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# Crystal structure and Hirshfeld surface analysis of dichlorido(methanol-κO)bis(2-methylpyridine-κN)-copper(II)

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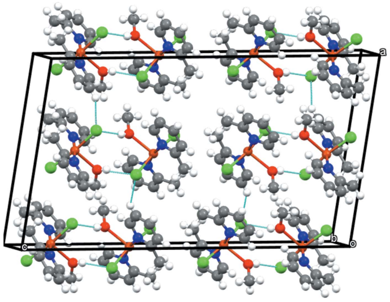
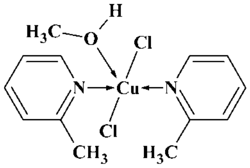
In the title complex, $[CuCl_2(C_6H_7N)_2(CH_3OH)]$, the copper atom is five-coordinated by two nitrogen atoms of 2-methylpyridine ligands, two chloro ligands and an oxygen atom of the methanol molecule, being in a tetragonal–pyramidal environment with N and Cl atoms forming the basal plane. In the crystal, complex molecules related by the twofold rotation axis are joined into dimeric units by pairs of O—H$\cdots$Cl hydrogen bonds. These dimeric units are assembled through C—H$\cdots$Cl interactions into layers parallel to (001).



## 1. Chemical context

Both organic (from simple molecules to peptides and proteins) and inorganic complexes have been known for more than a century and are central to modern chemistry because of their fascinating, aesthetic architectures and multiple applications (Gan *et al.*, 2011; Gellman, 1998; Thorat *et al.*, 2013; Vijayadas *et al.*, 2013; Ziach *et al.*, 2018). Recently, coordination compounds have been reported that find applications in fields such as catalysis, gas storage, separation technology and molecular sensing (Mueller *et al.*, 2006; Wan *et al.*, 2006; Férey *et al.*, 2003; James, 2003; Eddaoudi *et al.*, 2002; Ruben *et al.*, 2005, Kitagawa *et al.*, 2004). There are many reports of coordination complexes where solvent molecules are located in the voids of the crystal structure. However, reports describing the replacement of coordinated solvent molecules with other molecules are relatively scarce. As part of ongoing work in our laboratory, employing pyridine ligands in the preparation of various coordination networks (PrakashaReddy & Pedireddi, 2007), we have extended our work to the synthesis of other coordination networks. A literature survey revealed that coordination complex aquadichlorobis(2-methylpyridine)-copper(II) had been reported (Marsh *et al.*, 1982). Our interest was to see whether we could replace the coordinated water molecule in the complex with other solvent molecules such as methanol or ethanol *via* single-crystal-to-single-crystal transition (SCSCT) to investigate the structural changes. Although we could not succeed in SCSCT of the complex, we were successful in synthesizing the methanol-coordinated copper complex incorporating 2-methylpyridine as reported herein.



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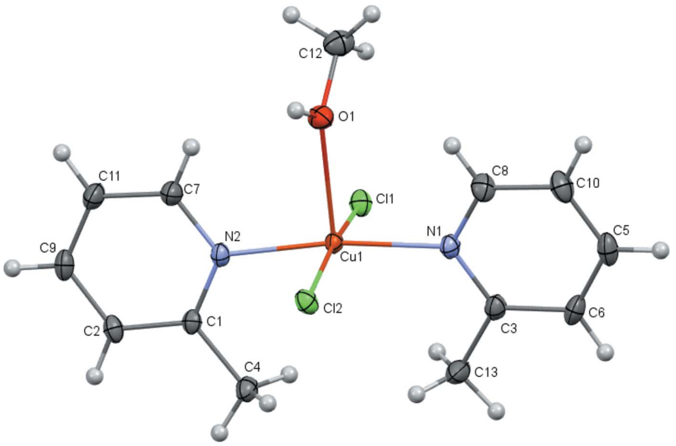

