# metal-organic papers

## Poly[di-$\mu_3$-chloro-$\mu_2$-1,2-di-4-pyridylethene-1:2$\kappa^2 N,N'$-dicopper(I)]

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**Key indicators**

Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.005 Å
$R$ factor = 0.040
$wR$ factor = 0.086
Data-to-parameter ratio = 13.4

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

The structure of the title compound, $[Cu_2Cl_2(C_{12}H_{10}N_2)]_n$, shows that each $Cu^I$ ion is tetrahedral, being coordinated by three Cl atoms and one N atom of the 1,2-bis(4-pyridyl)ethene ligand (BPE, $C_{12}H_{10}N_2$). Cl atoms and BPE molecules bridge the $Cu^I$ ions to form a two-dimensional layer structure through inversion centres located at the mid-point of the $Cu_2Cl_2$ bridge and at the mid-point of the C=C double bond of the BPE ligand.

## Comment

A contemporary focus in the chemistry of copper halides is the rational design and synthesis of organic–inorganic hybrid copper halides to explore potential applications in areas of molecular adsorption, catalysis, electromagnetism and photochemistry (Naether *et al.*, 2002; Meyer & Nockemann, 2001; Yaghi & Li, 1995). The architectures of copper halides can be tuned at the molecular level so as to possess interesting topological structures and unusual electronic properties, for use in various components and with potential applications in the above-mentioned areas (Wang *et al.*, 2003). More recently, owing to the introduction of the hydrothermal technique and various N-containing organic templating agents, a variety of novel organic–inorganic hybrid copper halides have been isolated with one-dimensional chain-like (Hammond *et al.*, 1999; Lu *et al.*, 1998) and two-dimensional layer-like structures (Chestnut *et al.*, 1999; Bailey & Pennington, 2000). We present here the title compound, (I).



(I)
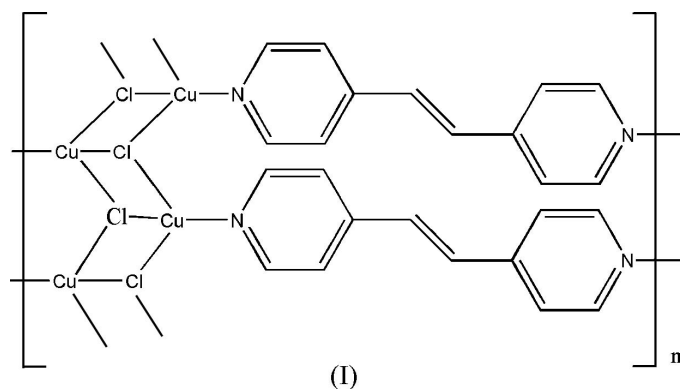
In (I), the Cu atom has a distorted tetrahedral coordination geometry, being coordinated by one N atom of a 1,2-bis(4-pyridyl)ethene (BPE) molecule and three Cl atoms. Each Cl atom is triply bridging to three Cu atoms, resulting in the formation of a ladder-like structure (Fig. 1). The BPE molecules act as bridging ligands, connecting two ladders to build up a two-dimensional layer structure (Fig. 2). This two-
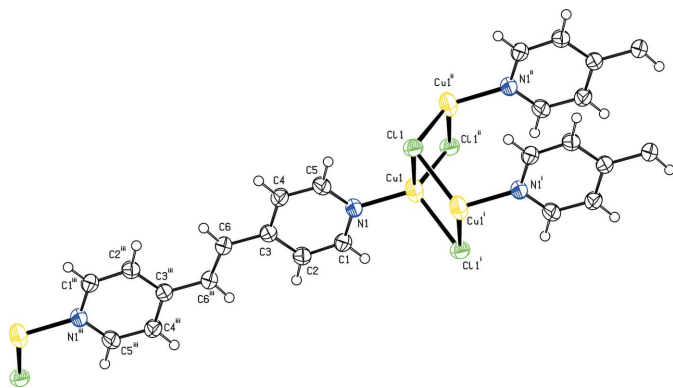
**Figure 1**
Part of the polymeric structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii. [Symmetry codes: (i) $-x, 1 - y, -z$; (ii) $1 - x, 1 - y, -z$; (iii) $-x, 2 - y, -z$.]

dimensional layer structure is arranged around inversion centres located at the mid-point of the $Cu_2Cl_2$ ring and at the mid-point of the C=C double bond of the BPE ligand.

## Experimental

The title compound was synthesized by the hydrothermal method from a mixture of biphenyl-4,4′-dicarboxylic acid (0.06 g, 0.25 mmol), copper(II) chloride dihydrate (0.04 g, 0.20 mmol), 1,2-bis(4-pyridyl)ethene (0.40 g, 2.20 mmol) and water (8.00 ml) in a 15 ml Telfon-lined stainless steel reactor. The solution was heated at 423 K for 4 d. After reaction, the vessel was slowly cooled to room temperature to give red plate crystals. The crystals were collected, washed with distilled water and dried in air. As shown by the crystal structure analysis, the biphenyl-4,4′-dicarboxylic acid was not incorporated into the product.

### Crystal data

| | |
|---|---|
| $[Cu_2Cl_2(C_{12}H_{10}N_2)]$ | $Z = 2$ |
| $M_r = 380.20$ | $D_x = 2.051$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 3.7824$ (4) Å | $\mu = 3.87$ mm$^{-1}$ |
| $b = 15.0560$ (17) Å | $T = 298$ (2) K |
| $c = 10.8776$ (12) Å | Platelet, red |
| $\beta = 96.301$ (2)° | $0.34 \times 0.20 \times 0.05$ mm |
| $V = 615.71$ (12) Å$^3$ | |

### Data collection

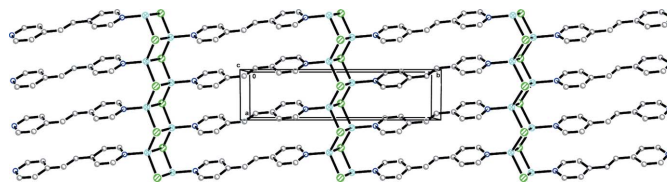| | |
|---|---|
| Bruker APEX area-detector diffractometer | 3198 measured reflections |
| $\varphi$ and $\omega$ scans | 1097 independent reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2000) | 1050 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.405$, $T_{max} = 0.822$ | $R_{int} = 0.018$ |
| | $\theta_{max} = 25.1°$ |



**Figure 2**
A perspective view of the two-dimensional layer-like structure. H atoms have been omitted for clarity.

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0271P)^2$ |
| $R[F^2 > 2\sigma(F^2)] = 0.040$ | $+ 1.1726P]$ |
| $wR(F^2) = 0.086$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.17$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 1097 reflections | $\Delta\rho_{max} = 0.64$ e Å$^{-3}$ |
| 82 parameters | $\Delta\rho_{min} = -0.53$ e Å$^{-3}$ |
| H-atom parameters constrained | |

All H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of C—H = 0.93 Å with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Bruker, 2002); software used to prepare material for publication: *SHELXTL* (Bruker, 2002).

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