Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

A one-dimensional coordination polymer of copper(II) with 2-pyrazinecarboxylate

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Received 24 January 2005
Accepted 2 February 2005
Online 12 February 2005

A new one-dimensional coordination polymer, *catena*-poly-[[aqua(nitrato-κ^2O,O')copper(II)]-μ-pyrazine-2-carboxylato-$\kappa^3N^1,O:N^4$], $[Cu(C_5H_3N_2O_2)(NO_3)(H_2O)]_n$, has been synthesized and characterized. The coordination environment of the copper(II) ion is distorted octahedral, arising from an *N*,*O*-bidentate 2-pyrazinecarboxylate ligand, an N atom from a symmetry-related 2-pyrazinecarboxylate ligand, a bidentate nitrate group and a water molecule. The chains interact by way of O—H···O hydrogen bonds and C—H···O interactions.

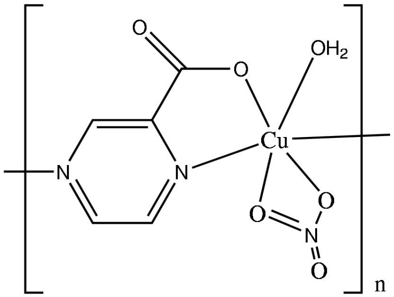
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.047
wR factor = 0.111
Data-to-parameter ratio = 13.7

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

Comment

The heterocyclic molecule 2-pyrazinecarboxylic acid can act as a versatile bridging or chelating ligand leading to extended metal-organic networks. For example, the one-dimensional polymeric copper(II) complexes $[Cu(pzca)(N_3)]_n$ (pzca = 2-pyrazinecarboxylate; Goher *et al.*, 1997), $[Cu(pzca)(N_3)(H_2O)]_n$ (Goher *et al.*, 1998) and $[Cu(pzca)Cl(H_2O)]_n$ (Nordell *et al.*, 2001) have been prepared. Cobalt(II) and manganese(II) complexes with pzca possess interesting magnetic properties (Liang *et al.*, 2002) and some bimetallic (Dong *et al.*, 2000*a*,*b*,*c*; Zheng *et al.*, 2000; Ciurtin *et al.*, 2001) coordination polymers have also been reported. In this paper, we report the crystal structure of the Cu^{II}/pzca coordination polymer, $[Cu(pzca)(NO_3)(H_2O)]_n$, (I).



(I)

The structure of (I) consists of copper(II) ions, 2-pyrazinecarboxylate anions, nitrate anions and water molecules (Fig. 1). The coordination environment of the copper(II) ion shows a distorted octahedral geometry, arising from an *N*,*O*-bidentate pzca ligand, an N atom from a symmetry-related pzca ligand, a bidentate nitrate group and a water molecule. The octahedron shows a typical Jahn–Teller axial distortion (Table 1), with the water O and one of the nitrate O atoms occupying the axial positions, and the two N atoms in *trans* conformation. The average Cu—N and Cu—O_{eq} bond lengths are 2.007 (4) and 1.965 (4) Å, respectively.

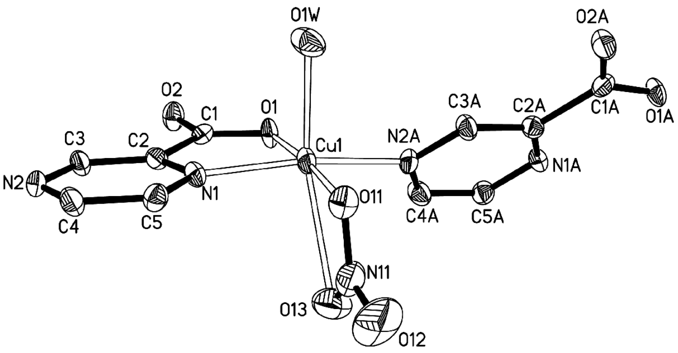


Figure 1
The coordination environment around the copper(II) ion in (I), shown with 30% probability displacement ellipsoids. H atoms have been omitted for clarity. Atoms with the A suffix were generated by the symmetry code (x, $-y$, $z - \frac{1}{2}$).

The different coordination behaviors of O11 (equatorial) and O13 (axial) are supported by the difference in bond lengths of N11—O11 [1.297 (7) Å] and N11—O13 [1.234 (7) Å], the latter being similar to the uncoordinated N11—O12 [1.220 (7) Å]. These differences suggest that the Cu1—O11 bond is much stronger than the Cu1—O13 bond. The copper(II) ion lies 0.132 (2) Å out of the square coordination plane toward atom O1*W*. Each pzca ligand links two copper(II) ions to form a one-dimensional chain structure extended along the *c* axis (Fig. 2).

