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catena-Poly[[(1,10-phenanthroline-κ^2N,N')-copper(II)]-μ-4-carboxyimidazole-5-carboxylato(2–)-$\kappa^4N,O:N',O'$]

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In the title coordination polymer, [Cu(HIDC)(1,10-phen)]$_n$ (HIDC^{2-} is the 4-carboxyimidazole-5-carboxylate dianion, $C_5H_2N_2O_4^{2-}$, and 1,10-phen is 1,10-phenanthroline, $C_{12}H_8N_2$), the Cu^{II} atom shows a distorted octahedral coordination configuration, defined by two N atoms from a terminal 1,10-phen molecule, two N atoms and two O atoms from two individual HIDC^{2-} groups. Adjacent Cu^{II} atoms are bridged by HIDC^{2-} groups, forming a one-dimensional chain structure. The Cu$\cdots$Cu separation within the polymer is 6.132 (4) Å. The chains are linked into a two-dimensional supramolecular network *via* π–π stacking interactions.

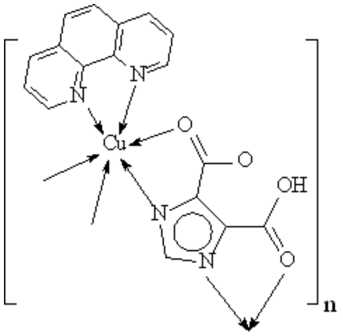
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.055
wR factor = 0.123
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

1H-Imidazole-4,5-dicarboxylic acid (H_3IDC) is recognized as an excellent candidate for the construction of supramolecular complexes owing to its versatile binding modes. It can be successively deprotonated to generate H_2IDC^-, HIDC^{2-} and IDC^{3-} anions, and hence may result in a large diversity of supramolecular architectures. So far some mononuclear (Zhang *et al.*, 2004; Xiao *et al.*, 2004; Liu *et al.*, 2004) and dinuclear (Rajendiran *et al.*, 2003) complexes have already been reported. However, coordination polymers based on the H_3IDC ligand remain largely unexplored (Wang *et al.*, 2004). We have recently reported two one-dimensional Cd^{II} polymers, [Cd(HIDC)(1,10-phen)]$_n$ (Gao, Gu *et al.*, 2004) and [Cd(HIDC)(2,2′-bipy)]$_n$ (Gao, Liu *et al.*, 2004). The present Cu^{II} complex, [Cu(HIDC)(1,10-phen)]$_n$, (I), is isomorphous with the [Cd(HIDC)(1,10-phen)]$_n$ analog. Similar structural descriptions of the analog apply to the present isomorphous complex.



(I)

As shown in Fig. 1, the uncoordinated carboxylate atoms O2 and O3 form an intramolecular hydrogen bond (Table 2). The Cu^{II} ion is coordinated by two N atoms from a terminal 1,10-phen ligand, two N atoms and two O atoms from two N,O-bidentate HIDC^{2-} groups (Table 1), and resides in a

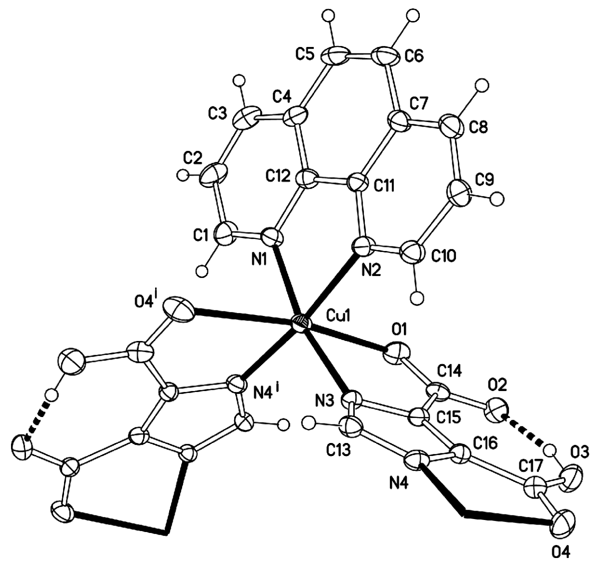


Figure 1
*ORTEP*II plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines (the symmetry code is as given in Table 1).

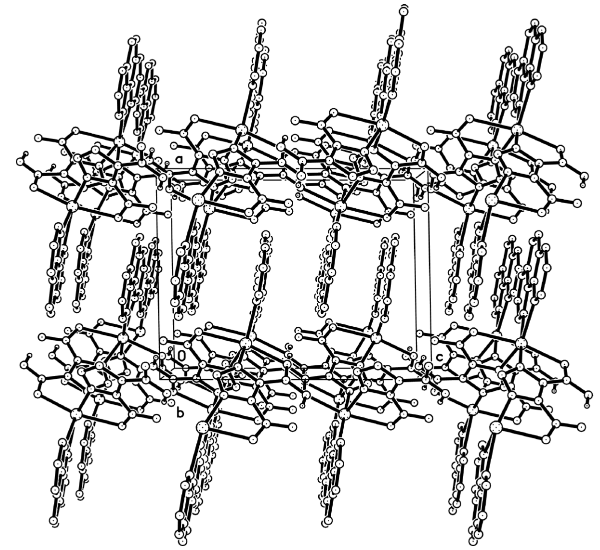


Figure 2
Packing diagram of the title complex. H atoms bound to C atoms have been omitted.

distorted octahedral environment. The Cu—O bonds are somewhat longer than those of the Cd^{II} analog [2.368 (2) and 2.432 (2) Å]. The Cu^{II} atom does not deviate significantly from the equatorial plane of atoms N3/N4^{i}/N1/N2 [symmetry code: (i) $1 - x$, $y + \frac{1}{2}$, $\frac{1}{2} - z$; r.m.s. deviation = 0.05 (4) Å; displacement of Cu atom from this plane = 0.02 (4) Å]. Atoms O1 and O4^{i} occupy the axial positions, with an angle of 167.12 (13)°. The HIDC^{2-} ligand is essentially planar, with an overall r.m.s. deviation of 0.05 (4) Å. The dihedral angle between the 1,10-phen and HIDC^{2-} ligands is 79.9 (5)°.

