catena-Poly[[bis(1-ethyl-1H-imidazole)-copper(II)]-μ-benzene-1,3-dicarboxylato]

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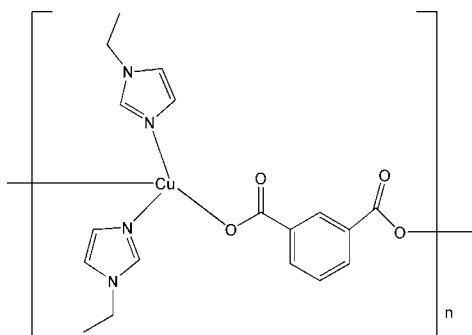
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In the title compound, $[Cu(C_8H_4O_4)(C_5H_8N_2)_2]_n$, each Cu^{II} atom (site symmetry $\bar{1}$) is four-coordinated by two carboxylate O atoms from two different benzene-1,3-dicarboxylate ligands and two N atoms from two 1-ethyl-1H-imidazole ligands in a trans-CuN_2O_2 square-planar arrangement. Each benzene-1,3-dicarboxylate ligand, which possesses crystallographic twofold rotation symmetry, links two adjacent Cu^{II} atoms in a bis-monodentate mode, resulting in a chain with the 1-ethyl-1H-imidazole ligands attached on both sides.

Related literature

For related literature, see: Qi et al. (2003).

Experimental

Crystal data

$[Cu(C_8H_4O_4)(C_5H_8N_2)_2]$	V = 1899.9 (7) Å³
M_r = 419.92	Z = 4
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 15.817 (3) Å	μ = 1.18 mm⁻¹
b = 7.2249 (14) Å	T = 293 (2) K
c = 17.509 (4) Å	0.33 × 0.21 × 0.19 mm
β = 108.29 (3)°	

Data collection

Rigaku R-AXIS RAPID diffractometer	9040 measured reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	2178 independent reflections
T_{min} = 0.671, T_{max} = 0.798	1801 reflections with $I > 2\sigma(I)$
	R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035	125 parameters
$wR(F^2)$ = 0.112	H-atom parameters constrained
S = 1.15	$\Delta\rho_{max}$ = 0.28 e Å⁻³
2178 reflections	$\Delta\rho_{min}$ = −0.38 e Å⁻³

Table 1
Selected bond lengths (Å).

Cu1—N1	1.9881 (18)	Cu1—O1	1.9858 (16)

Data collection: PROCESS-AUTO (Rigaku, 1998); cell refinement: PROCESS-AUTO; data reduction: PROCESS-AUTO; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-Plus (Sheldrick, 1990); software used to prepare material for publication: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2560).

References

Higashi, T. (1995). ABSCOR. Rigaku Corporation, Tokyo, Japan.
Qi, Y., Wang, Y., Hu, C., Cao, M., Mao, L. & Wang, E. (2003). Inorg. Chem. **42**, 8519–8523.
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Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.

supplementary materials

catena-Poly[[bis(1-ethyl-1*H*-imidazole)copper(II)]-*μ*-benzene-1,3-dicarboxylato]

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Comment

In the presence of secondary ligands, such as 2,2'-bipyridine (bipy) and 1,10-phenanthroline (phen), bidentate organic carboxylic acid ligands can construct polymeric structures (Qi *et al.*, 2003). Two coordination positions of metal ions can be occupied by the N atoms from the secondary ligand. The rest of the coordination positions are available for the carboxylate ligands, leading to the formation of a chain structure. We have now selected 1,3-benzenedicarboxylic acid (1,3-H$_2$BDC) as a bridging ligand and 1-ethyl-1*H*-imidazole (*L*) as a secondary ligand, generating the title coordination polymer, [Cu(1,3-BDC)(*L*)$_2$], (I), (Table 1) which is reported here.

In compound (I), the Cu^{II} atom (site symmetry $\bar{1}$) is four-coordinated by two carboxylate O atoms from two different 1,3-BDC ligands, and two N atoms from two *L* ligands in a square-planar coordination environment (Fig. 1). The Cu—O and Cu—N distances are within their normal ranges (Table 1). A very long Cu1—O2 contact of 2.652 (2)Å would lead to a very distorted CuN$_2$O$_4$ octahedron. The complete 1,3-BDC dianion is generated by crystallographic 2-fold symmetry. As shown in Fig. 2, each 1,4-BDC acts as a bis-modentate ligand that binds two Cu^{II} atoms, generating a unique chain. Interestingly, the *L* ligands are attached on both sides of the chains.

Experimental

A mixture of CuCl$_2$·2H$_2$O (0.5 mmol), 1,3-H$_2$BDC (0.5 mmol), *L* (0.5 mmol), and H$_2$O (500 mmol) was adjusted to pH = 5.8 by addition of aqueous NaOH solution, and heated at 458 K for 2 days. After the mixture was slowly cooled to room temperature, blue crystals of (I) were yielded (29% yield).