The Cu1···Cu1^{i} [symmetry code; (i) $x, -y, z - \frac{1}{2}$] distance within a chain is 6.7458 (19) Å and the shortest Cu1···Cu1^{ii} [symmetry code: (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$] distance between chains is 5.9490 (15) Å. Adjacent chains are linked by hydrogen bonds between the O atoms of coordinated water and the uncoordinated O atom of carboxylate groups *via* H1*WB* (Table 2), forming two-dimensional sheets. A three-dimensional framework is constructed alternately from hydrogen bonds between the O atoms of coordinated water and the O atoms of coordinated carboxylate groups (*via* H1*WA*) and between the aromatic C atom of the pyrazine ring and the O atom of the nitrate anion (*via* H5*A*).

Experimental

To a solution of 2-pyrazinecarboxylic acid (124 mg, 1.0 mmol) in tetrahydrofuran (20 ml) was added a solution of $Cu(NO_3)_2\cdot 3H_2O$ (242 mg, 1.0 mmol) in ethanol (20 ml) with stirring. The resulting solution was refluxed for about 4 h and then filtered. Deep-blue crystals of (I) were obtained by evaporating the filtrate at room temperature. Elemental analysis found: C 23.10, H 1.86, N 15.80%; calculated for $C_5H_5CuN_3O_6$: C 22.50, H 1.89, N 15.75%.

Crystal data

$[Cu(C_5H_3N_2O_2)(NO_3)(H_2O)]$
$M_r = 266.66$
Monoclinic, $C2/c$
$a = 21.027$ (5) Å
$b = 6.3196$ (17) Å
$c = 13.382$ (4) Å
$\beta = 102.354$ (16)°
$V = 1737.0$ (8) Å^3
$Z = 8$
$D_x = 2.039$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3139 reflections
$\theta = 3.1$–27.5°
$\mu = 2.53$ mm^{-1}
$T = 293$ (2) K
Rod, blue
0.34 × 0.09 × 0.07 mm

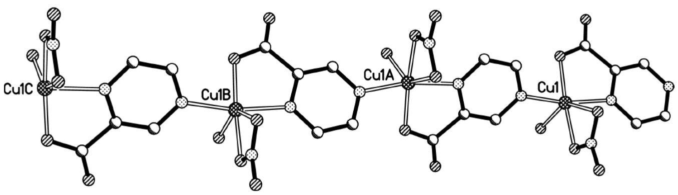


Figure 2
The one-dimensional chain structure of (I). Atoms Cu1A, Cu1B and Cu1C are generated by the symmetry codes ($x, -y, -\frac{1}{2} + z$), ($x, y, -1 + z$) and ($x, -y, -\frac{3}{2} + z$), respectively.

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Oscillation scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.761$, $T_{max} = 0.838$
3139 measured reflections
1966 independent reflections
948 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 27.5°$
$h = -27 \rightarrow 27$
$k = -7 \rightarrow 8$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.111$
$S = 0.81$
1966 reflections
143 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.84$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0006 (2)

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.963 (4)	Cu1—N2^{i}	2.011 (4)
Cu1—O11	1.968 (4)	Cu1—O1*W*	2.196 (4)
Cu1—N1	2.002 (4)	Cu1—O13	2.589 (5)
O1—Cu1—O11	174.34 (16)	N1—Cu1—O1*W*	93.00 (16)
O1—Cu1—N1	82.36 (16)	N2^{i}—Cu1—O1*W*	97.26 (17)
O11—Cu1—N1	95.06 (17)	O1—Cu1—O13	119.93 (19)
O1—Cu1—N2^{i}	90.15 (16)	O11—Cu1—O13	54.89 (19)
O11—Cu1—N2^{i}	91.51 (16)	N1—Cu1—O13	90.68 (16)
N1—Cu1—N2^{i}	167.77 (19)	N2^{i}—Cu1—O13	84.68 (17)
O1—Cu1—O1*W*	94.81 (18)	O1*W*—Cu1—O13	145.2 (2)
O11—Cu1—O1*W*	90.35 (18)		

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1^{ii}	0.845 (10)	2.02 (3)	2.817 (5)	156 (6)
O1*W*—H1*WB*···O2^{iii}	0.89 (6)	1.86 (6)	2.751 (6)	173 (7)
C5—H5*A*···O12^{iv}	0.93	2.25	2.977 (8)	135

Symmetry codes: (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$; (iii) $x, 1 + y, z$; (iv) $1 - x, 1 - y, 2 - z$.

The crystal was a weak scatterer, leading to a low percentage of observed $[I > 2\sigma(I)]$ reflections. The water H atoms were located in a difference Fourier map and refined with restrained O—H bond lengths [0.85 (2) Å] and fixed isotropic displacement parameters (0.080 Å^2). The C—H H atoms were placed at calculated positions and refined as riding, with C—H distances in the range 0.93–0.96 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

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Data collection: *RAPID-AUTO* (Rigaku, 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXTL* (Siemens, 1995).

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