**Figure 1**
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| O1—H1$\cdots$Cl2$^{i}$ | 0.75 (3) | 2.37 (3) | 3.1033 (16) | 169 (3) |
| C7—H7$\cdots$O1 | 0.93 | 2.46 | 3.148 (3) | 130 |
| C8—H8$\cdots$O1 | 0.93 | 2.34 | 3.036 (3) | 131 |
| C11—H11$\cdots$Cl2$^{ii}$ | 0.93 | 2.83 | 3.624 (2) | 143 |

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

## 2. Structural commentary

The title complex crystallizes in the monoclinic space group $C2/c$ with one complex molecule per asymmetric unit. Two nitrogen atoms of 2-methylpyridine and two chloride ligands, which are *trans* to each other, form a rectangle around the copper atom, and its coordination is accomplished by the methanol oxygen atom, thus giving a tetragonal pyramid with the oxygen atom in the apical position (Fig. 1). The copper atom deviates by 0.161 (1) Å from the basal plane, and the angles around the copper atom are close to 90 and 180°. A plausible reason why the formation of a dimeric unit, as observed in [Cu(2-pic)$_2$Cl$_2$] (Marsh *et al.*, 1982), was precluded might be the presence of the coordinated methanol molecule on one side of the coordination rectangle and the methyl groups on the other side. The methylpyridine rings form angles of 83.96 (8) and 85.70 (8)° with respect to the basal plane of the coordination polyhedron, thereby plausibly blocking the sixth coordination position at the copper atom. The Cu—O bond distance of 2.353 (2) Å is relatively short for an apical atom in typical copper(II) tetragonal–pyramidal structure, whereas the Cu—N bond lengths [Cu1—N1= 2.031 (2) Å, Cu1—N2 = 2.017 (2) Å] agree well with those reported for related structures (Wang *et al.*, 2006; Gong *et al.*, 2009; Hu & Zhang, 2010; Li, 2011; Sun *et al.*, 2013; Sanram *et al.*, 2016).

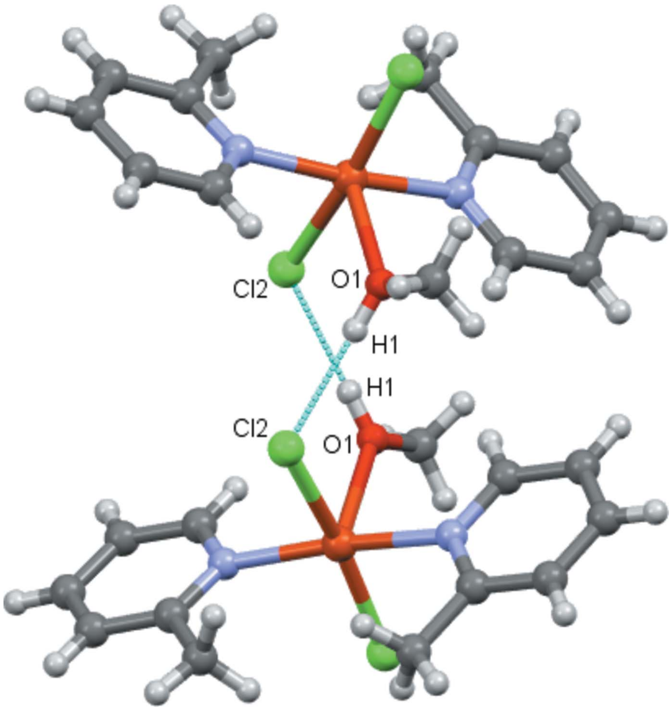

**Figure 2**
The O—H$\cdots$Cl interactions between two molecules in the crystal of the title compound. The molecules are related by the symmetry operation $-x+1, y, -z+\frac{1}{2}$.

