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catena-Poly[copper(II)-bis(μ-3-cyano-2-hydroxypropionato)-κ^3N:O^1,O^2;-κ^3O^1,O^2:N-copper(II)]

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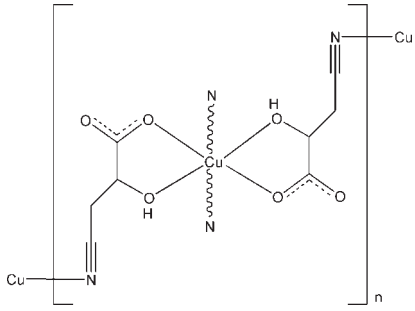
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.064; data-to-parameter ratio = 12.3.

The title compound, $[Cu(C_4H_4NO_3)_2]_n$, exhibits a double-chain structure extending along [100]. The Cu^{II} atom, lying on an inversion center, is coordinated by two cyano N atoms from two 3-cyano-2-hydroxypropionate ligands and two hydroxy O atoms and two carboxylate O atom from two other two ligands in a distorted octahedral geometry. Intermolecular C—H···O and O—H···O hydrogen bonds connect the chains into a three-dimensional structure.

Related literature

For the synthesis and studies of β-hydroxynitriles, see: Conti *et al.* (2003); Seo *et al.* (1994). For related structures, see: Klein *et al.* (1982); Wang *et al.* (2009).



Experimental

Crystal data

$[Cu(C_4H_4NO_3)_2]$
M_r = 291.71
Monoclinic, $P2_1/c$
a = 6.3704 (7) Å
b = 8.4382 (10) Å
c = 10.0412 (12) Å
β = 104.492 (2)°
V = 522.59 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.11 mm^{-1}
T = 293 K
0.28 × 0.19 × 0.12 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.624, T_{max} = 0.776
2803 measured reflections
1031 independent reflections
973 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.064
S = 1.11
1031 reflections
83 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O2	1.9159 (12)	Cu1—N1^{i}	2.545 (2)
Cu1—O1	1.9579 (11)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O2^{ii}	0.98	2.54	3.240 (2)	128
O1—H1W···O3^{ii}	0.83 (2)	1.75 (2)	2.560 (2)	165 (4)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2278).

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supporting information

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S1. Comment

β-Hydroxynitriles are potentially important intermediates in the synthesis of complex organic compounds (Seo *et al.*, 1994). The study of coordination polymers with *β*-hydroxynitrile is rarely reported according to Cambridge Structural Database. Herein we report the structure of the title compound.

In the title compound, the Cu^{II} atom, lying on an inversion center, is six-coordinated in a distorted octahedral geometry defined by two carboxylate O atoms and two hydroxy O atoms in the equatorial plane and two N atoms from the cyano groups in the axial positions (Table 1 and Fig. 1). Weak coordination between the Cu^{II} atom and the N atoms is indicated by a Cu—N distance of 2.545 (2) Å, due to Jahn-Teller effects. The bond lengths and angles are in normal ranges (Klein *et al.*, 1982; Wang *et al.*, 2009). Adjacent Cu^{II} centers are bridged by two ligands, forming a double-chain structure, which is further extended by intermolecular C—H···O and O—H···O hydrogen bonds (Table 2) into a three-dimentional supramolecular structure.

S2. Experimental

2-Isoxazoline-3,5-dicarboxylic acid was synthesized according to the previously reported procedure (Conti *et al.*, 2003). 3-Cyano-2-hydroxypropionic acid was obtained from 2-isoxazoline-3,5-dicarboxylic acid by selective cleavage of the N—O bond and decarboxylation under basic condition (Seo *et al.*, 1994). A solution of $Cu(NO_3)_2.3H_2O$ (0.048 g, 0.2 mmol) in H_2O (4 ml) was added to a solution of 3-cyano-2-hydroxypropionic acid (0.046 g, 0.4 mmol) in H_2O (8 ml), then aqueous triethylamine (0.07 ml) was added dropwise to the above solution accompanied with stirring. The mixture was flitered and placed at room temperature. Blue block crystals of the title compound were obtained in three days (yield 0.046 g, 78% based on Cu).

S3. Refinement

C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.98 (CH) and 0.97 (CH_2) Å and with U_{iso}(H) = 1.2U_{eq}(C). The hydroxy H atom was found in a difference Fourier map and refined isotropically.

