) = 1624

D_x = 1.554 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 25414 reflections

θ = 3.7–37.4°

μ = 1.33 mm⁻¹

T = 100 K

Plate, dark green

0.59 × 0.47 × 0.10 mm

Data collection

Oxford Diffraction Gemini diffractometer

Graphite monochromator

Detector resolution: 10.4738 pixels mm⁻¹

ω scans

Absorption correction: analytical

[*CrysAlis PRO* (Agilent, 2011) based on Clark & Reid (1995)]

T_{min} = 0.597, *T_{max}* = 0.88

110425 measured reflections

8673 independent reflections

7021 reflections with *I* > 2σ(*I*)

R_{int} = 0.045

θ_{max} = 37.5°, θ_{min} = 3.7°

h = -17→17

k = -25→25

l = -36→36

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.084$
 $S = 1.05$
 8673 reflections
 231 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.9858P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 0.64 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.402856 (11)	0.587478 (7)	0.514407 (5)	0.01235 (3)
C11	0.32361 (9)	0.46134 (6)	0.42192 (4)	0.01446 (14)
O11	0.42030 (7)	0.50521 (5)	0.44728 (3)	0.01630 (12)
C12	0.33769 (10)	0.43410 (6)	0.35910 (4)	0.01654 (15)
O12	0.45029 (8)	0.46267 (6)	0.33152 (3)	0.02223 (15)
C121	0.47672 (13)	0.43092 (8)	0.27121 (5)	0.0262 (2)
H12A	0.4814	0.3665	0.272	0.039*
H12B	0.5606	0.4548	0.2567	0.039*
H12C	0.4064	0.4494	0.2431	0.039*
C13	0.24123 (11)	0.38471 (7)	0.33053 (5)	0.02007 (17)
H13	0.2522	0.3668	0.2888	0.024*
C14	0.12726 (12)	0.36098 (7)	0.36284 (5)	0.02237 (19)
H14	0.0614	0.3269	0.343	0.027*
C15	0.11093 (10)	0.38700 (7)	0.42308 (5)	0.01978 (17)
H15	0.0337	0.3705	0.4448	0.024*
C16	0.20753 (9)	0.43801 (6)	0.45312 (4)	0.01527 (15)
C17	0.18368 (9)	0.46319 (6)	0.51653 (4)	0.01637 (15)
H17	0.1114	0.4362	0.5367	0.02*
N17	0.25120 (8)	0.51886 (5)	0.54829 (4)	0.01518 (13)
C18	0.21142 (10)	0.53316 (7)	0.61269 (4)	0.01945 (17)
H18A	0.1379	0.4942	0.6228	0.029*
H18B	0.1843	0.5945	0.6181	0.029*
H18C	0.2855	0.5204	0.6402	0.029*
C21	0.44917 (9)	0.73470 (6)	0.59567 (4)	0.01441 (14)
O21	0.37172 (7)	0.67187 (5)	0.57781 (4)	0.01810 (13)
C22	0.41886 (9)	0.78000 (6)	0.65201 (4)	0.01576 (15)