Refinement

All H atoms on C atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).
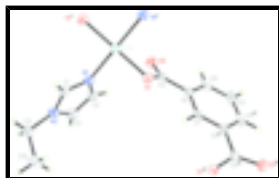
Figures

Fig. 1. A fragment of the chain structure of (I). Displacement ellipsoids are drawn at the 30% probability level. (H atoms have been omitted). Symmetry codes: (i) 2 − *x*, *y*, 1.5 − *z*; (ii) 2 − *x*, −*y*, 1 − *z*;
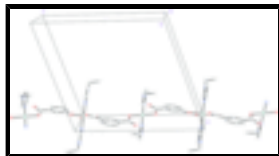
 Fig. 2. View of the chain structure of (I).

catena-Poly[[bis(1-ethyl-1_H_-imidazole)copper(II)]-μ-benzene-1,3-dicarboxylato]

Crystal data

[Cu(C$_8$H$_4$O$_4$)(C$_5$H$_8$N$_2$)$_2$]	$F_{000} = 868$
$M_r = 419.92$	$D_x = 1.468$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 7827 reflections
$a = 15.817$ (3) Å	$\theta = 3.0–27.5º$
$b = 7.2249$ (14) Å	$\mu = 1.18$ mm^{-1}
$c = 17.509$ (4) Å	$T = 293$ (2) K
$\beta = 108.29$ (3)º	Block, blue
$V = 1899.9$ (7) Å^3	0.33 × 0.21 × 0.19 mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID diffractometer	2178 independent reflections
Radiation source: rotating anode	1801 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.033$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.5º$
$T = 293(2)$ K	$\theta_{min} = 3.1º$
ω scans	$h = -18 \rightarrow 20$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -9 \rightarrow 9$
$T_{min} = 0.671$, $T_{max} = 0.798$	$l = -22 \rightarrow 22$
9040 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 0.6587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.15$	$(\Delta/\sigma)_{max} = 0.001$
2178 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
125 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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	$U_{iso}*/U_{eq}$
C1	1.14471 (14)	−0.2801 (3)	0.55401 (13)	0.0411 (5)
H1	1.1061	−0.3779	0.5332	0.049*
C2	1.2802 (2)	−0.4741 (4)	0.6142 (2)	0.0550 (7)
H2A	1.3402	−0.4590	0.6118	0.066*
H2B	1.2508	−0.5680	0.5753	0.066*
C3	1.26507 (16)	−0.1258 (4)	0.61419 (16)	0.0538 (6)
H3	1.3238	−0.0954	0.6420	0.065*
C4	1.19657 (18)	−0.0070 (4)	0.58733 (19)	0.0528 (7)
H4	1.2000	0.1208	0.5937	0.063*
C5	1.02334 (13)	0.2495 (3)	0.61465 (13)	0.0382 (5)
C6	1.01289 (13)	0.3540 (3)	0.68534 (13)	0.0364 (5)
C7	1.0000	0.2586 (4)	0.7500	0.0328 (6)
H7	1.0000	0.1299	0.7500	0.039*
C8	1.01330 (17)	0.5460 (4)	0.68607 (19)	0.0514 (7)
H8	1.0225	0.6109	0.6435	0.062*
C9	1.0000	0.6412 (5)	0.7500	0.0596 (10)
H9	1.0000	0.7699	0.7500	0.072*
C10	1.2842 (2)	−0.5379 (5)	0.6975 (2)	0.0709 (9)
H10A	1.3160	−0.6528	0.7095	0.106*
H10B	1.2248	−0.5549	0.6998	0.106*
H10C	1.3142	−0.4463	0.7363	0.106*
N1	1.12108 (11)	−0.1053 (3)	0.54914 (11)	0.0399 (4)
N2	1.23206 (12)	−0.2991 (3)	0.59294 (12)	0.0432 (5)
O1	0.99755 (10)	0.0808 (2)	0.60769 (9)	0.0419 (4)
O2	1.05357 (11)	0.3279 (3)	0.56545 (10)	0.0507 (4)
Cu1	1.0000	0.0000	0.5000	0.03463 (15)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0336 (10)	0.0512 (14)	0.0385 (11)	−0.0042 (9)	0.0114 (9)	0.0039 (10)

