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**Key indicators**

Single-crystal X-ray study  
 T = 150 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$   
 R factor = 0.028  
 wR factor = 0.075  
 Data-to-parameter ratio = 19.0

For details of how these key indicators were  
 automatically derived from the article, see  
<http://journals.iucr.org/e>.

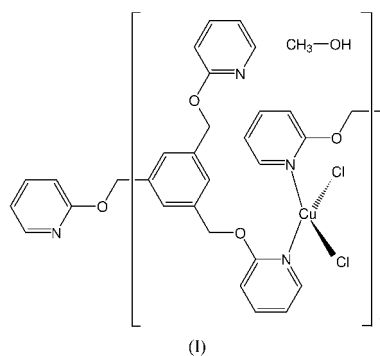
**catena-Poly[[[dichlorocopper(II)]- $\mu$ -1,3,5-  
 tris(2-pyridyloxymethyl)benzene] methanol  
 solvate]**

In the title compound,  $\{[\text{CuCl}_2(\text{tpomb})] \cdot \text{CH}_3\text{OH}\}_n$  [where  
 tpomb = 1,3,5-tris(2-pyridyloxymethyl)benzene,  $\text{C}_{24}\text{H}_{21}\text{N}_3\text{O}_3$ ],  
 two pyridyloxymethyl pendant arms of the tpomb ligand  
 bridge  $\text{Cu}^{\text{II}}$  centres *via* Cu–N bonds to form one-dimensional  
 coordination polymer chains.

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**Comment**

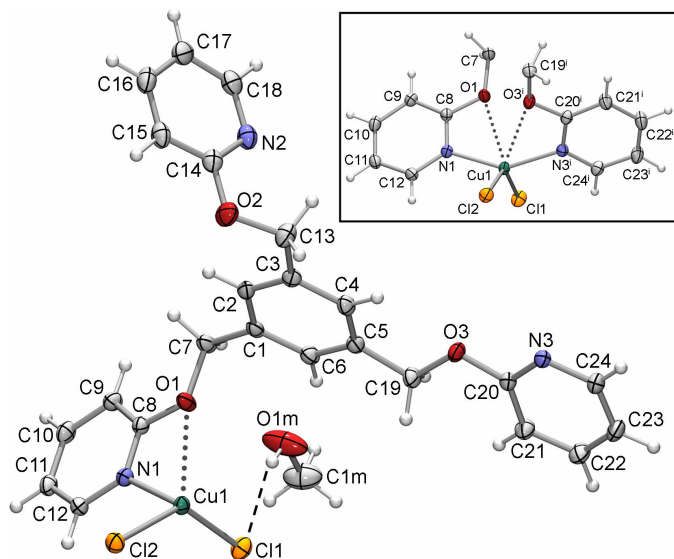
We have been investigating the molecular and polymeric  
 structures of metal complexes with tripodal ligands and,  
 in particular, those that incorporate pyridyl donors. The structure  
 reported here, (I), was obtained during those investigations.



In (I), two pyridyloxymethyl pendant arms of 1,3,5-tris(2-pyridyloxymethyl)benzene (tpomb) bridge  $\text{Cu}^{\text{II}}$  atoms *via* Cu–N bonds, forming a one-dimensional coordination polymer chain. The remaining pyridyloxymethyl pendant arm does not coordinate to a metal centre but is instead involved in an offset face-to-face aryl–aryl interaction with a coordinated pyridyl ring in an adjacent chain.

The coordination sphere of each  $\text{Cu}^{\text{II}}$  atom comprises two pyridyl donors (from two different ligands in the polymer chain), as well as two chloride ligands. The resulting Cu coordination stereochemistry is intermediate between tetrahedral and square planar (see Fig. 1 for a graphical illustration and Table 1 for pertinent bond lengths and angles). There are two weaker Cu  $\cdots$  O contacts that, at 2.6445 (11) (Cu1  $\cdots$  O1) and 2.8146 (11)  $\text{Å}$  [Cu1  $\cdots$  O3<sup>i</sup>; symmetry code: (i)  $\frac{1}{2} + x, y, \frac{3}{2} - z$ ], are longer than typical Cu–O coordinate bonds. While possibly not true coordinate bonds, these Cu to O contacts are almost certainly significant in the observed configurational organization of the pyridyloxymethyl pendant arms around the  $\text{Cu}^{\text{II}}$  atoms.

