Acta Crystallographica Section E
**Structure Reports**
**Online**

ISSN 1600-5368

# A polymeric copper(II) complex bridged by benzene-1,3,5-tricarboxylate

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Received 8 July 2005
Accepted 11 August 2005
Online 17 August 2005

**Key indicators**

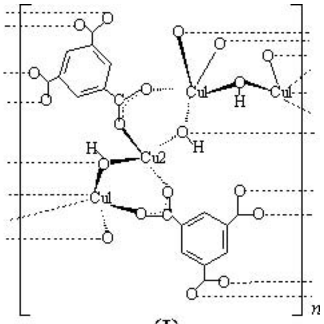
Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.023
$wR$ factor = 0.065
Data-to-parameter ratio = 9.9

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

The asymmetric unit of the title polymer, poly[copper(II)-$\mu_6$-benzene-1,3,5-tricarboxylato-tri-$\mu_3$-hydroxo], $[Cu_3(C_9H_3O_6)(OH)_3]_n$, contains two independent Cu$^{II}$ atoms, one located in a general position assuming a pyramidal coordination geometry, and the other located on an inversion center assuming a square-planar geometry. The benzenetricarboxylate and hydroxo groups bridge the Cu$^{II}$ atoms to form a three-dimensional polymeric structure.

## Comment

Benzenetricarboxylate (BTC) usually plays the role of a bridging ligand in metal complexes. We present here the structure of the title Cu$^{II}$ complex $[Cu_3(OH)_3BTC]_n$, (I), in which BTC ligands link the Cu$^{II}$ atoms to form a three-dimensional polymeric complex.



(I)

A sheet of the three-dimentional polymeric structure of (I) is shown in Fig. 1. The asymmetric unit contains two Cu$^{II}$ atoms; atom Cu1 is located on a general position and assumes a pyramidal coordination geometry formed by two BTC and three hydroxo groups (O2), while atom Cu2 is located at an inversion center and assumes a distorted square-planar coordination geometry formed by two BTC and two hydroxo groups (Table 1). Each BTC bridges six Cu$^{II}$ atoms to form the two-dimentional polymeric sheet, all carboxylate groups of the BTC coordinating to Cu$^{II}$ atoms in a bidentate chelating fashion. The O1 hydroxo group is located on a twofold axis and bridges two neighboring Cu1 atoms. The O2 hydroxo group is located at a general position and bridges three Cu atoms (two Cu1 and one Cu2); thus the two-dimensional polymeric sheets are linked to form the three-dimensional polymeric structure.

## Experimental

An aqueous solution (20 ml) of benzene-1,3,5-tricarboxylic acid ($H_3BTC$) (0.105 g), adipic acid (0.073 g) and NaOH (0.04 g) was mixed with an aqueous solution (10 ml) of $Cu(NO_3)_2 \cdot 3H_2O$ with continuous stirring. The mixture was sealed in a 40 ml Teflon-lined stainless steel vessel and heated at 453 K for 96 h under autogenous conditions. After cooling to room temperature, the resulting product was filtered off to obtain blue crystals of (I) (about 90% yield based on the Cu source). IR (KBr, $\nu$ $cm^{-1}$): 3450, 3068, 1612, 1540, 1437, 1379, 754, 723, 589, 484; Elemental analysis calculated for $C_9H_6Cu_3O_9$: C 24.09, H 1.35%; found: C 23.94, H 1.46%.

*Crystal data*

$[Cu_3(C_9H_3O_6)(OH)_3]$
$M_r = 448.76$
Monoclinic, $P2_1/m$
$a = 3.6100$ (11) Å
$b = 14.110$ (4) Å
$c = 10.915$ (3) Å
$\beta = 97.060$ (4)°
$V = 551.8$ (3) Å$^3$
$Z = 2$

$D_x = 2.701$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1551 reflections
$\theta = 2.4$–24.9°
$\mu = 5.78$ mm$^{-1}$
$T = 293$ (2) K
Block, blue
0.14 × 0.12 × 0.08 mm

*Data collection*

Bruker APEX-II CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.376$, $T_{max} = 0.630$
2985 measured reflections

1020 independent reflections
914 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.0°$
$h = -4 \rightarrow 3$
$k = -16 \rightarrow 16$
$l = -9 \rightarrow 12$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.065$
$S = 1.01$
1020 reflections
103 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.6748P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.75$ e Å$^{-3}$
$\Delta\rho_{min} = -0.38$ e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.9444 (18) | Cu1—O5 | 1.953 (2) |
| Cu1—O2 | 1.925 (2) | Cu2—O2 | 1.875 (2) |
| Cu1—O2$^{i}$ | 2.496 (3) | Cu2—O3 | 1.983 (2) |
| Cu1—O4 | 1.950 (2) | | |

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

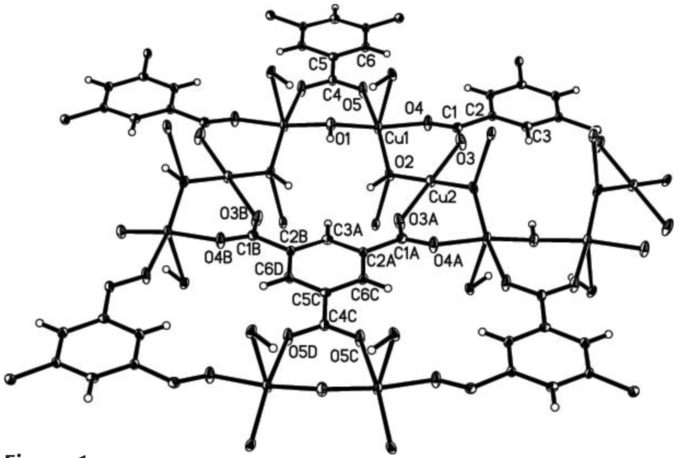


**Figure 1**
A sheet of the polymeric molecular structure of (I), shown with 50% probability displacement ellipsoids (arbitrary spheres for H atoms). [Symmetry codes: (*A*) $-x, 1-y, 1-z$; (*B*) $-x, -\frac{1}{2}+y, 1-z$; (*C*) $x, -2+y, -1+z$; (*D*) $-2+x, -y+\frac{1}{2}, -1+z$.]

C-bound H atoms were placed in geometrically idealized positions, with C—H = 0.93 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms on hydroxo groups were located in a difference Fourier map and refined as riding in their as-found position relative to the O atoms, with $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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