C2	0.0433 (14)	0.0570 (17)	0.0656 (18)	0.0091 (11)	0.0181 (13)	0.0106 (12)
C3	0.0326 (11)	0.0609 (16)	0.0605 (15)	−0.0072 (11)	0.0041 (11)	−0.0050 (13)
C4	0.0374 (14)	0.0526 (16)	0.0620 (17)	−0.0073 (10)	0.0064 (13)	−0.0069 (12)
C5	0.0279 (9)	0.0486 (13)	0.0346 (10)	0.0005 (8)	0.0049 (9)	0.0071 (9)
C6	0.0232 (9)	0.0399 (12)	0.0430 (11)	−0.0007 (8)	0.0057 (8)	0.0031 (9)
C7	0.0241 (12)	0.0329 (15)	0.0368 (14)	0.000	0.0027 (11)	0.000
C8	0.0448 (13)	0.0417 (13)	0.0746 (19)	0.0004 (10)	0.0287 (13)	0.0125 (12)
C9	0.060 (2)	0.0329 (19)	0.097 (3)	0.000	0.040 (2)	0.000
C10	0.0600 (19)	0.078 (2)	0.067 (2)	0.0048 (15)	0.0088 (16)	0.0277 (16)
N1	0.0298 (8)	0.0495 (12)	0.0382 (9)	−0.0041 (8)	0.0075 (7)	0.0015 (8)
N2	0.0311 (9)	0.0544 (12)	0.0437 (10)	0.0017 (8)	0.0108 (8)	0.0065 (9)
O1	0.0425 (8)	0.0473 (10)	0.0361 (8)	−0.0061 (7)	0.0127 (7)	−0.0019 (7)
O2	0.0496 (9)	0.0599 (12)	0.0455 (9)	−0.0032 (8)	0.0189 (8)	0.0111 (8)
Cu1	0.0287 (2)	0.0414 (2)	0.0322 (2)	−0.00322 (13)	0.00727 (16)	0.00134 (14)

Geometric parameters (Å, °)

Cu1—N1	1.9881 (18)	C4—H4	0.9300
Cu1—O1	1.9858 (16)	C5—O2	1.245 (3)
Cu1—O1^i	1.9858 (16)	C5—O1	1.280 (3)
Cu1—N1^i	1.9881 (18)	C5—C6	1.502 (3)
C1—N1	1.313 (3)	C6—C8	1.387 (3)
C1—N2	1.342 (3)	C6—C7	1.394 (3)
C1—H1	0.9300	C7—C6^{ii}	1.394 (3)
C2—N2	1.462 (3)	C7—H7	0.9300
C2—C10	1.513 (4)	C8—C9	1.385 (4)
C2—H2A	0.9700	C8—H8	0.9300
C2—H2B	0.9700	C9—C8^{ii}	1.385 (4)
C3—C4	1.346 (4)	C9—H9	0.9300
C3—N2	1.362 (3)	C10—H10A	0.9600
C3—H3	0.9300	C10—H10B	0.9600
C4—N1	1.370 (3)	C10—H10C	0.9600
O1^i—Cu1—O1	180.0	C8—C6—C5	120.6 (2)
O1^i—Cu1—N1^i	90.26 (8)	C7—C6—C5	120.2 (2)
O1—Cu1—N1^i	89.74 (8)	C6^{ii}—C7—C6	120.8 (3)
O1^i—Cu1—N1	89.74 (8)	C6^{ii}—C7—H7	119.6
O1—Cu1—N1	90.26 (8)	C6—C7—H7	119.6
N1^i—Cu1—N1	180.0	C9—C8—C6	120.2 (3)
N1—C1—N2	111.0 (2)	C9—C8—H8	119.9
N1—C1—H1	124.5	C6—C8—H8	119.9
N2—C1—H1	124.5	C8—C9—C8^{ii}	120.5 (4)
N2—C2—C10	111.7 (3)	C8—C9—H9	119.8
N2—C2—H2A	109.3	C8^{ii}—C9—H9	119.8
C10—C2—H2A	109.3	C2—C10—H10A	109.5
N2—C2—H2B	109.3	C2—C10—H10B	109.5
C10—C2—H2B	109.3	H10A—C10—H10B	109.5
H2A—C2—H2B	107.9	C2—C10—H10C	109.5

C4—C3—N2	107.0 (2)	H10A—C10—H10C	109.5
C4—C3—H3	126.5	H10B—C10—H10C	109.5
N2—C3—H3	126.5	C1—N1—C4	106.3 (2)
C3—C4—N1	108.8 (2)	C1—N1—Cu1	127.75 (15)
C3—C4—H4	125.6	C4—N1—Cu1	125.94 (18)
N1—C4—H4	125.6	C1—N2—C3	106.9 (2)
O2—C5—O1	123.2 (2)	C1—N2—C2	126.0 (2)
O2—C5—C6	120.5 (2)	C3—N2—C2	126.9 (2)
O1—C5—C6	116.28 (18)	C5—O1—Cu1	105.65 (14)
C8—C6—C7	119.2 (2)		

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1; (ii) −*x*+2, *y*, −*z*+3/2.

Fig. 1

Fig. 2