## 3. Supramolecular features and Hirshfeld surface analysis

Complex molecules related by the twofold rotation axis are connected by pairs of O—H$\cdots$Cl interactions (Table 1) involving the apical methanol ligand of one complex and a chloride ligand of the other, thus forming dimers (Fig. 2). The O$\cdots$Cl and H$\cdots$Cl distances and associated O—H$\cdots$Cl angle lie within the ranges observed for other O—H$\cdots$Cl interactions reported in the literature (Veal *et al.*, 1972; Taylor,

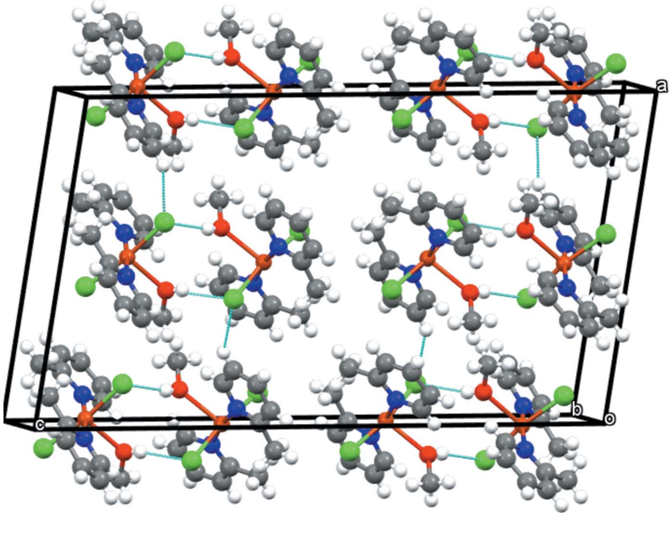

**Figure 3**
A general view of the crystal packing of the title compound along the $b$-axis direction with intermolecular contacts shown as dashed lines.

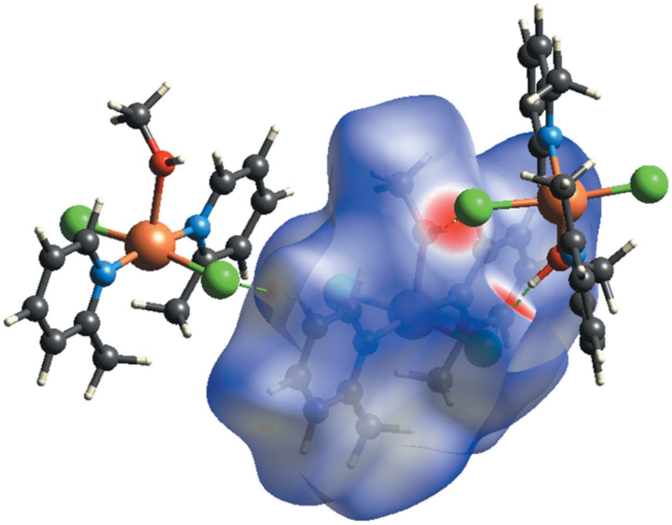

**Figure 4**
Hirshfeld surface mapped over $d_{\rm norm}$ highlighting the regions of O—H···Cl and C—H···Cl intermolecular contacts.

2016; Ristić *et al.*, 2020; Estes *et al.*, 1976). These dimers are further connected through C—H···Cl interactions, generating layers parallel to (001) (Fig. 3, Table 1).

A Hirshfeld surface analysis was performed and two-dimensional fingerprint plots were prepared using *Crystal Explorer17* (Turner *et al.*, 2017) to further investigate the intermolecular interactions in the title structure. The Hirshfeld surface mapped over $d_{\rm norm}$ with corresponding colours representing intermolecular interactions is shown in Fig. 4. The red spots on the surface correspond to the O—H···Cl, C—H···Cl and C—H···O interactions (Table 1). The two-dimensional fingerprint plots (McKinnon *et al.*, 2007) are shown in Fig. 5. Weak van der Waals H···H contacts make the largest contribution (53.1%) to the Hirshfeld surface. The two-dimensional fingerprint plot shows two spikes that correspond to H···Cl/Cl···H (25.2%) interactions, which highlight the hydrogen bonds between adjacent molecules. The C···H/H···C (15.5%) interactions also appear as two spikes. These interactions play a crucial role in the overall cohesion of the crystal packing.

