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Polymeric bis(hydrogen pyrazine-2,3-dicarboxylato)copper(II) *N*,*N*′-dimethylformamide disolvate

Guang-Qi Xiang,[a] Nan-Wen Zhu,[b] Mao-Lin Hu,[a] Hong-Ping Xiao[a]* and Xiao-Xia Chen[a]

[a]Department of Chemistry and Materials Science, Wenzhou Normal College, Wenzhou 325027, People's Republic of China, and [b]School of Environmental Science and Engineering, Shanghai Jiao Tong University, Shanghai 200240, People's Republic of China

Correspondence e-mail: hp_xiao@wznc.zj.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.013 Å
R factor = 0.096
wR factor = 0.264
Data-to-parameter ratio = 12.3

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

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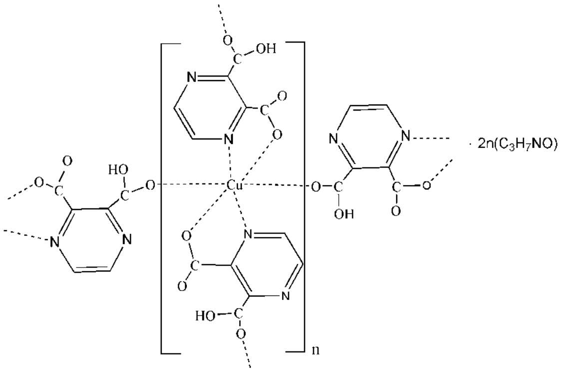
In the title compound, $\{[Cu(C_6H_3N_2O_4)_2]\cdot 2C_3H_7NO\}_n$, each copper(II) center is surrounded by two N atoms, two bridging carboxylate O atoms from two pyrazine-2,3-dicarboxylate anions, and two bridging carboxylate O atoms of two pyrazine-2,3-dicarboxylate anions from neighboring units, forming an elongated CuN_2O_4 octahedron. The $[Cu(C_6H_3N_2O_4)_2]$ blocks, with the copper(II) cation located on a center of inversion, are connected together by four μ-carboxylate bridges, creating a one-dimensional intersecting double chain.

Comment

Polymeric compounds play an important role in the field of molecular magnetism, and di- and polycarboxylates are good candidates for exhibiting such phenomena (Eddaoudi *et al.*, 2001; Konar *et al.*, 2004; Ptasiewicz-Bak & Leciejewicz, 2000; Zou *et al.*, 1999). In our previous work, we have been engaged in synthesizing polynuclear metal-organic frameworks using 1,4-benzenedicarboxylate and 1,2,4,5-benzenetetracarboxylate (Xiao *et al.*, 2004; Zhu *et al.*, 2004). We present here the structure of the title compound, $[Cu(Hpzdc)_2]\cdot(DMF)_2$, (I), formed with pyrazine-2,3-dicarboxylic acid (H_2pzdc).



(I)

In (I), each copper(II) cation, on an inversion center, is at the center of a distorted octahedron (Fig. 1), with a distinct Jahn–Teller effect. The basal plane [O1, O1^{ii}, N1, N1^{ii}; symmetry code: (ii) $-x, -y, 2-z$] consists of two N atoms and two carboxylate O atoms from two pyrazine-2,3-dicarboxylate ligands. The two apical positions are filled by the other two carboxylate O atoms [O4^{i} and O4^{iv}; symmetry code: (i) $x-1, y, z$; (iv) $1-x, 2-y, 2-z$] of neighboring units, the axial bonds distances [2.565 (2) Å] being longer than the equatorial Cu—O bond distances [1.919 (5) Å; Table 1]. The carboxylate group involved in chelation is almost coplanar with the pyrazine ring [dihedral angle of 3.70 (2)°], and the other carboxylate group is almost perpendicular to the pyrazine ring [dihedral angle of 93.90 (1)°]. This conformation was also observed in a series of transition metal complexes formed with pyrazine-2,3-dicarboxlate (Konar *et al.*, 2004). The hydrogenpyrazine-2,3-dicarboxylate anion chelates the copper(II) cation *via* the heterocyclic N atom and the deprotoned carboxylate O atom, and the unprotoned carboxylate group coordinates to another copper(II) cation of a neighboring unit, thus forming a novel kind of intersecting double-chain structure with a Cu···Cu separation of 6.289 (2) Å (Fig. 2).

