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catena-Poly[[bis(1-vinyl-1*H*-imidazole-κN^3)copper(II)]-μ-phthalato-$\kappa^2 O:O'$]

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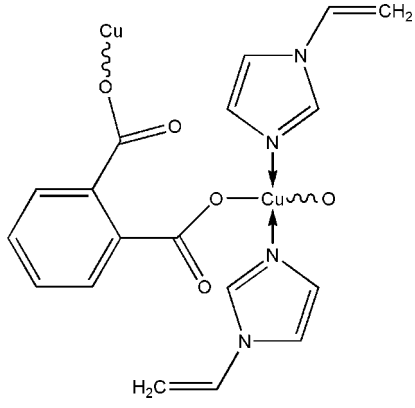
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.048; wR factor = 0.135; data-to-parameter ratio = 14.3.

The title compound, $[Cu(C_8H_4O_4)(C_5H_6N_2)_2]_n$, exhibits a polymeric zigzag chain structure extended along the c axis in the solid state. Each Cu^{II} ion is located on a crystallographic center of symmetry and is coordinated by two N [Cu—N = 1.993 (3) Å] and two O [Cu—O = 1.952 (2) Å] atoms in a distorted square-planar geometry. Weak C—H···O interactions contribute to the crystal packing stability.

Related literature

In the related compound [Cu(phthalato)(1-methylimidazole)$_2$] (Baca *et al.*, 2004), the Cu^{II} ions have a distorted tetrahedral environment.



Experimental

Crystal data

$[Cu(C_8H_4O_4)(C_5H_6N_2)_2]$
M_r = 415.90
Monoclinic, $C2/c$
a = 16.527 (3) Å
b = 8.1800 (16) Å
c = 14.463 (3) Å
β = 113.19 (3)°
V = 1797.3 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.25 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.706, T_{max} = 0.885
3525 measured reflections
1768 independent reflections
1344 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.136
S = 1.00
1768 reflections
124 parameters
40 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···O1^{i}	0.93	2.33	3.243 (5)	167
C6—H6A···O1^{ii}	0.93	2.50	3.158 (5)	128
C8—H8A···O2^{iii}	0.93	2.43	3.342 (6)	168
C9—H9C···O1^{iv}	0.93	2.45	3.349 (8)	162

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2291).

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supplementary materials

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catena-Poly[[bis(1-vinyl-1*H*-imidazole-κN^3)copper(II)]-μ-phthalato-$\kappa^2 O:O'$]

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Comment

In the title compound, (I) (Fig. 1), the copper(II) centers are bridged by the carboxylate groups of *o*-phthalate ligiands and saturated by two 1-vinylimidazole ligands. Each Cu^{II} ion is located on a crystallographic center of symmetry being coordinated by two N [Cu—N 1.993 (3) Å] and two O [Cu—O 1.952 (2) Å] atoms in a distorted square-planar geometry. All these values agree well with those observed in [Cu(phthalato)(1-methylimidazole)$_2$] (Baca *et al.*, 2004), where Cu^{II} ions have a distorted tetrahedral environment. Each *o*-phthalate dianion acts as a bidentate ligand to bridge two Cu^{II} ions through two monodentate carboxylate groups, building a zigzag infinate chain structure along the *c* axis. The metal-metal distances across each polymer backbone are 7.231 (6) Å.

In the crystal, weak C—H···O (Table 1) interactions contribute to the crystal packing stability.

Experimental

The reaction of $CuCl_2{\cdot}2H_2O$(0.85 g, 5 mmol) with *o*-phthalic acid (0.83 g, 5 mmol) in an aqueous-alcohol(3:1) solution(40 ml) at 363 K for 30 min produced a blue solution, to which 1-vinylimidazole (0.94 g, 10 mmol) was added. The reaction solution was kept at room temperature after stirring for an hour at 333 K. Blue crystals were obtained after a few days.