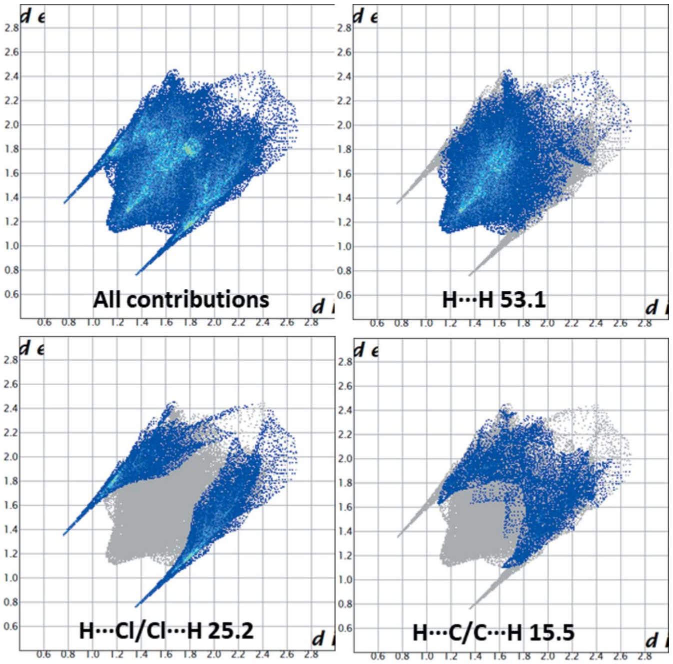

**Figure 5**
The full two-dimensional fingerprint plot for the title compound and those delineated into H···H (53.1%), Cl···H/H···Cl (25.2%) and C···H/H···C (15.5%) contacts.

## 4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.40, update of August 2019; Groom *et al.*, 2016) revealed three closely related complexes: dichlorobis(2-methylpyridine)copper(II) (refcode CMPYCU01; Marsh *et al.*, 1982), aquadichlorobis(2-methylpyridine)copper(II) (BIJWUM; Marsh *et al.*, 1982) and bis(isothiocyanato)-methanolbis(2-methylpyridine)copper(II) (ABOSIW; Handy *et al.*, 2017). Structures CMPYCU01 and BIJWUM display dimeric arrangements of the complex molecules arising from C—H···Cl and O—H···Cl interactions, respectively, while in the copper(II) thiocyanate complex ABOSIW, the three-dimensional network is formed as a result of O—H···S, C—H···S and C—H···C interactions.

## 5. Synthesis and crystallization

2-Methylpyridine and anhydrous copper(II) chloride were obtained from Aldrich, and HPLC grade methanol was used for reaction. Anhydrous copper(II) chloride (0.675 g, 0.005 mol) was dissolved in 15 ml of methanol. To this solution, 2-methylpyridine (0.93 g, 0.01 mol) dissolved in 15 mL of methanol was added. The resulting mixture was stirred for *ca* 40 min. at room temperature and filtered to remove the greenish precipitate. The blue filtrate was then allowed to stand at room temperature for a few hours, before being filtered and left at room temperature for crystallization. A mixture of dark-blue crystals of different sizes was obtained after 24 h.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were located in a difference map. The C-bound H atoms were placed in calculated positions with C—H = 0.93-0.96 Å and refined as riding, whereas the coordinates of O-bound H atom were freely refined. All hydrogen atoms were refined with fixed isotropic displacement parameters [$U_{\rm iso}$(H) = 1.2–1.5$U_{\rm eq}$(C,O)]

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[CuCl_2(C_6H_7N)_2(CH_4O)]$ |
| $M_r$ | 352.73 |
| Crystal system, space group | Monoclinic, $C2/c$ |
| Temperature (K) | 120 |
| $a$, $b$, $c$ (Å) | 14.4554 (4), 8.5865 (2), 24.8055 (8) |
| $\beta$ (°) | 99.209 (3) |
| $V$ (Å$^3$) | 3039.22 (16) |
| $Z$ | 8 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.78 |
| Crystal size (mm) | 0.21 × 0.16 × 0.11 |
| | |
| Data collection | |
| Diffractometer | Agilent XCalibur diffractometer |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018) |
| $T_{min}$, $T_{max}$ | 0.549, 1.000 |
| No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections | 15974, 5137, 4251 |
| $R_{int}$ | 0.040 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.758 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.038, 0.081, 1.13 |
| No. of reflections | 5137 |
| No. of parameters | 178 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.54, −0.51 |

