

# catena-Poly[[bis(1-ethyl-1*H*-imidazole- $\kappa$ <sup>N</sup><sup>3</sup>)copper(II)]- $\mu$ -oxalato- $\kappa^4$ O<sup>1</sup>,O<sup>2</sup>:O<sup>1'</sup>,O<sup>2'</sup>]

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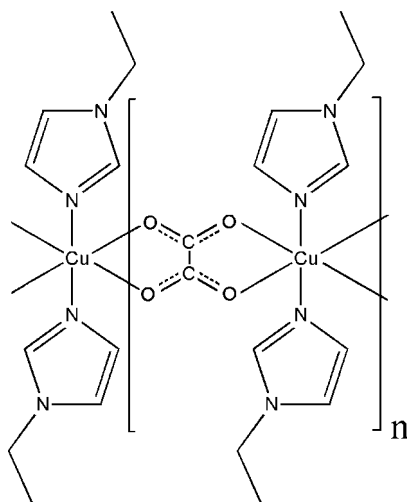
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.040;  $wR$  factor = 0.092; data-to-parameter ratio = 16.9.

The title compound,  $[\text{Cu}(\text{C}_2\text{O}_4)(\text{C}_5\text{H}_8\text{N}_2)_2]_n$ , is composed of one-dimensional linear chains running parallel to the  $a$  axis. In the chain,  $\text{trans}[\text{Cu}(\text{imidazole})_2]^{2+}$  units are sequentially bridged by bis-bidentate oxalate ligands, resulting in an octahedral  $\text{CuO}_4\text{N}_2$  donor set. The  $\text{Cu}\cdots\text{Cu}$  separation through the oxalate bridge is 5.620 (5) Å. Both the Cu atoms and the C—C bond of the oxalate bridge are bisected by inversion centres.

## Related literature

For general background on ferroelectric organic compounds with framework structures, see: Fu *et al.* (2009); Ye *et al.* (2006); Zhang *et al.* (2008, 2010).



## Experimental

### Crystal data

$[\text{Cu}(\text{C}_2\text{O}_4)(\text{C}_5\text{H}_8\text{N}_2)_2]$   
 $M_r = 343.83$   
Monoclinic,  $P2_1/n$   
 $a = 5.6200$  (11) Å  
 $b = 8.8577$  (18) Å  
 $c = 14.481$  (3) Å  
 $\beta = 96.55$  (3)°

$V = 716.2$  (2) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 1.55$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.30 \times 0.25 \times 0.20$  mm

### Data collection

Rigaku SCXmini diffractometer  
Absorption correction: multi-scan  
(*CrystalClear*; Rigaku, 2005)  
 $T_{\min} = 0.635$ ,  $T_{\max} = 0.734$

7300 measured reflections  
1653 independent reflections  
1267 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.062$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.092$   
 $S = 1.05$   
1653 reflections

98 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.48$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.33$  e Å<sup>-3</sup>

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2425).

## References

- Fu, D.-W., Ge, J.-Z., Dai, J., Ye, H.-Y. & Qu, Z.-R. (2009). *Inorg. Chem. Commun.* **12**, 994–997.  
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Ye, Q., Song, Y.-M., Wang, G.-X., Chen, K. & Fu, D.-W. (2006). *J. Am. Chem. Soc.* **128**, 6554–6555.  
Zhang, W., Xiong, R.-G. & Huang, S.-P. D. (2008). *J. Am. Chem. Soc.* **130**, 10468–10469.  
Zhang, W., Ye, H.-Y., Cai, H.-L., Ge, J.-Z. & Xiong, R.-G. (2010). *J. Am. Chem. Soc.* **132**, 7300–7302.

