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catena-Poly[[tetrakis(μ-2,4-dichlorophenoxyacetato-κ^2O:O')dicopper(II)]-μ-pyrazine-κ^2N:N']

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Key indicators

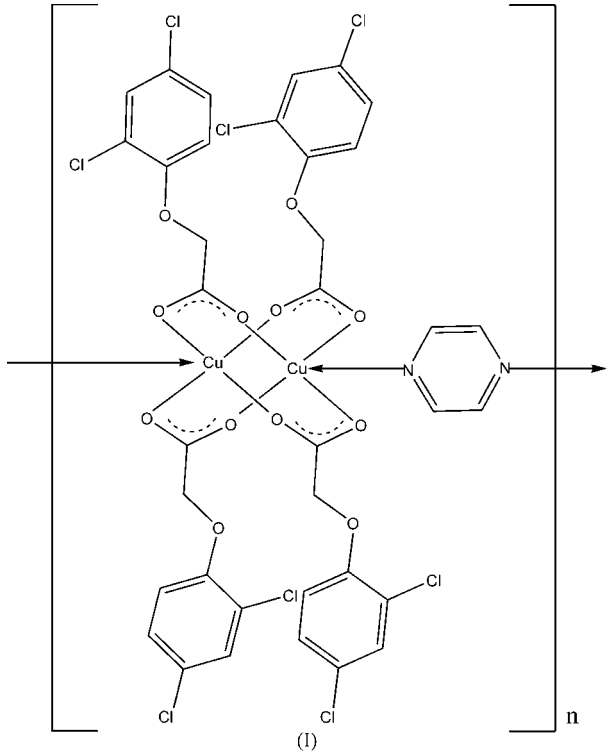
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.085
Data-to-parameter ratio = 12.7

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

The title complex, $[Cu_2(C_8H_5Cl_2O_3)_4(C_4H_4N_2)]_n$, crystallizes as a chain of alternating tetrakis(2,4-dichlorophenoxyacetato)dicopper(II) and pyrazine units in which square-pyramidal copper(II) centers are alternately linked by four bridging 2,4-dichlorophenoxyacetate anions and a single bridging pyrazine molecule. Both the dinuclear copper unit and the pyrazine ligand have a center of symmetry.

Comment

Phenoxyacetic acid and its derivatives are biologically active compounds which are widely used as herbicides and plant-growth substances. Due to their versatile bonding modes with metal ions, they have also been used in the synthesis of metal-organic frameworks (Psomas *et al.*, 2000; Liu *et al.*, 2004; Gao *et al.*, 2005). We report here the crystal structure of a new copper(II) complex, (I), obtained by reacting a copper salt with 2,4-dichlorophenoxyacetic acid and a pyrazine ligand.



(I)

As can be seen from Fig. 1, the asymmetric unit comprises one half of the tetrakis(2,4-dichlorophenoxyacetato)-dicopper(II) unit, and one half-pyrazine ligand; the complete dinuclear unit and pyrazine are generated by an inversion center. The square-pyramidal coordination geometry of the

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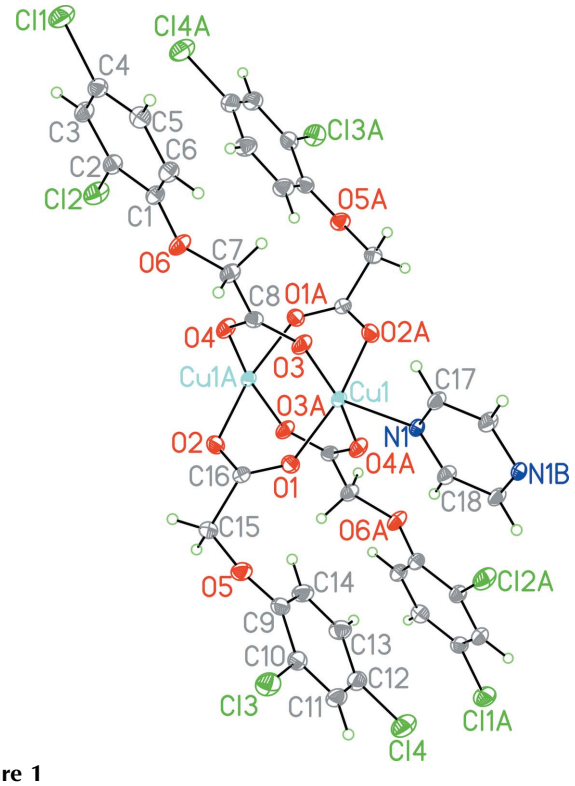

Figure 1
Part of the polymeric structure of the title complex with the atom-labeling scheme. Displacement ellipsoids are drawn at the 35% probability level. [Symmetry codes: (A) $1-x, 1-y, 1-z$; (B) $-x, 1-y, 1-z$.]