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2009), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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# supporting information

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## Crystal structure and Hirshfeld surface analysis of dichlorido(methanol-*κO*)bis(2-methylpyridine-*κN*)copper(II)

**J. Prakasha Reddy**

### Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); program(s) used to solve structure: ShelXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

### Dichlorido(methanol-*κO*)bis(2-methylpyridine-*κN*)copper(II)

*Crystal data*

$[CuCl_2(C_6H_7N)_2(CH_4O)]$
$M_r = 352.73$
Monoclinic, $C2/c$
$a = 14.4554\ (4)$ Å
$b = 8.5865\ (2)$ Å
$c = 24.8055\ (8)$ Å
$\beta = 99.209\ (3)°$
$V = 3039.22\ (16)$ Å$^3$
$Z = 8$

$F(000) = 1448$
$D_x = 1.542$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4621 reflections
$\theta = 3.1$–$32.0°$
$\mu = 1.78$ mm$^{-1}$
$T = 120$ K
Block, blue
0.21 × 0.16 × 0.11 mm

*Data collection*

Agilent XCalibur
diffractometer
Detector resolution: 16.1511 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan
(CrysAlisPro; Rigaku OD, 2018)
$T_{min} = 0.549$, $T_{max} = 1.000$
15974 measured reflections

5137 independent reflections
4251 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 32.6°$, $\theta_{min} = 2.8°$
$h = -20 \rightarrow 21$
$k = -12 \rightarrow 11$
$l = -37 \rightarrow 37$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.081$
$S = 1.13$
5137 reflections
178 parameters
0 restraints
Primary atom site location: dual

Hydrogen site location: mixed
H atoms treated by a mixture of independent
and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0199P)^2 + 4.4488P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å$^{-3}$
$\Delta\rho_{min} = -0.51$ e Å$^{-3}$