## supporting information

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***catena*-Poly[[bis(1-ethyl-1*H*-imidazole- $\kappa$ N<sup>3</sup>)copper(II)]- $\mu$ -oxalato- $\kappa^4$ O<sup>1</sup>,O<sup>2</sup>:O<sup>1'</sup>,O<sup>2'</sup>]**

**Qian Xu**

### S1. Comment

As part of our ongoing study of potential ferroelectric materials we have determined the structure of the present copper complex and examined its dielectric behaviour with temperature. This is the usual method for detecting these materials (Fu *et al.*, 2009; Ye *et al.*, 2006; Zhang *et al.*, 2008; Zhang *et al.*, 2010). Unfortunately, the dielectric constant for the title compound, Cu[C<sub>5</sub>H<sub>8</sub>N]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>, (I) does not show any behavior indicating the onset of a ferroelectric phase change over the range 80 K to 298 K (m.p.319–329).

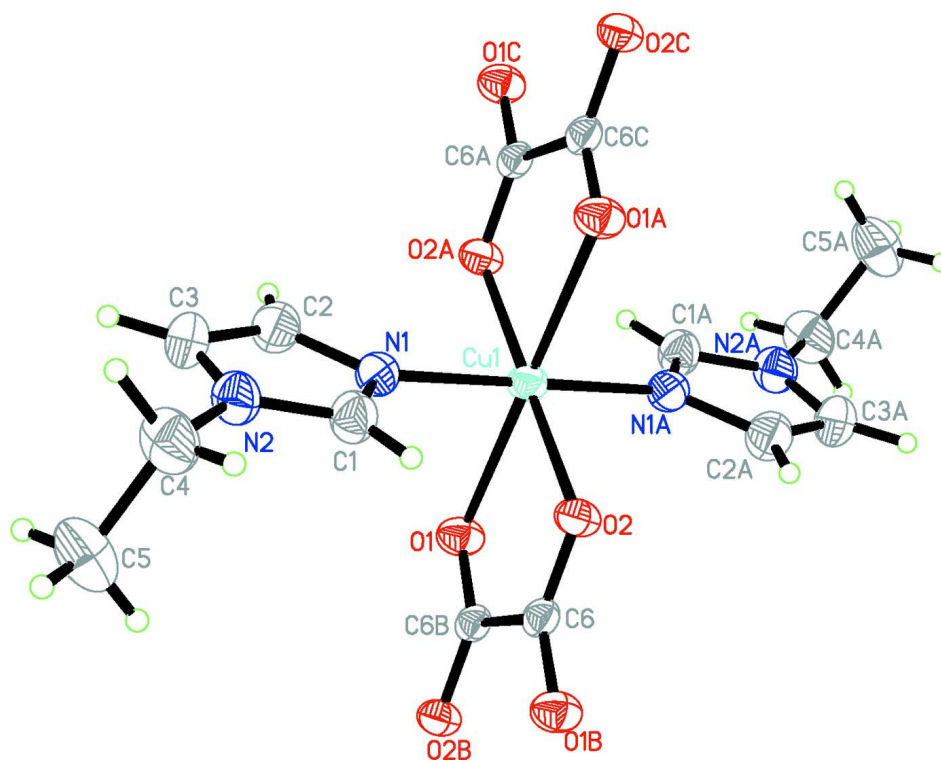
The Cu atoms are located on crystallographic inversion centers, and are coordinated to four oxygen atoms of two bridging oxalato ligands, also bisected by inversion centres, and two endocyclic nitrogen atoms from two crystallographically related imidazole molecules, resulting in octahedral MO<sub>4</sub>N<sub>2</sub> donor sets. Fig. 2 suggests the way in which oxalato-bridged chains build up. The Cu — Cu intrachain separation is 5.620 (5) Å.