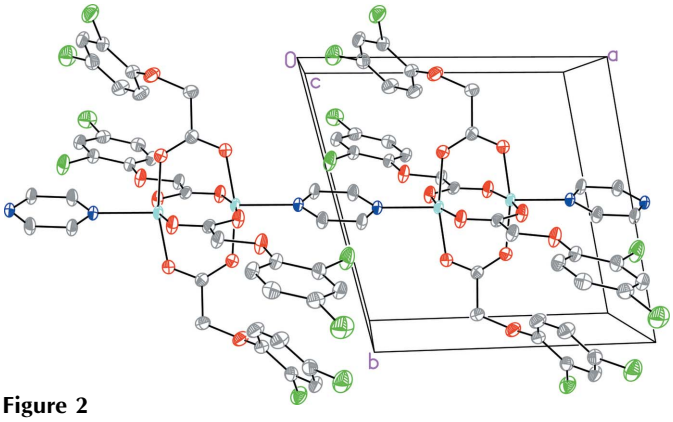

Figure 2
The one-dimensional chain structure of the title complex. H atoms have been omitted for clarity.

copper(II) atom comprises four basal O atoms from four bridging 2,4-dichlorophenoxyacetate anions and an apical N atom from a single bridging pyrazine molecule. The basic architectural motif of the extended structure is a one-dimensional chain of alternating tetrakis(2,4-dichlorophenoxyacetato)dicopper(II) and pyrazine units, as shown in Fig. 2.

Experimental

The title compound was obtained from a solvothermal reaction. Copper(II) nitrate trihydrate (0.06 g, 0.25 mmol), 2,4-dichlorophenoxyacetic acid (0.11 g, 0.5 mmol), pyrazine (0.04 g, 0.5 mmol), and acetonitrile (10 ml) were placed in a Teflon-lined stainless steel Parr bomb and heated at 353 K for 3 d, and then cooled slowly to room temperature, yielding green single crystals of the title compound.

Crystal data

$[Cu_2(C_8H_5Cl_2O_3)_4(C_4H_4N_2)]$
$M_r = 1087.26$
Triclinic, $P\overline{1}$
$a = 9.8662$ (3) Å
$b = 10.9610$ (4) Å
$c = 11.0262$ (3) Å
$\alpha = 63.467$ (2)°
$\beta = 78.764$ (2)°
$\gamma = 72.876$ (2)°
$V = 1016.73$ (6) Å^3
$Z = 1$
$D_x = 1.776$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.64$ mm^{-1}
$T = 296$ (2) K
Block, green
0.24 × 0.14 × 0.10 mm

Data collection

Bruker SMART APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.699$, $T_{max} = 0.859$
8012 measured reflections
3444 independent reflections
2807 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.085$
$S = 1.01$
3444 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O2^{i}	1.9573 (18)	Cu1—O3	1.9734 (19)
Cu1—O1	1.9713 (17)	Cu1—N1	2.204 (2)
Cu1—O4^{i}	1.9734 (19)		
O2^{i}—Cu1—O1	166.77 (8)	O4^{i}—Cu1—O3	166.87 (8)
O2^{i}—Cu1—O4^{i}	89.96 (8)	O2^{i}—Cu1—N1	101.10 (8)
O1—Cu1—O4^{i}	88.11 (8)	O1—Cu1—N1	92.09 (7)
O2^{i}—Cu1—O3	89.09 (8)	O4^{i}—Cu1—N1	93.73 (8)
O1—Cu1—O3	89.83 (8)	O3—Cu1—N1	99.30 (7)

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

All H atoms were placed in idealized positions and constrained to ride on their parent C atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic, and C—H = 0.97 Å and U_{iso}(H)= 1.2U_{eq}(C) for methylene H atoms.

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

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