*Special details*

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

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

| | *x* | *y* | *z* | $U_{\rm iso}$*/$U_{\rm eq}$ |
|---|---|---|---|---|
| Cu1 | 0.50986 (2) | 0.75598 (3) | 0.37062 (2) | 0.01272 (6) |
| Cl1 | 0.41953 (3) | 0.66088 (6) | 0.43059 (2) | 0.01703 (10) |
| Cl2 | 0.61677 (3) | 0.86629 (5) | 0.32152 (2) | 0.01706 (10) |
| O1 | 0.40656 (10) | 0.69534 (18) | 0.29006 (6) | 0.0192 (3) |
| H1 | 0.408 (2) | 0.738 (3) | 0.2640 (12) | 0.029* |
| N2 | 0.45788 (11) | 0.97058 (19) | 0.38001 (7) | 0.0145 (3) |
| N1 | 0.57721 (11) | 0.54847 (19) | 0.37032 (7) | 0.0149 (3) |
| C1 | 0.49779 (13) | 1.0690 (2) | 0.41912 (8) | 0.0141 (3) |
| C2 | 0.45939 (14) | 1.2154 (2) | 0.42581 (8) | 0.0168 (4) |
| H2 | 0.488544 | 1.282802 | 0.452631 | 0.020* |
| C3 | 0.64638 (14) | 0.5067 (2) | 0.41102 (9) | 0.0175 (4) |
| C4 | 0.58446 (14) | 1.0157 (2) | 0.45567 (8) | 0.0188 (4) |
| H4A | 0.571444 | 0.921107 | 0.473669 | 0.028* |
| H4B | 0.604355 | 1.094501 | 0.482496 | 0.028* |
| H4C | 0.633209 | 0.997353 | 0.434317 | 0.028* |
| C5 | 0.66783 (15) | 0.2646 (2) | 0.36638 (9) | 0.0220 (4) |
| H5 | 0.698699 | 0.170012 | 0.364995 | 0.026* |
| C6 | 0.69292 (14) | 0.3650 (2) | 0.40943 (9) | 0.0216 (4) |
| H6 | 0.740983 | 0.338329 | 0.437494 | 0.026* |
| C7 | 0.37914 (14) | 1.0160 (2) | 0.34693 (9) | 0.0201 (4) |
| H7 | 0.351990 | 0.948582 | 0.319564 | 0.024* |
| C8 | 0.55316 (15) | 0.4492 (2) | 0.32849 (8) | 0.0190 (4) |
| H8 | 0.505512 | 0.477838 | 0.300461 | 0.023* |
| C9 | 0.37781 (15) | 1.2600 (2) | 0.39241 (9) | 0.0192 (4) |
| H9 | 0.350701 | 1.356328 | 0.396982 | 0.023* |
| C10 | 0.59622 (16) | 0.3063 (2) | 0.32532 (9) | 0.0220 (4) |
| H10 | 0.577215 | 0.239722 | 0.296070 | 0.026* |
| C11 | 0.33724 (15) | 1.1589 (3) | 0.35209 (9) | 0.0223 (4) |
| H11 | 0.282686 | 1.186387 | 0.328834 | 0.027* |
| C12 | 0.32370 (15) | 0.6023 (3) | 0.28385 (9) | 0.0231 (4) |
| H12A | 0.326320 | 0.525448 | 0.256034 | 0.035* |
| H12B | 0.269827 | 0.667541 | 0.273541 | 0.035* |
| H12C | 0.319211 | 0.551434 | 0.317792 | 0.035* |
| C13 | 0.67215 (16) | 0.6175 (3) | 0.45740 (10) | 0.0271 (5) |
| H13A | 0.691508 | 0.714806 | 0.443729 | 0.041* |
| H13B | 0.722622 | 0.574607 | 0.482943 | 0.041* |
| H13C | 0.618872 | 0.634370 | 0.475334 | 0.041* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.01378 (11) | 0.01059 (11) | 0.01375 (11) | 0.00289 (8) | 0.00206 (8) | −0.00104 (8) |