Experimental

A mixed solution (15 ml) of dimethylformamide and water (2:1 *v*:*v*) containing $Cu_2Cl_2·2H_2O$ (0.25 mol, 0.043 g) and pyrazine-2,3-dicarboxylic acid (0.25 mol, 0.043 g) was added slowly to a solution (10 ml) of methanol containing 1,10-phenanthroline (0.5 mmol, 0.099 g). The mixture was stirred for a few minutes and left to stand at room temperature for about five days; blue crystals were obtained.

Crystal data

$[Cu(C_6H_3N_2O_4)_2]·2C_3H_7NO$
$M_r = 543.94$
Triclinic, $P\overline{1}$
$a = 6.289$ (2) Å
$b = 7.679$ (3) Å
$c = 12.686$ (5) Å
$\alpha = 76.147$ (7)°
$\beta = 88.002$ (7)°
$\gamma = 70.902$ (7)°
$V = 561.5$ (4) Å^3

$Z = 1$
$D_x = 1.609$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1209 reflections
$\theta = 2.9$–23.3°
$\mu = 1.04$ mm^{-1}
$T = 293$ (2) K
Prism, blue
0.33 × 0.12 × 0.05 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.861$, $T_{max} = 0.950$
4122 measured reflections

2005 independent reflections
1921 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.2°$
$h = -7 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.096$
$wR(F^2) = 0.264$
$S = 1.23$
2005 reflections
163 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1029P)^2 + 3.7409P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.29$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.919 (5)	Cu1—O4^i	2.565 (5)
Cu1—N1	1.974 (6)		
O1—Cu1—N1	83.7 (3)	O4^i—Cu1—O1	84.8 (3)
O1^{ii}—Cu1—N1	96.3 (3)	O4^i—Cu1—N1	81.1 (3)

Symmetry codes: (i) $x - 1, y, z$; (ii) $-x, 2 - y, 2 - z$.

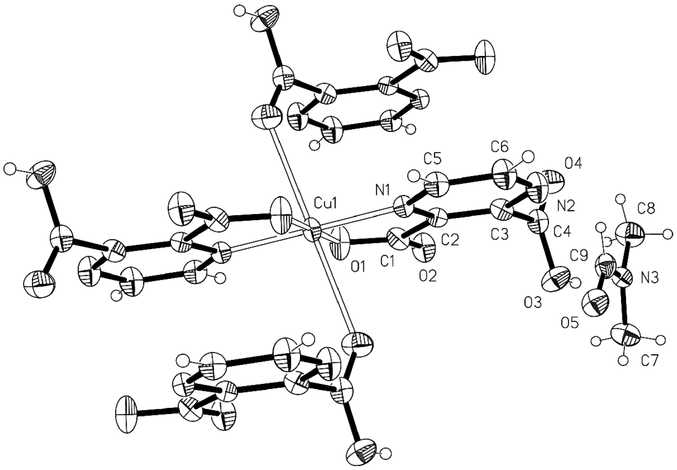


Figure 1
The coordination environment of the Cu^{II} cation in (I), with the atom numbering scheme, showing displacement ellipsoids at the 50% probability level.

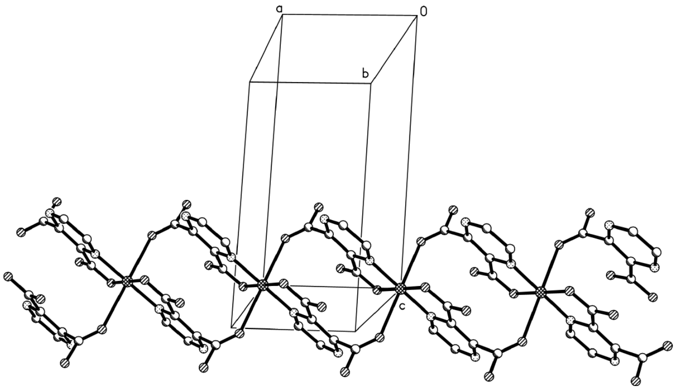


Figure 2
The double-chain structure of (I).

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O5^{iii}	0.82	1.72	2.512 (9)	162

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

H atoms were positioned geometrically (C—H = 0.93 Å and O—H = 0.82 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}$(parent atom). The maximum positive peak in the difference Fourier map is situated 1.6 Å from atom O2. The probable reason for the relatively high values of the *R* factors is the poor quality of the crystal.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXL*97.

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