### S2. Experimental

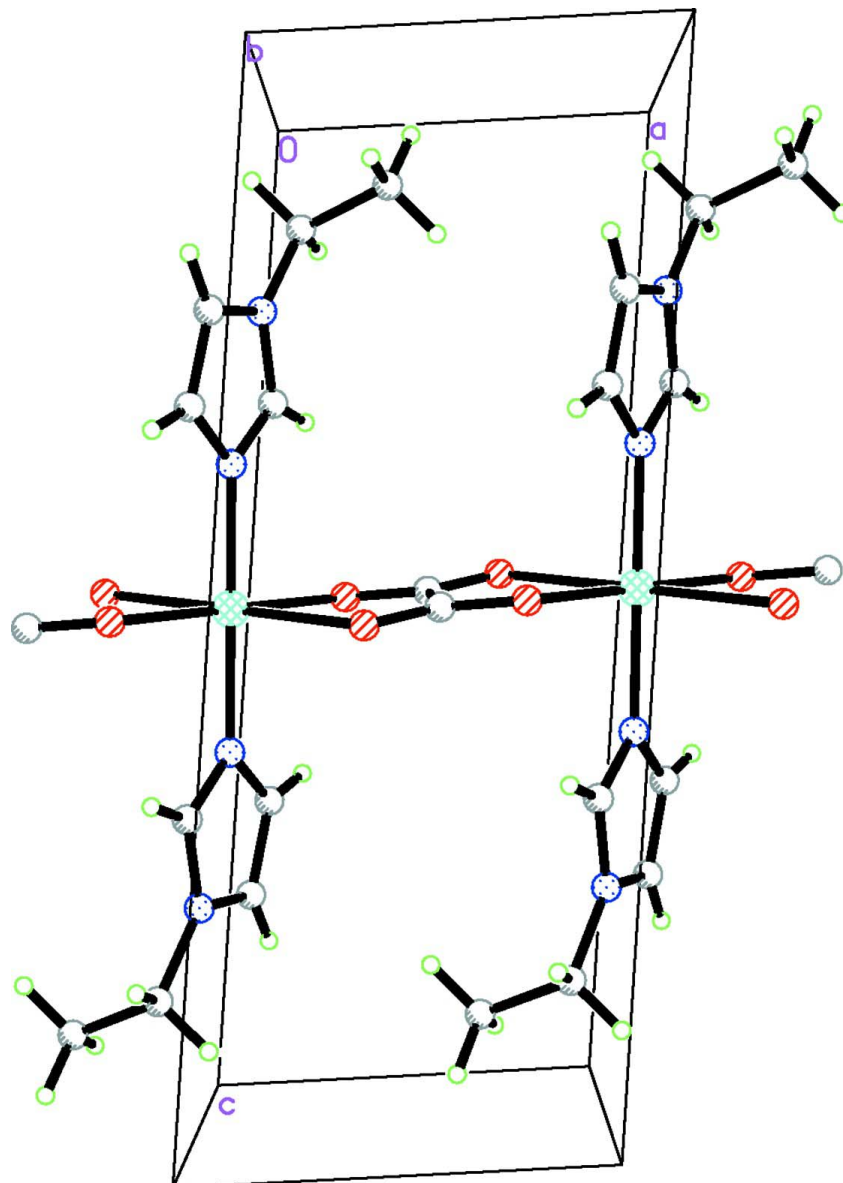
A mixture of 1-ethyl imidazole (1.9 g, 20 mmol), cupric oxalate (1.5 g, 10 mmol) in water was stirred for several days at ambient temperature; blue block crystals were obtained on standing.

### S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93–0.96 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{iso}}(\text{C})$  or  $1.5 U_{\text{iso}}(\text{C})$  for ethy H atoms..

**Figure 1**

Ellipsoid plot of (I), ( 50% probability level). Symmetry codes A:  $-x, 1-y, 1-z$ . B:  $1-x, 1-y, 1-z$ . C:  $-1+x, y, z$ .



**Figure 2**

Packing diagram of the title compound showing the way in which chains are built up.