| Cl1 | 0.0200 (2) | 0.0157 (2) | 0.0161 (2) | 0.00216 (17) | 0.00497 (17) | 0.00003 (17) |
| Cl2 | 0.0182 (2) | 0.0149 (2) | 0.0192 (2) | −0.00028 (16) | 0.00627 (17) | −0.00322 (17) |
| O1 | 0.0226 (7) | 0.0190 (7) | 0.0152 (7) | −0.0020 (6) | 0.0008 (6) | 0.0024 (6) |
| N2 | 0.0145 (7) | 0.0122 (7) | 0.0175 (8) | 0.0024 (6) | 0.0047 (6) | 0.0004 (6) |
| N1 | 0.0152 (7) | 0.0133 (7) | 0.0168 (8) | 0.0020 (6) | 0.0045 (6) | −0.0011 (6) |
| C1 | 0.0168 (8) | 0.0135 (8) | 0.0128 (8) | 0.0014 (7) | 0.0049 (7) | 0.0018 (7) |
| C2 | 0.0226 (9) | 0.0128 (9) | 0.0165 (9) | 0.0015 (7) | 0.0075 (8) | −0.0011 (7) |
| C3 | 0.0157 (9) | 0.0155 (9) | 0.0217 (10) | 0.0024 (7) | 0.0041 (7) | 0.0004 (8) |
| C4 | 0.0216 (9) | 0.0175 (9) | 0.0164 (9) | 0.0042 (8) | 0.0005 (8) | −0.0029 (8) |
| C5 | 0.0252 (10) | 0.0135 (9) | 0.0304 (11) | 0.0057 (8) | 0.0138 (9) | 0.0027 (8) |
| C6 | 0.0186 (9) | 0.0196 (10) | 0.0264 (11) | 0.0077 (8) | 0.0030 (8) | 0.0034 (8) |
| C7 | 0.0178 (9) | 0.0175 (9) | 0.0237 (10) | 0.0031 (7) | −0.0009 (8) | −0.0033 (8) |
| C8 | 0.0235 (10) | 0.0190 (10) | 0.0154 (9) | 0.0031 (8) | 0.0055 (8) | −0.0020 (8) |
| C9 | 0.0233 (10) | 0.0138 (9) | 0.0225 (10) | 0.0058 (7) | 0.0094 (8) | 0.0022 (8) |
| C10 | 0.0293 (11) | 0.0163 (9) | 0.0222 (10) | 0.0021 (8) | 0.0101 (9) | −0.0044 (8) |
| C11 | 0.0198 (9) | 0.0205 (10) | 0.0252 (11) | 0.0076 (8) | −0.0007 (8) | −0.0007 (8) |
| C12 | 0.0202 (10) | 0.0289 (11) | 0.0202 (10) | 0.0001 (8) | 0.0033 (8) | −0.0023 (9) |
| C13 | 0.0236 (10) | 0.0235 (11) | 0.0303 (12) | 0.0082 (9) | −0.0081 (9) | −0.0069 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—Cl1 | 2.2818 (5) | C4—H4C | 0.9600 |
| Cu1—Cl2 | 2.3175 (5) | C5—H5 | 0.9300 |
| Cu1—O1 | 2.3534 (15) | C5—C6 | 1.375 (3) |
| Cu1—N2 | 2.0174 (16) | C5—C10 | 1.378 (3) |
| Cu1—N1 | 2.0310 (16) | C6—H6 | 0.9300 |
| O1—H1 | 0.75 (3) | C7—H7 | 0.9300 |
| O1—C12 | 1.427 (3) | C7—C11 | 1.383 (3) |
| N2—C1 | 1.345 (2) | C8—H8 | 0.9300 |
| N2—C7 | 1.350 (3) | C8—C10 | 1.384 (3) |
| N1—C3 | 1.351 (3) | C9—H9 | 0.9300 |
| N1—C8 | 1.345 (3) | C9—C11 | 1.382 (3) |
| C1—C2 | 1.395 (3) | C10—H10 | 0.9300 |
| C1—C4 | 1.496 (3) | C11—H11 | 0.9300 |
| C2—H2 | 0.9300 | C12—H12A | 0.9600 |
| C2—C9 | 1.382 (3) | C12—H12B | 0.9600 |
| C3—C6 | 1.394 (3) | C12—H12C | 0.9600 |
| C3—C13 | 1.494 (3) | C13—H13A | 0.9600 |
| C4—H4A | 0.9600 | C13—H13B | 0.9600 |
| C4—H4B | 0.9600 | C13—H13C | 0.9600 |