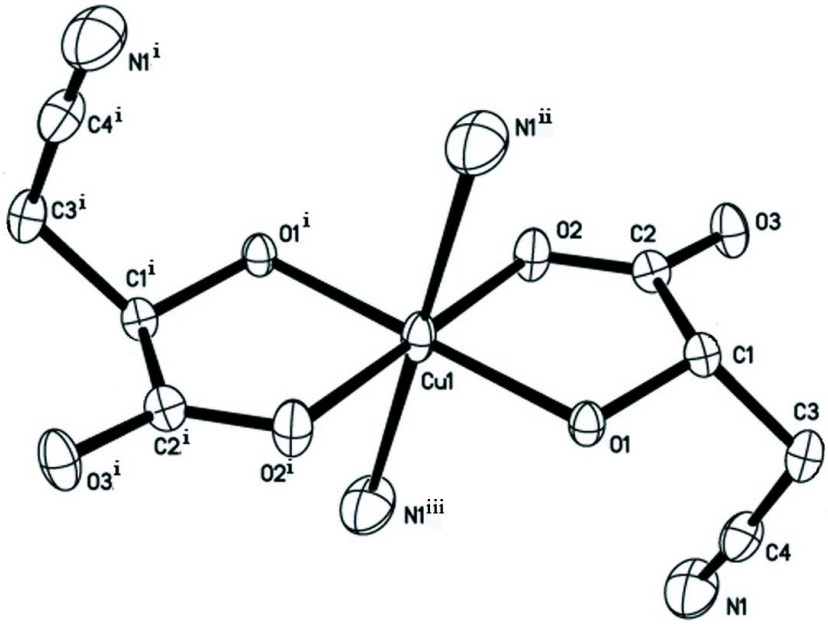

Figure 1

The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) 1-x, -y, -z; (ii) x-1, y, z; (iii) 2-x, -y, -z.]

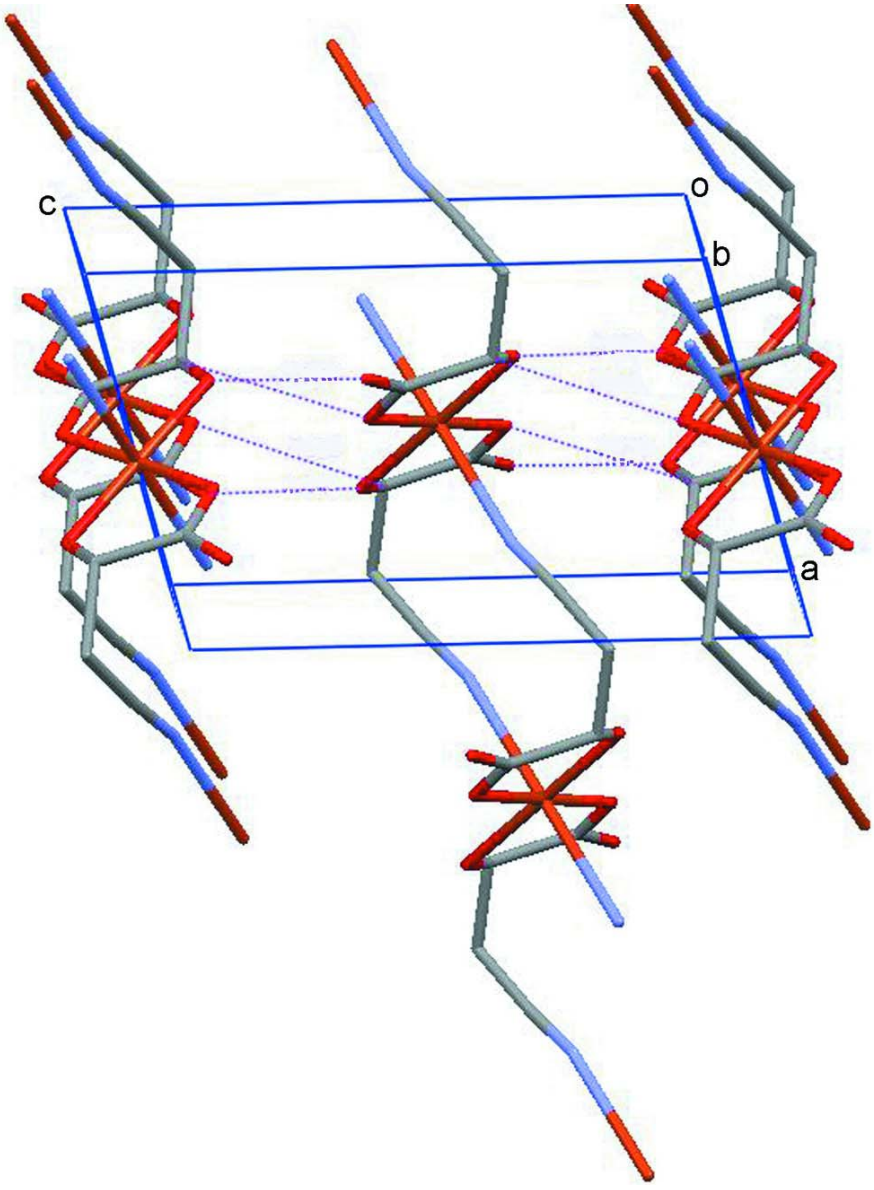

Figure 2

The one-dimensional double-chain in the title compound. Dashed lines denote hydrogen bonds.