Refinement

All H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

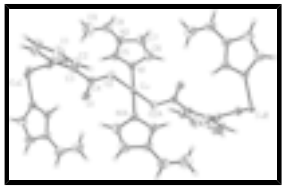

Fig. 1. A portion of polymeric chain in (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme [symmetry codes: (A) −*x*, −*y*, −*z*; (B) *x* + 1/2, *y* + 1/2, *z*; (C) *x* + 1/2, *y* + 1/2, *z* − 1].

Fig. 2. The packing of (I), viewed down the *b* axis. Dashed lines denote hydrogen bonds.

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Crystal data

$[Cu(C_8H_4O_4)(C_5H_6N_2)_2]$	F_{000} = 852
M_r = 415.90	D_x = 1.537 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3318 reflections
a = 16.527 (3) Å	θ = 2.5–25.1º
b = 8.1800 (16) Å	μ = 1.25 mm^{-1}
c = 14.463 (3) Å	*T* = 293 (2) K
β = 113.19 (3)º	Block, blue
V = 1797.3 (7) Å^3	0.30 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	1768 independent reflections
Radiation source: fine-focus sealed tube	1344 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.023
T = 293(2) K	θ_{max} = 26.0º
thin–slice ω scans	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	*h* = −20→20
T_{min} = 0.706, T_{max} = 0.885	*k* = 0→10
3525 measured reflections	*l* = −17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.136	$w = 1/[\sigma^2(F_o^2) + (0.0844P)^2 + 0.9237P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
1768 reflections	$\Delta\rho_{max}$ = 0.75 e Å^{-3}
124 parameters	$\Delta\rho_{min}$ = −0.63 e Å^{-3}
40 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu	0.0000	0.0000	0.0000	0.0333 (2)
O1	−0.06590 (16)	−0.0922 (3)	0.14946 (17)	0.0480 (6)
O2	0.01489 (15)	−0.2039 (3)	0.07497 (16)	0.0423 (5)
N1	0.11711 (18)	0.0724 (4)	0.0994 (2)	0.0431 (6)
C6	0.1839 (3)	0.1421 (6)	0.0812 (3)	0.0679 (12)
H6A	0.1818	0.1666	0.0175	0.081*
C1	−0.0087 (3)	−0.6538 (5)	0.1984 (3)	0.0627 (11)
H1A	−0.0156	−0.7519	0.1637	0.075*
C2	−0.0155 (3)	−0.5079 (4)	0.1493 (3)	0.0486 (9)
H2B	−0.0253	−0.5085	0.0814	0.058*
C3	−0.00809 (19)	−0.3593 (4)	0.1982 (2)	0.0341 (7)
C4	−0.0211 (2)	−0.2048 (4)	0.1387 (2)	0.0375 (7)
C5	0.1469 (2)	0.0592 (5)	0.1980 (3)	0.0478 (8)
H5A	0.1153	0.0148	0.2328	0.057*
N2	0.22960 (19)	0.1189 (4)	0.2419 (2)	0.0533 (8)
C7	0.2538 (3)	0.1709 (7)	0.1679 (3)	0.0728 (13)
H7A	0.3074	0.2169	0.1752	0.087*
C8	0.2838 (3)	0.1327 (6)	0.3459 (3)	0.0695 (12)
H8A	0.3422	0.1638	0.3639	0.083*
C9	0.2577 (4)	0.1057 (9)	0.4147 (4)	0.107 (2)
H9C	0.1997	0.0745	0.3990	0.128*
H9A	0.2963	0.1168	0.4816	0.128*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0317 (3)	0.0411 (4)	0.0270 (3)	0.0012 (2)	0.0114 (2)	0.0024 (2)
O1	0.0608 (15)	0.0420 (14)	0.0393 (13)	0.0160 (11)	0.0178 (11)	0.0031 (10)
O2	0.0444 (12)	0.0481 (14)	0.0360 (11)	0.0018 (10)	0.0176 (10)	0.0065 (10)
N1	0.0390 (14)	0.0504 (16)	0.0354 (14)	−0.0037 (13)	0.0098 (11)	0.0025 (13)
C6	0.050 (2)	0.103 (3)	0.047 (2)	−0.020 (2)	0.0159 (17)	0.002 (2)
C1	0.090 (3)	0.038 (2)	0.070 (3)	−0.0032 (19)	0.042 (3)	−0.0090 (18)