| | | | |
|---|---|---|---|
| Cl1—Cu1—Cl2 | 171.17 (2) | C6—C5—H5 | 120.5 |
| Cl1—Cu1—O1 | 97.06 (4) | C6—C5—C10 | 118.99 (19) |
| Cl2—Cu1—O1 | 91.73 (4) | C10—C5—H5 | 120.5 |

| | | | |
|---|---|---|---|
| N2—Cu1—Cl1 | 89.37 (5) | C3—C6—H6 | 120.0 |
| N2—Cu1—Cl2 | 88.82 (5) | C5—C6—C3 | 120.0 (2) |
| N2—Cu1—O1 | 95.90 (6) | C5—C6—H6 | 120.0 |
| N2—Cu1—N1 | 171.61 (7) | N2—C7—H7 | 118.7 |
| N1—Cu1—Cl1 | 90.74 (5) | N2—C7—C11 | 122.6 (2) |
| N1—Cu1—Cl2 | 89.79 (5) | C11—C7—H7 | 118.7 |
| N1—Cu1—O1 | 92.42 (6) | N1—C8—H8 | 118.6 |
| Cu1—O1—H1 | 121 (2) | N1—C8—C10 | 122.9 (2) |
| C12—O1—Cu1 | 128.53 (13) | C10—C8—H8 | 118.6 |
| C12—O1—H1 | 109 (2) | C2—C9—H9 | 120.6 |
| C1—N2—Cu1 | 122.19 (13) | C2—C9—C11 | 118.84 (19) |
| C1—N2—C7 | 118.63 (17) | C11—C9—H9 | 120.6 |
| C7—N2—Cu1 | 119.16 (14) | C5—C10—C8 | 118.7 (2) |
| C3—N1—Cu1 | 121.89 (13) | C5—C10—H10 | 120.7 |
| C8—N1—Cu1 | 119.60 (13) | C8—C10—H10 | 120.7 |
| C8—N1—C3 | 118.50 (17) | C7—C11—H11 | 120.6 |
| N2—C1—C2 | 121.29 (18) | C9—C11—C7 | 118.87 (19) |
| N2—C1—C4 | 117.75 (17) | C9—C11—H11 | 120.6 |
| C2—C1—C4 | 120.96 (18) | O1—C12—H12A | 109.5 |
| C1—C2—H2 | 120.1 | O1—C12—H12B | 109.5 |
| C9—C2—C1 | 119.71 (19) | O1—C12—H12C | 109.5 |
| C9—C2—H2 | 120.1 | H12A—C12—H12B | 109.5 |
| N1—C3—C6 | 120.91 (19) | H12A—C12—H12C | 109.5 |
| N1—C3—C13 | 118.02 (17) | H12B—C12—H12C | 109.5 |
| C6—C3—C13 | 121.06 (19) | C3—C13—H13A | 109.5 |
| C1—C4—H4A | 109.5 | C3—C13—H13B | 109.5 |
| C1—C4—H4B | 109.5 | C3—C13—H13C | 109.5 |
| C1—C4—H4C | 109.5 | H13A—C13—H13B | 109.5 |
| H4A—C4—H4B | 109.5 | H13A—C13—H13C | 109.5 |
| H4A—C4—H4C | 109.5 | H13B—C13—H13C | 109.5 |
| H4B—C4—H4C | 109.5 | | |

| | | | |
|---|---|---|---|
| Cu1—N2—C1—C2 | −178.36 (14) | C1—C2—C9—C11 | −1.5 (3) |
| Cu1—N2—C1—C4 | 1.1 (2) | C2—C9—C11—C7 | 0.6 (3) |
| Cu1—N2—C7—C11 | 177.53 (17) | C3—N1—C8—C10 | −0.1 (3) |
| Cu1—N1—C3—C6 | −178.70 (15) | C4—C1—C2—C9 | −178.23 (18) |
| Cu1—N1—C3—C13 | 0.6 (3) | C6—C5—C10—C8 | 1.1 (3) |
| Cu1—N1—C8—C10 | 179.63 (16) | C7—N2—C1—C2 | 0.0 (3) |
| N2—C1—C2—C9 | 1.2 (3) | C7—N2—C1—C4 | 179.42 (18) |
| N2—C7—C11—C9 | 0.5 (3) | C8—N1—C3—C6 | 1.0 (3) |
| N1—C3—C6—C5 | −0.9 (3) | C8—N1—C3—C13 | −179.70 (19) |
| N1—C8—C10—C5 | −1.0 (3) | C10—C5—C6—C3 | −0.2 (3) |
| C1—N2—C7—C11 | −0.9 (3) | C13—C3—C6—C5 | 179.8 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···Cl2$^{i}$ | 0.75 (3) | 2.37 (3) | 3.1033 (16) | 169 (3) |

| | | | | |
|---|---|---|---|---|
| C7—H7···O1 | 0.93 | 2.46 | 3.148 (3) | 130 |
| C8—H8···O1 | 0.93 | 2.34 | 3.036 (3) | 131 |
| C11—H11···Cl2$^{ii}$ | 0.93 | 2.83 | 3.624 (2) | 143 |

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