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Poly[[(isonicotinic acid-κN)copper(I)]-μ_3-chloro]

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The crystal structure of the title compound, $[CuCl(C_6H_5O_2)]_n$, exhibits polymeric chains extended in the *b*-axis direction, with a shortest Cu···Cu distance of 2.885 (2) Å. The Cu atom is tetrahedrally coordinated by three Cl atoms, each of which bridges three metal atoms, and the N atom of isonicotinic acid. The Cu and Cl atoms lie on mirror planes, across which the isonicotinic acid ligands are disordered. Each Cu_2Cl_2 ring is centrosymmetric. The carboxyl groups are connected by O—H···O hydrogen bonds into an infinite chain running in the [101] direction. The Cu—Cl bond distances are 2.343 (1) and 2.483 (2) Å, while Cu—N is 1.976 (5) Å.

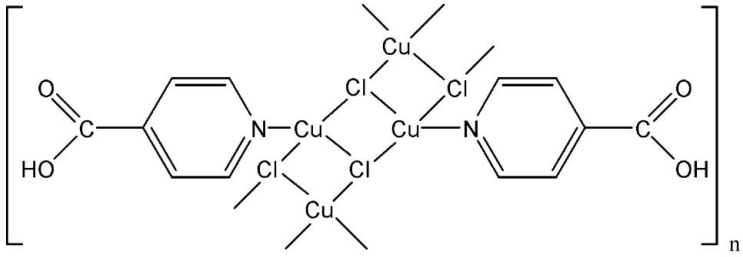
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
Disorder in main residue
R factor = 0.038
wR factor = 0.112
Data-to-parameter ratio = 10.0

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

Comment

Recently, much effort in metal-organic frameworks has been focused on coordination polymers with organic rod–like rigid ligands containing either *N*- or *O*-donors; the isonicotinic acid ligand is a combination of both. Until now, a large number of metal-organic framework structures containing isonicotinic acid ligands have been reported, including copper isonicotinates (Chapman *et al.*, 2001; Yu *et al.*, 2002; Kang *et al.*, 2004; Lu *et al.*, 2003; Goher & Mak, 1987), cobalt isonicotinate (Feng *et al.*, 2006) and rare-earth isonicotinates (Zhang *et al.*, 2005).



(I)

We present here the synthesis and crystal structure of the title polymeric compound, (I) (Fig. 1). The Cu atom is tetra-

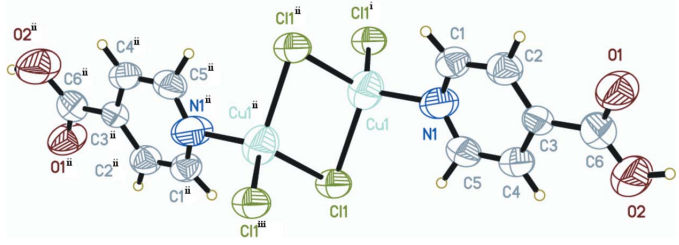


Figure 1
Part of the polymeric structure of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, -y, 1-z$; (iii) $x, 1-y, z$.]

hedrally coordinated by three Cl^- ions and one N atom from an isonicotinic acid ligand (Fig. 1 and Table 1); each of the Cl^- ions bridges three Cu atoms, generating a polymeric $[Cu-Cl]_n$ chain. The Cu and Cl atoms lie on mirror planes, across which the isonicotinic acid ligands are disordered. Each Cu_2Cl_2 ring is centrosymmetric. The geometric parameters are in agreement with those found in reported copper nicotinates (Bai *et al.*, 2005).

The carboxyl groups of isonicotinic acid are involved in O—H···O hydrogen bonds [O2—H2···O1^{i}: O2—H2 = 0.88 (5) Å, H2···O1^{i} = 1.88 (5) Å, O2···O1^{i} = 2.676 (7) Å and O2—H2···O1^{i} = 151 (4)°; symmetry code: (i) $-1-x, \frac{1}{2}+y, -z$] (Fig. 2). It is generally accepted that Cu^{II} cations can be reduced to Cu^{I} by pyridine derivatives under hydrothermal conditions. Although $Cu(OAc)_2$ was used as a starting material, copper(I) is observed in (I). Cu^{II} can be reduced to Cu^{I} by reduction involving isonicotinic acid (Zhang *et al.*, 2005).

Experimental

Orange needle-like crystals were hydrothermally synthesized from a mixture of $CuCl_2$ (0.0637 g), $MnCl_2$ (0.3541 g), isonicotinic acid (0.2438 g), H_3BO_3(0.0219 g), HCl (0.165 g), and H_2O (8 g). The mixture was kept in a 25 ml Teflon-lined steel autoclave at 443 K for 10 d. The autoclave was slowly cooled to room temperature, and then the product was filtered, washed with distilled water, and dried at room temperature.

Crystal data

$[CuCl(C_6H_5NO_2)]$
M_r = 222.10
Monoclinic, $P2_1/m$
a = 7.109 (4) Å
b = 3.732 (2) Å
c = 14.073 (7) Å
β = 101.381 (6)°
V = 366.1 (3) Å^3
Z = 2
D_x = 2.015 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.29 mm^{-1}
T = 293 (2) K
Needle, orange
0.20 × 0.08 × 0.06 mm

Data collection

Bruker APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.559, T_{max} = 0.827
3328 measured reflections
836 independent reflections
657 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.112
S = 1.06
836 reflections
84 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 0.1373P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

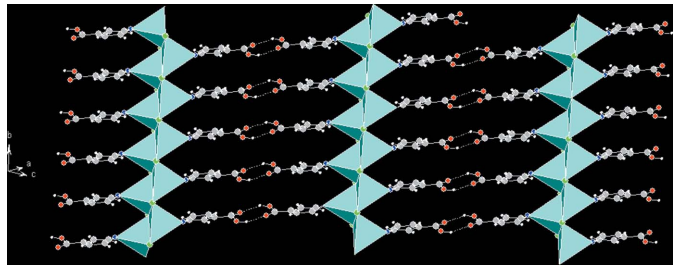


Figure 2
The crystal structure of (I), showing the polymeric tehrahedra with hydrogen-bonded (dashed lines) carboxyl groups of nicotinic acid.

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.976 (5)	Cu1—Cl1	2.4831 (18)
N1—Cu1—Cl1^{i}	116.43 (8)	Cu1^{i}—Cl1—Cu1^{ii}	105.58 (7)
N1—Cu1—Cl1	104.35 (15)	Cu1^{i}—Cl1—Cu1	73.36 (4)

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

Because of the symmetry, the isonicotinic acid molecule was refined using a split model with an occupancy of 0.5 for atoms C1, C2, C3, C6 and O1. C-bound H atoms were positioned geometrically (C—H = 0.96 Å) and refined using a riding model. The hydroxy H atom was located in a difference map and refined with U_{iso}(H) = 1.2U_{eq}(O); O—H = 0.67 (2) Å.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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