**catena-Poly[[bis(1-ethyl-1H-imidazole- $\kappa$ N<sup>3</sup>)copper(II)]- $\mu$ -oxalato- $\kappa^4$ O<sup>1</sup>,O<sup>2</sup>:O<sup>1'</sup>,O<sup>2'</sup>]**

*Crystal data*

[Cu(C<sub>2</sub>O<sub>4</sub>)(C<sub>5</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>]

$M_r = 343.83$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 5.6200$  (11) Å

$b = 8.8577$  (18) Å

$c = 14.481$  (3) Å

$\beta = 96.55$  (3)°

$V = 716.2$  (2) Å<sup>3</sup>

$Z = 2$

$F(000) = 354$

$D_x = 1.594$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1653 reflections

$\theta = 2.3$ – $27.5$ °

$\mu = 1.55$  mm<sup>-1</sup>

$T = 293$  K

Block, blue

$0.30 \times 0.25 \times 0.20$  mm

*Data collection*

Rigaku SCXmini  
diffractometer  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
 $\omega$  scans  
Absorption correction: multi-scan  
(*CrystalClear*; Rigaku, 2005)  
 $T_{\min} = 0.635$ ,  $T_{\max} = 0.734$   
7300 measured reflections

1653 independent reflections  
1267 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.062$   
 $\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.7^\circ$   
 $h = -7 \rightarrow 7$   
 $k = -11 \rightarrow 11$   
 $l = -18 \rightarrow 18$   
2 standard reflections every 150 reflections  
intensity decay: none

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.092$   
 $S = 1.05$   
1653 reflections  
98 parameters  
0 restraints  
Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map  
Hydrogen site location: inferred from  
neighbouring sites  
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 0.3394P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.0000	0.5000	0.5000	0.02341 (16)
C1	0.0677 (5)	0.4366 (4)	0.3025 (2)	0.0326 (7)
H1	0.1452	0.3463	0.3194	0.039*
C2	-0.1151 (5)	0.6469 (4)	0.3090 (2)	0.0365 (7)
H2	-0.1900	0.7304	0.3318	0.044*
C3	-0.0853 (6)	0.6229 (4)	0.2184 (2)	0.0397 (8)
H3	-0.1337	0.6861	0.1685	0.048*
C4	0.1083 (6)	0.4132 (4)	0.1331 (2)	0.0439 (8)
H4A	-0.0227	0.4136	0.0833	0.053*
H4B	0.1477	0.3088	0.1482	0.053*
C5	0.3213 (7)	0.4885 (4)	0.0999 (3)	0.0534 (9)
H5A	0.2801	0.5899	0.0809	0.080*
H5B	0.3701	0.4333	0.0482	0.080*
H5C	0.4505	0.4906	0.1494	0.080*
C6	0.4839 (4)	0.4123 (3)	0.49195 (17)	0.0210 (5)

N1	-0.0177 (4)	0.5292 (3)	0.36168 (15)	0.0282 (6)
N2	0.0296 (4)	0.4876 (3)	0.21516 (16)	0.0339 (6)
O1	0.3372 (3)	0.6619 (2)	0.52150 (13)	0.0291 (5)
O2	0.2754 (3)	0.3599 (2)	0.49398 (12)	0.0259 (4)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0188 (2)	0.0301 (3)	0.0218 (2)	0.0016 (2)	0.00409 (16)	-0.0002 (2)
C1	0.0357 (16)	0.0345 (16)	0.0279 (16)	0.0039 (14)	0.0056 (13)	0.0016 (13)
C2	0.0367 (16)	0.0403 (18)	0.0333 (16)	0.0065 (14)	0.0067 (13)	0.0027 (14)
C3	0.0414 (17)	0.0478 (19)	0.0291 (16)	0.0012 (16)	0.0010 (13)	0.0095 (15)
C4	0.050 (2)	0.056 (2)	0.0266 (16)	-0.0079 (17)	0.0082 (14)	-0.0087 (15)
C5	0.063 (2)	0.050 (2)	0.052 (2)	-0.0054 (19)	0.0277 (19)	0.0000 (18)
C6	0.0211 (12)	0.0244 (14)	0.0172 (12)	0.0034 (12)	0.0008 (10)	0.0010 (11)
N1	0.0265 (12)	0.0336 (15)	0.0248 (12)	0.0027 (10)	0.0048 (10)	0.0015 (10)
N2	0.0358 (13)	0.0422 (15)	0.0238 (12)	-0.0023 (12)	0.0042 (10)	-0.0010 (11)
O1	0.0235 (9)	0.0270 (11)	0.0374 (11)	0.0020 (8)	0.0069 (8)	-0.0030 (9)
O2	0.0197 (9)	0.0269 (10)	0.0316 (10)	-0.0014 (8)	0.0054 (8)	-0.0003 (9)