***catena*-Poly[copper(II)-bis(*μ*-3-cyano-2-hydroxypropionato)- κ^3N:O^1,O^2;κ^3O^1,O^2:N- copper(II)]**

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$c = 10.0412\ (12)$ Å
$\beta = 104.492\ (2)°$
$V = 522.59\ (11)$ Å^3
$Z = 2$
$F(000) = 294$
$D_x = 1.854$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2150 reflections
$\theta = 3.2–26.0°$
$\mu = 2.11$ mm^{-1}
$T = 293$ K
Block, blue
0.28 × 0.19 × 0.12 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.624, T_{max} = 0.776
2803 measured reflections
1031 independent reflections
973 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 26.0°, θ_{min} = 3.2°
$h = -5 \rightarrow 7$
$k = -9 \rightarrow 10$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.064
S = 1.11
1031 reflections
83 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.2506P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.0000	0.0000	0.03130 (14)
N1	1.1980 (3)	0.1558 (3)	0.0646 (2)	0.0635 (6)
O1	0.69000 (19)	0.11889 (14)	0.15024 (11)	0.0264 (3)
H1W	0.671 (4)	0.117 (3)	0.2292 (14)	0.057 (7)*
O2	0.5444 (2)	0.17730 (15)	−0.10898 (11)	0.0364 (3)
O3	0.6908 (2)	0.41604 (15)	−0.09635 (12)	0.0384 (3)
C1	0.7140 (3)	0.28079 (19)	0.11473 (16)	0.0256 (3)
H1	0.6192	0.3473	0.1545	0.031*
C2	0.6441 (3)	0.2934 (2)	−0.04252 (16)	0.0274 (4)
C3	0.9491 (3)	0.3336 (2)	0.17056 (18)	0.0345 (4)
H3A	0.9641	0.4433	0.1454	0.041*
H3B	0.9880	0.3266	0.2701	0.041*
C4	1.0950 (3)	0.2340 (3)	0.1150 (2)	0.0419 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0435 (2)	0.0282 (2)	0.02069 (19)	−0.01409 (12)	0.00516 (14)	0.00079 (10)
N1	0.0422 (10)	0.0728 (14)	0.0791 (14)	−0.0038 (10)	0.0222 (10)	−0.0190 (12)
O1	0.0346 (6)	0.0251 (6)	0.0203 (5)	−0.0059 (5)	0.0080 (5)	−0.0001 (4)
O2	0.0537 (8)	0.0323 (7)	0.0217 (6)	−0.0152 (6)	0.0065 (5)	0.0008 (5)
O3	0.0626 (9)	0.0272 (7)	0.0284 (6)	−0.0107 (6)	0.0170 (6)	0.0016 (5)
C1	0.0333 (9)	0.0228 (8)	0.0232 (7)	−0.0030 (6)	0.0116 (6)	−0.0017 (6)
C2	0.0327 (8)	0.0276 (8)	0.0244 (8)	−0.0008 (7)	0.0120 (7)	0.0001 (6)
C3	0.0385 (10)	0.0351 (9)	0.0306 (8)	−0.0119 (8)	0.0099 (7)	−0.0069 (7)

C4	0.0307 (9)	0.0476 (11)	0.0465 (11)	−0.0109 (9)	0.0081 (8)	−0.0063 (9)

Geometric parameters (Å, º)

Cu1—O2	1.9159 (12)	O3—C2	1.238 (2)
Cu1—O1	1.9579 (11)	C1—C3	1.528 (2)
Cu1—N1^{i}	2.545 (2)	C1—C2	1.533 (2)
N1—C4	1.135 (3)	C1—H1	0.9800
O1—C1	1.4298 (19)	C3—C4	1.464 (3)
O1—H1W	0.832 (10)	C3—H3A	0.9700
O2—C2	1.264 (2)	C3—H3B	0.9700
O2^{ii}—Cu1—O2	180.0	C3—C1—C2	111.28 (14)
O2^{ii}—Cu1—O1	96.39 (5)	O1—C1—H1	109.3
O2—Cu1—O1	83.62 (5)	C3—C1—H1	109.3
O2—Cu1—O1^{ii}	96.38 (5)	C2—C1—H1	109.3
O1—Cu1—O1^{ii}	179.999 (1)	O3—C2—O2	124.17 (15)
O1—Cu1—N1^{i}	84.25 (6)	O3—C2—C1	117.92 (14)
O2—Cu1—N1^{i}	88.35 (6)	O2—C2—C1	117.90 (14)
O1^{ii}—Cu1—N1^{i}	95.74 (6)	C4—C3—C1	110.51 (15)
O2^{ii}—Cu1—N1^{i}	91.65 (6)	C4—C3—H3A	109.5
C1—O1—Cu1	112.43 (9)	C1—C3—H3A	109.5
C1—O1—H1W	108.0 (19)	C4—C3—H3B	109.5
Cu1—O1—H1W	120.9 (19)	C1—C3—H3B	109.5
C2—O2—Cu1	115.49 (10)	H3A—C3—H3B	108.1
O1—C1—C3	110.09 (14)	N1—C4—C3	175.7 (2)
O1—C1—C2	107.56 (12)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O2^{iii}	0.98	2.54	3.240 (2)	128
O1—H1*W*···O3^{iii}	0.83 (2)	1.75 (2)	2.560 (2)	165 (4)

Symmetry code: (iii) $x, -y+1/2, z+1/2$.