C2	0.059 (2)	0.045 (2)	0.046 (2)	−0.0037 (16)	0.0252 (18)	−0.0069 (15)
C3	0.0355 (15)	0.0318 (16)	0.0368 (16)	−0.0003 (12)	0.0161 (13)	0.0005 (13)
C4	0.0365 (15)	0.0401 (17)	0.0311 (15)	−0.0041 (13)	0.0082 (13)	−0.0012 (13)
C5	0.0463 (19)	0.0520 (19)	0.0411 (17)	−0.0077 (16)	0.0129 (15)	0.0031 (16)
N2	0.0452 (16)	0.063 (2)	0.0390 (15)	−0.0081 (14)	0.0029 (13)	−0.0029 (14)
C7	0.048 (2)	0.105 (4)	0.063 (2)	−0.026 (2)	0.0194 (19)	0.000 (2)
C8	0.052 (2)	0.090 (3)	0.052 (2)	−0.018 (2)	0.0054 (19)	−0.002 (2)
C9	0.084 (4)	0.165 (6)	0.061 (3)	−0.039 (4)	0.017 (3)	−0.019 (4)

Geometric parameters (Å, °)

Cu—O2	1.952 (2)	C2—C3	1.387 (4)
Cu—O2^{i}	1.952 (2)	C2—H2B	0.9300
Cu—N1^{i}	1.993 (3)	C3—C3^{ii}	1.415 (6)
Cu—N1	1.993 (3)	C3—C4	1.496 (4)
O1—C4	1.228 (4)	C5—N2	1.351 (4)
O2—C4	1.280 (4)	C5—H5A	0.9300
N1—C5	1.317 (4)	N2—C7	1.351 (5)
N1—C6	1.358 (5)	N2—C8	1.420 (5)
C6—C7	1.350 (6)	C7—H7A	0.9300
C6—H6A	0.9300	C8—C9	1.250 (7)
C1—C2	1.371 (5)	C8—H8A	0.9300
C1—C1^{ii}	1.405 (8)	C9—H9C	0.9300
C1—H1A	0.9300	C9—H9A	0.9300
O2—Cu—O2^{i}	180.00 (13)	C2—C3—C4	118.9 (3)
O2—Cu—N1^{i}	91.21 (11)	C3^{ii}—C3—C4	122.22 (16)
O2^{i}—Cu—N1^{i}	88.79 (11)	O1—C4—O2	124.1 (3)
O2—Cu—N1	88.79 (11)	O1—C4—C3	121.2 (3)
O2^{i}—Cu—N1	91.21 (11)	O2—C4—C3	114.6 (3)
N1^{i}—Cu—N1	180.0 (2)	N1—C5—N2	110.9 (3)
C4—O2—Cu	114.3 (2)	N1—C5—H5A	124.5
C5—N1—C6	105.0 (3)	N2—C5—H5A	124.5
C5—N1—Cu	126.9 (2)	C7—N2—C5	107.6 (3)
C6—N1—Cu	128.1 (2)	C7—N2—C8	123.6 (3)
C7—C6—N1	110.9 (4)	C5—N2—C8	128.8 (3)
C7—C6—H6A	124.6	C6—C7—N2	105.6 (3)
N1—C6—H6A	124.6	C6—C7—H7A	127.2
C2—C1—C1^{ii}	119.4 (2)	N2—C7—H7A	127.2
C2—C1—H1A	120.3	C9—C8—N2	123.8 (4)
C1^{ii}—C1—H1A	120.3	C9—C8—H8A	118.1
C1—C2—C3	121.7 (4)	N2—C8—H8A	118.1
C1—C2—H2B	119.2	C8—C9—H9C	120.0
C3—C2—H2B	119.2	C8—C9—H9A	120.0
C2—C3—C3^{ii}	118.8 (2)	H9C—C9—H9A	120.0
N1^{i}—Cu—O2—C4	−84.6 (2)	C2—C3—C4—O1	135.5 (3)
N1—Cu—O2—C4	95.4 (2)	C3^{ii}—C3—C4—O1	−42.0 (5)