The conformation of the tpomb ligand is not only influenced by the coordination geometry of the pyridyloxymethyl groups



**Figure 1**

The asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level. The dotted line represents the Cu1...O1 contact and the dashed line represents the CH<sub>3</sub>OH to Cl hydrogen bond. The insert shows the complete coordination sphere of the Cu<sup>II</sup> centre. [Symmetry code: (i)  $\frac{1}{2} + x, y, \frac{3}{2} - z$ .]

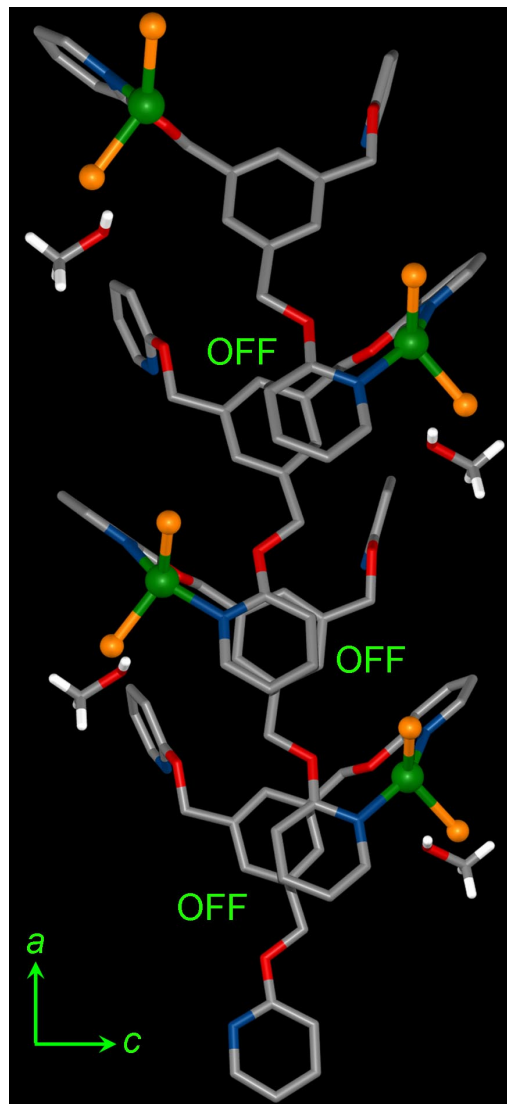
around the Cu<sup>II</sup> centres but also by an intrachain offset face-to-face aryl-aryl interaction between the central benzene ring and a pyridyl arm from an adjacent ligand, as illustrated in Fig. 2.

The methanol solvent molecule is involved in a hydrogen bond to one of the chloride ligands (geometrical details of which are provided in Table 2).

## Experimental

For the preparation of 1,3,5-tris(2-pyridyloxymethyl)benzene (tpomb), a mixture of 1,3,5-tris(hydroxymethyl)benzene (0.75 g, 4.5 mmol), 2-bromopyridine (2.21 g, 14 mmol) and potassium hydroxide (2.5 g, 45 mmol) was refluxed in toluene (30 ml) for 48 h. The solvent was then removed under vacuum and the residue partitioned between chloroform (50 ml) and water (50 ml). The organic layer was separated, washed with saturated aqueous NaCl and then dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> before removing the solvent under vacuum. The solid residue was then triturated with cold methanol to give tpomb as a pale-yellow powder (0.5 g, 30%) (m.p. 339–340 K). <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>, 300 K): δ 5.41 (s, CH<sub>2</sub>, 6H), 6.7–8–6.91 (m, pyridine, 6H), 7.51 (s, C<sub>6</sub>H<sub>3</sub>, 3H), 7.54–7.63 (m, pyridine, 3H), 8.18 (d, pyridine, 3H). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>, 300 K): δ 67.28 (CH<sub>2</sub>), 111.36, 116.95, 126.91, 138.63, 146.85 (aromatic), 137.91, 163.58 (quarternary aromatic). MS (ES) *m/z* = 400.0 (*M* + H)<sup>+</sup>. Found (%): C 71.65, H 5.31, N 10.28; C<sub>24</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>·0.25CH<sub>4</sub>O requires: C 71.47, H 5.45, N 10.32.

CuCl<sub>2</sub>·2H<sub>2</sub>O (0.060 g, 0.35 mmol) in ethanol (6 ml) was added to a solution of tpomb (0.15 g, 0.37 mmol) in ethanol (12 ml) to give a finely divided blue precipitate with empirical formula [Cu(tpomb)Cl<sub>2</sub>]<sub>0.5</sub>H<sub>2</sub>O (0.10 g, 50%). Found (%): C 53.00, H 4.07, N 7.62; C<sub>24</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>·0.5H<sub>2</sub>O requires: C 53.10, H 4.08, N 7.74. Small pale-green crystals of the title compound were obtained by recrystallization of the above fine blue solid from a methanol solution.