Each HIDC^{2-} ligand acts as a bis-bidentate bridging group to link two Cu^{II} ions, giving rise to a one-dimensional chain running along the *b* axis. The antiparallel 1,10-phen ligands lie on alternate sides of the chain. In the chain, the closest Cu$\cdots$Cu distance of 6.132 (4) Å, is slightly shorter than the corresponding Cd$\cdots$Cd distance of 6.661 (2) Å in the Cd^{II} analog. In addition, there are strong π–π stacking interactions between 1,10-phen molecules at a centroid–centroid distance of 3.463 (4) Å, leading to a two-dimensional supramolecular network structure (Fig. 2).

Experimental

$Cu(OAc)_2 \cdot H_2O$ (4.00 g, 20 mmol), 1,10-phenanthroline (3.98 g, 20 mmol) and 1*H*-imidazole-4,5-dicarboxylic acid (4.60 g, 20 mmol) were dissolved in ethanol/water (1:5 *v*/*v*). The mixture was sealed in a 25 ml Teflon-lined stainless steel bomb and held at 403 K for 3 d. The bomb was cooled naturally to room temperature and blue prismatic crystals were obtained after several days. Analysis calculated for $C_{17}H_{10}CuN_4O_4$: C 51.32, H 2.53, N 14.08%; found: C 51.49, H 2.59, N 14.11%.

Crystal data

$[Cu(C_5H_2N_2O_4)(C_{12}H_8N_2)]$
$M_r = 397.84$
Monoclinic, $P2_1/c$
$a = 10.360$ (2) Å
$b = 9.6427$ (19) Å
$c = 14.352$ (3) Å
$\beta = 91.36$ (3)°
$V = 1433.3$ (5) Å^3
$Z = 4$
$D_x = 1.844$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12710 reflections
$\theta = 3.2$–27.5°
$\mu = 1.56$ mm^{-1}
$T = 293$ (2) K
Prism, blue
0.24 × 0.18 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.706$, $T_{\max} = 0.859$
13223 measured reflections
3265 independent reflections
2385 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.098$
$\theta_{\max} = 27.5°$
$h = -13 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -18 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.124$
$S = 1.02$
3265 reflections
238 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.8363P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.51$ e Å^{-3}
$\Delta\rho_{\min} = -0.56$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.035 (4)	Cu1—O4^{i}	2.509 (4)
Cu1—N2	2.080 (4)	O1—C14	1.245 (5)
Cu1—N3	2.007 (3)	O2—C14	1.275 (5)
Cu1—N4^{i}	2.017 (4)	O3—C17	1.300 (6)
Cu1—O1	2.383 (3)	O4—C17	1.227 (5)
N1—Cu1—N2	79.88 (15)	N4^{i}—Cu1—N2	172.63 (14)
N1—Cu1—O1	98.11 (13)	N4^{i}—Cu1—O1	92.82 (13)
N2—Cu1—O1	90.14 (13)	O4^{i}—Cu1—N1	83.22 (13)
N3—Cu1—N1	167.00 (14)	O4^{i}—Cu1—N2	102.72 (13)
N3—Cu1—N2	88.00 (14)	O4^{i}—Cu1—N3	104.32 (13)
N3—Cu1—N4^{i}	99.24 (13)	O4^{i}—Cu1—N4^{i}	74.33 (15)
N3—Cu1—O1	77.07 (12)	O4^{i}—Cu1—O1	167.12 (13)
N4^{i}—Cu1—N1	93.01 (14)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H18···O2	0.85 (4)	1.65 (4)	2.485 (5)	167 (6)

The H atoms of C atoms were placed in calculated positions, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atom of the carboxy group was located in a difference Fourier map and refined with an O—H distance restraint of 0.85 (1) Å and $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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References

Gao, S., Gu, C. S., Huo, L. H., Zhao, H. & Zhao, J. G. (2004). *Acta Cryst.* E**60**, m1672–m1674.

Gao, S., Liu, J. W., Huo, L. H. & Zhao, J. G. (2004). *Acta Cryst.* E**60**, m1728–m1730.

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Liu, J. W., Gao, S., Huo, L. H., Gu, C. S., Zhao, H. & Zhao, J. G. (2004). *Acta Cryst.* E**60**, m1697–m1699.

Rajendiran, T. M., Kirk, M. L., Setyawati, I. A., Caudle, M. T., Kampf, J. W. & Pecoraro, V. L. (2003). *Chem. Commun.* pp. 824–825.

Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.

Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Wang, C. F., Gao, E. Q., He, Z. & Yan, C. H. (2004). *Chem. Commun.* pp. 720–721.

Xiao, H. P., Li, X. H. & Shi, Q. (2004). *Acta Cryst.* E**60**, m1519–m1521.

Zhang, X. M., Fang, R. Q., Wu, H. S. & Ng, S. W. (2004). *Acta Cryst.* E**60**, m12–m13.

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