O22	0.30820 (7)	0.75006 (5)	0.68125 (3)	0.01921 (13)
C221	0.25933 (13)	0.80269 (8)	0.73029 (5)	0.0256 (2)
H22A	0.3214	0.8015	0.7649	0.038*
H22B	0.1743	0.7796	0.744	0.038*
H22C	0.2485	0.8634	0.7159	0.038*
C23	0.49660 (11)	0.84784 (6)	0.67335 (5)	0.01998 (17)
H23	0.4745	0.8767	0.7109	0.024*
C24	0.60788 (11)	0.87448 (7)	0.64016 (5)	0.0236 (2)
H24	0.6615	0.9209	0.6552	0.028*
C25	0.63872 (11)	0.83310 (7)	0.58585 (5)	0.02131 (18)
H25	0.7141	0.8513	0.5634	0.026*
C26	0.56052 (9)	0.76367 (6)	0.56242 (4)	0.01585 (15)
C27	0.58954 (9)	0.73111 (7)	0.50142 (5)	0.01682 (16)
H27	0.6603	0.7582	0.4801	0.02*
N27	0.52864 (8)	0.66860 (5)	0.47287 (4)	0.01607 (14)
C28	0.56176 (12)	0.65605 (7)	0.40743 (5)	0.02199 (19)
H28A	0.6356	0.6943	0.3964	0.033*
H28B	0.4856	0.671	0.3818	0.033*
H28C	0.5862	0.5945	0.4003	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01144 (5)	0.01349 (5)	0.01214 (5)	-0.00031 (3)	0.00112 (3)	-0.00053 (3)
C11	0.0148 (3)	0.0148 (3)	0.0138 (3)	0.0015 (3)	-0.0024 (3)	-0.0005 (3)
O11	0.0141 (3)	0.0204 (3)	0.0145 (3)	-0.0013 (2)	-0.0003 (2)	-0.0039 (2)
C12	0.0177 (4)	0.0175 (4)	0.0145 (4)	0.0035 (3)	-0.0022 (3)	-0.0015 (3)
O12	0.0198 (3)	0.0319 (4)	0.0149 (3)	0.0009 (3)	0.0021 (3)	-0.0060 (3)
C121	0.0323 (6)	0.0315 (5)	0.0147 (4)	0.0057 (4)	0.0027 (4)	-0.0042 (4)
C13	0.0247 (4)	0.0186 (4)	0.0169 (4)	0.0022 (3)	-0.0059 (3)	-0.0037 (3)
C14	0.0264 (5)	0.0189 (4)	0.0218 (4)	-0.0045 (4)	-0.0071 (4)	-0.0014 (3)
C15	0.0209 (4)	0.0183 (4)	0.0201 (4)	-0.0050 (3)	-0.0040 (3)	0.0008 (3)
C16	0.0156 (4)	0.0148 (3)	0.0153 (4)	-0.0013 (3)	-0.0022 (3)	0.0011 (3)
C17	0.0159 (4)	0.0165 (4)	0.0167 (4)	-0.0024 (3)	-0.0003 (3)	0.0023 (3)
N17	0.0148 (3)	0.0170 (3)	0.0137 (3)	-0.0011 (3)	0.0009 (2)	0.0004 (3)
C18	0.0201 (4)	0.0232 (4)	0.0151 (4)	-0.0040 (3)	0.0041 (3)	-0.0008 (3)
C21	0.0138 (3)	0.0128 (3)	0.0166 (4)	0.0005 (3)	-0.0003 (3)	0.0008 (3)
O21	0.0164 (3)	0.0173 (3)	0.0206 (3)	-0.0037 (2)	0.0050 (2)	-0.0050 (2)
C22	0.0177 (4)	0.0136 (3)	0.0160 (4)	0.0016 (3)	-0.0013 (3)	0.0010 (3)
O22	0.0204 (3)	0.0189 (3)	0.0183 (3)	0.0008 (3)	0.0036 (2)	-0.0030 (2)
C221	0.0350 (6)	0.0231 (5)	0.0187 (4)	0.0054 (4)	0.0062 (4)	-0.0026 (4)
C23	0.0256 (5)	0.0150 (4)	0.0193 (4)	-0.0008 (3)	-0.0057 (3)	-0.0003 (3)
C24	0.0269 (5)	0.0191 (4)	0.0248 (5)	-0.0074 (4)	-0.0070 (4)	0.0022 (4)
C25	0.0197 (4)	0.0198 (4)	0.0244 (5)	-0.0064 (3)	-0.0025 (3)	0.0046 (3)
C26	0.0145 (3)	0.0147 (3)	0.0184 (4)	-0.0011 (3)	-0.0010 (3)	0.0028 (3)
C27	0.0145 (4)	0.0166 (4)	0.0194 (4)	0.0007 (3)	0.0023 (3)	0.0042 (3)
N27	0.0162 (3)	0.0158 (3)	0.0162 (3)	0.0018 (3)	0.0034 (3)	0.0028 (3)
C28	0.0268 (5)	0.0220 (4)	0.0172 (4)	0.0019 (4)	0.0078 (4)	0.0030 (3)

Geometric parameters (Å, °)