**Figure 2**

The coordination polymer chains propagate parallel to the *a* axis (C grey, Cu green, Cl orange, N blue and O red; H atoms omitted). A section of one such chain is illustrated above. The conformation of the tpomb ligand is determined by the coordinate bonding of the pyridyloxymethyl pendant arms as well as by intrachain Offset Face-to-Face (OFF) interaction.

### Crystal data

[CuCl<sub>2</sub>(C<sub>24</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>)]·CH<sub>4</sub>O  
*M<sub>r</sub>* = 565.92  
 Orthorhombic, *Pbca*  
*a* = 12.7397 (8) Å  
*b* = 15.6191 (10) Å  
*c* = 25.0173 (15) Å  
*V* = 4978.0 (5) Å<sup>3</sup>  
*Z* = 8  
*D<sub>x</sub>* = 1.510 Mg m<sup>-3</sup>

Mo Kα radiation  
 Cell parameters from 16 661 reflections  
 $\theta$  = 2.2–28.2°  
 $\mu$  = 1.13 mm<sup>-1</sup>  
*T* = 150 (2) K  
 Plate, pale-green  
 0.35 × 0.34 × 0.15 mm

### Data collection

Siemens SMART 1000 CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1999)  
 $T_{\min}$  = 0.717,  $T_{\max}$  = 0.844  
 46 409 measured reflections

6076 independent reflections  
 5070 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}}$  = 0.031  
 $\theta_{\text{max}}$  = 28.4°  
 $h$  = -16 → 17  
 $k$  = -20 → 20  
 $l$  = -33 → 33

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.075$   
 $S = 1.03$   
 6076 reflections  
 320 parameters  
 H atoms treated by a mixture of  
 independent and constrained  
 refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 2.1134P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.003$   
 $\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cu1—N1	1.9782 (12)	Cu1—Cl1	2.2782 (4)
Cu1—N3 <sup>i</sup>	1.9888 (12)	Cu1—O1	2.6445 (11)
Cu1—Cl2	2.2352 (4)	Cu1—O3 <sup>i</sup>	2.8146 (11)
N1—Cu1—N3 <sup>i</sup>	147.39 (5)	Cl2—Cu1—O1	130.62 (3)
N1—Cu1—Cl2	96.48 (4)	Cl1—Cu1—O1	92.73 (3)
N3 <sup>i</sup> —Cu1—Cl2	98.47 (4)	N1—Cu1—O3 <sup>i</sup>	102.71 (4)
N1—Cu1—Cl1	93.40 (4)	N3 <sup>i</sup> —Cu1—O3 <sup>i</sup>	51.95 (4)
N3 <sup>i</sup> —Cu1—Cl1	97.78 (4)	Cl2—Cu1—O3 <sup>i</sup>	80.79 (3)
Cl2—Cu1—Cl1	131.983 (17)	Cl1—Cu1—O3 <sup>i</sup>	141.76 (3)
N1—Cu1—O1	54.92 (4)	O1—Cu1—O3 <sup>i</sup>	70.05 (3)
N3 <sup>i</sup> —Cu1—O1	93.87 (4)		

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

**Table 2**

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1m-H1m\cdots Cl1$	0.793 (9)	2.463 (13)	3.2161 (16)	159 (2)

C-bound H atoms were included in idealized positions and refined using a riding-model approximation with methylene, methyl and aromatic bond lengths fixed at 0.99, 0.98 and 0.95  $\text{\AA}$ , respectively.  $U_{\text{iso}}(\text{H})$  values were fixed at  $1.2U_{\text{eq}}$  of the parent C atoms for methylene and aromatic H atoms, and at  $1.5U_{\text{eq}}$  of the parent C atoms for methyl H atoms. The hydroxy H atom was located in a Fourier difference map and refined with the following restraints: O—H = 0.8 (1)  $\text{\AA}$ , C···H = 1.95 (2)  $\text{\AA}$  and  $U_{\text{iso}}$  fixed at  $1.5U_{\text{eq}}$  of the parent O atom.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINTE* (Siemens, 1995); data reduction: *SAINTE* and *XPREP* (Siemens, 1995); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *enCIFer* (Version 1.0; Allen *et al.*, 2004) and *WinGX-32* (Farrugia, 1999).

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