O2—Cu—N1—C5	−44.5 (3)	C2—C3—C4—O2	−42.0 (4)
O2^{i}—Cu—N1—C5	135.5 (3)	C3^{ii}—C3—C4—O2	140.5 (4)
O2—Cu—N1—C6	133.9 (4)	C6—N1—C5—N2	0.3 (5)
O2^{i}—Cu—N1—C6	−46.1 (4)	Cu—N1—C5—N2	179.1 (3)
C5—N1—C6—C7	0.1 (5)	N1—C5—N2—C7	−0.6 (5)
Cu—N1—C6—C7	−178.7 (3)	N1—C5—N2—C8	177.6 (4)
C1^{ii}—C1—C2—C3	−1.9 (8)	N1—C6—C7—N2	−0.4 (6)
C1—C2—C3—C3^{ii}	0.9 (6)	C5—N2—C7—C6	0.6 (5)
C1—C2—C3—C4	−176.6 (4)	C8—N2—C7—C6	−177.7 (4)
Cu—O2—C4—O1	4.0 (4)	C7—N2—C8—C9	169.9 (6)
Cu—O2—C4—C3	−178.59 (18)	C5—N2—C8—C9	−8.1 (9)

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5A···O1^{ii}	0.93	2.33	3.243 (5)	167
C6—H6A···O1^{i}	0.93	2.50	3.158 (5)	128
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Symmetry codes: (ii) −*x*, *y*, −*z*+1/2; (i) −*x*, −*y*, −*z*; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iv) −*x*, *y*, −*z*+1/2.

Fig. 1

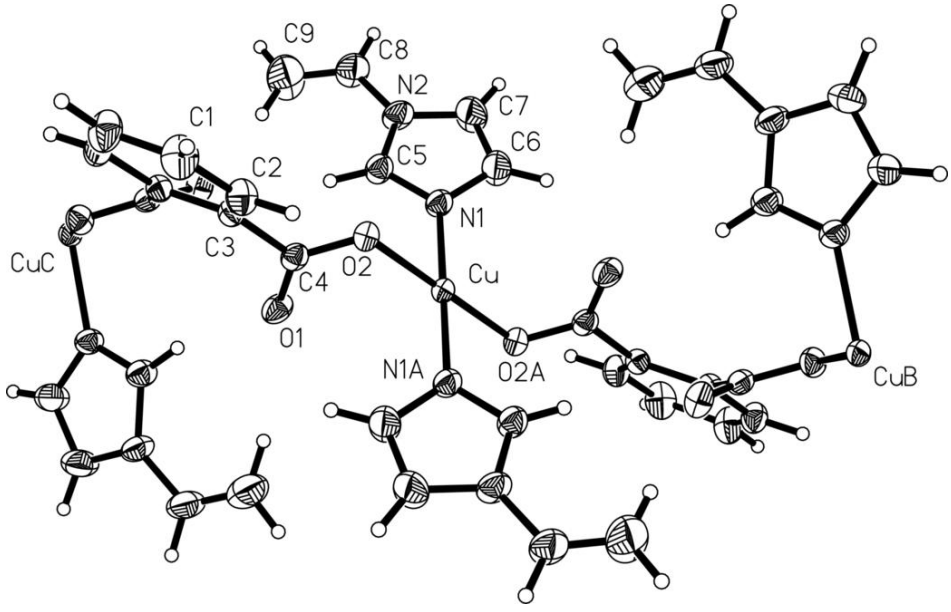

Fig. 2