*Geometric parameters (Å, °)*

Cu1—O2	1.9935 (18)	C3—H3	0.9300
Cu1—O2 <sup>i</sup>	1.9935 (18)	C4—N2	1.470 (4)
Cu1—N1	2.011 (2)	C4—C5	1.497 (4)
Cu1—N1 <sup>i</sup>	2.011 (2)	C4—H4A	0.9700
Cu1—O1 <sup>i</sup>	2.3684 (18)	C4—H4B	0.9700
Cu1—O1	2.3684 (19)	C5—H5A	0.9600
C1—N1	1.316 (4)	C5—H5B	0.9600
C1—N2	1.337 (4)	C5—H5C	0.9600
C1—H1	0.9300	C6—O1 <sup>ii</sup>	1.235 (3)
C2—C3	1.359 (4)	C6—O2	1.264 (3)
C2—N1	1.368 (4)	C6—C6 <sup>ii</sup>	1.579 (5)
C2—H2	0.9300	O1—C6 <sup>ii</sup>	1.235 (3)
C3—N2	1.365 (4)		
O2—Cu1—O2 <sup>i</sup>	180.000 (1)	N2—C4—C5	112.7 (3)
O2—Cu1—N1	89.27 (8)	N2—C4—H4A	109.1
O2 <sup>i</sup> —Cu1—N1	90.73 (8)	C5—C4—H4A	109.1
O2—Cu1—N1 <sup>i</sup>	90.73 (8)	N2—C4—H4B	109.1
O2 <sup>i</sup> —Cu1—N1 <sup>i</sup>	89.27 (8)	C5—C4—H4B	109.1
N1—Cu1—N1 <sup>i</sup>	180.000 (1)	H4A—C4—H4B	107.8
O2—Cu1—O1 <sup>i</sup>	103.35 (7)	C4—C5—H5A	109.5
O2 <sup>i</sup> —Cu1—O1 <sup>i</sup>	76.65 (7)	C4—C5—H5B	109.5
N1—Cu1—O1 <sup>i</sup>	89.94 (8)	H5A—C5—H5B	109.5
N1 <sup>i</sup> —Cu1—O1 <sup>i</sup>	90.06 (8)	C4—C5—H5C	109.5
O2—Cu1—O1	76.65 (7)	H5A—C5—H5C	109.5
O2 <sup>i</sup> —Cu1—O1	103.35 (7)	H5B—C5—H5C	109.5

N1—Cu1—O1	90.06 (8)	O1 <sup>ii</sup> —C6—O2	125.6 (2)
N1 <sup>i</sup> —Cu1—O1	89.94 (8)	O1 <sup>ii</sup> —C6—C6 <sup>ii</sup>	117.7 (3)
O1 <sup>i</sup> —Cu1—O1	180.00 (7)	O2—C6—C6 <sup>ii</sup>	116.7 (3)
N1—C1—N2	112.0 (3)	C1—N1—C2	105.3 (2)
N1—C1—H1	124.0	C1—N1—Cu1	126.0 (2)
N2—C1—H1	124.0	C2—N1—Cu1	128.6 (2)
C3—C2—N1	109.5 (3)	C1—N2—C3	106.8 (2)
C3—C2—H2	125.2	C1—N2—C4	125.6 (3)
N1—C2—H2	125.2	C3—N2—C4	127.5 (3)
C2—C3—N2	106.3 (3)	C6 <sup>ii</sup> —O1—Cu1	108.12 (16)
C2—C3—H3	126.8	C6—O2—Cu1	119.93 (16)
N2—C3—H3	126.8		

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