Cu1—O21	1.9044 (7)	C18—H18A	0.98
Cu1—O11	1.9243 (7)	C18—H18B	0.98
Cu1—N27	1.9925 (8)	C18—H18C	0.98
Cu1—N17	2.0032 (8)	C21—O21	1.2979 (11)
Cu1—O11 ⁱ	2.4329 (8)	C21—C26	1.4135 (13)
C11—O11	1.3101 (11)	C21—C22	1.4333 (13)
C11—C16	1.4071 (13)	C22—O22	1.3705 (12)
C11—C12	1.4274 (13)	C22—C23	1.3799 (14)
O11—Cu1 ⁱ	2.4329 (8)	O22—C221	1.4187 (13)
C12—O12	1.3640 (13)	C221—H22A	0.98
C12—C13	1.3825 (14)	C221—H22B	0.98
O12—C121	1.4165 (13)	C221—H22C	0.98
C121—H12A	0.98	C23—C24	1.4017 (16)
C121—H12B	0.98	C23—H23	0.95
C121—H12C	0.98	C24—C25	1.3689 (17)
C13—C14	1.4026 (16)	C24—H24	0.95
C13—H13	0.95	C25—C26	1.4163 (14)
C14—C15	1.3716 (15)	C25—H25	0.95
C14—H14	0.95	C26—C27	1.4396 (14)
C15—C16	1.4115 (14)	C27—N27	1.2922 (14)
C15—H15	0.95	C27—H27	0.95
C16—C17	1.4444 (14)	N27—C28	1.4673 (13)
C17—N17	1.2890 (12)	C28—H28A	0.98
C17—H17	0.95	C28—H28B	0.98
N17—C18	1.4667 (13)	C28—H28C	0.98
O21—Cu1—O11	175.12 (3)	N17—C18—H18A	109.5
O21—Cu1—N27	90.84 (3)	N17—C18—H18B	109.5
O11—Cu1—N27	90.16 (3)	H18A—C18—H18B	109.5
O21—Cu1—N17	87.65 (3)	N17—C18—H18C	109.5
O11—Cu1—N17	90.50 (3)	H18A—C18—H18C	109.5
N27—Cu1—N17	169.53 (3)	H18B—C18—H18C	109.5
O21—Cu1—O11 ⁱ	105.57 (3)	O21—C21—C26	124.47 (9)
O11—Cu1—O11 ⁱ	79.17 (3)	O21—C21—C22	118.40 (8)
N27—Cu1—O11 ⁱ	92.04 (3)	C26—C21—C22	117.11 (8)
N17—Cu1—O11 ⁱ	98.34 (3)	C21—O21—Cu1	127.51 (6)
O11—C11—C16	124.03 (8)	O22—C22—C23	124.49 (9)
O11—C11—C12	118.08 (9)	O22—C22—C21	114.20 (8)
C16—C11—C12	117.89 (8)	C23—C22—C21	121.32 (9)
C11—O11—Cu1	125.26 (6)	C22—O22—C221	116.50 (8)
C11—O11—Cu1 ⁱ	113.86 (6)	O22—C221—H22A	109.5
Cu1—O11—Cu1 ⁱ	100.84 (3)	O22—C221—H22B	109.5
O12—C12—C13	125.13 (9)	H22A—C221—H22B	109.5
O12—C12—C11	114.10 (8)	O22—C221—H22C	109.5
C13—C12—C11	120.76 (9)	H22A—C221—H22C	109.5
C12—O12—C121	117.00 (9)	H22B—C221—H22C	109.5
O12—C121—H12A	109.5	C22—C23—C24	120.60 (10)
O12—C121—H12B	109.5	C22—C23—H23	119.7

H12A—C121—H12B	109.5	C24—C23—H23	119.7
O12—C121—H12C	109.5	C25—C24—C23	119.49 (10)
H12A—C121—H12C	109.5	C25—C24—H24	120.3
H12B—C121—H12C	109.5	C23—C24—H24	120.3
C12—C13—C14	120.37 (9)	C24—C25—C26	121.35 (10)
C12—C13—H13	119.8	C24—C25—H25	119.3
C14—C13—H13	119.8	C26—C25—H25	119.3
C15—C14—C13	119.97 (10)	C21—C26—C25	120.12 (9)
C15—C14—H14	120	C21—C26—C27	121.59 (9)
C13—C14—H14	120	C25—C26—C27	117.94 (9)
C14—C15—C16	120.73 (10)	N27—C27—C26	126.30 (9)
C14—C15—H15	119.6	N27—C27—H27	116.8
C16—C15—H15	119.6	C26—C27—H27	116.8
C11—C16—C15	120.26 (9)	C27—N27—C28	116.49 (9)
C11—C16—C17	122.00 (8)	C27—N27—Cu1	123.28 (7)
C15—C16—C17	117.72 (9)	C28—N27—Cu1	120.15 (7)
N17—C17—C16	126.16 (9)	N27—C28—H28A	109.5
N17—C17—H17	116.9	N27—C28—H28B	109.5
C16—C17—H17	116.9	H28A—C28—H28B	109.5
C17—N17—C18	117.11 (8)	N27—C28—H28C	109.5
C17—N17—Cu1	123.97 (7)	H28A—C28—H28C	109.5
C18—N17—Cu1	118.90 (6)	H28B—C28—H28C	109.5

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