

Poly[bis(μ_2 -formato- κ^2 O:O')-(quinoxaline- κ N)copper(II)]

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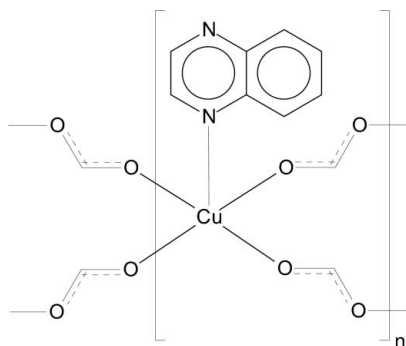
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 Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.027; wR factor = 0.070; data-to-parameter ratio = 15.3.

In the polymeric title copper(II) compound, $[\text{Cu}(\text{CHO}_2)_2(\text{C}_8\text{H}_6\text{N}_2)]_n$, both formate ligands are O-bidentate anions and act as bridging ligands, creating a planar polymeric arrangement. The slightly distorted square-pyramidal coordination around Cu^{II} comprises four O atoms from two different formate anions as the base and a quinoxaline molecule in the apical position.

Related literature

For related literature, see: Addison *et al.* (1984); Borthwick (1980); Sieroń (2003, 2007).



Experimental

Crystal data

 $[\text{Cu}(\text{CHO}_2)_2(\text{C}_8\text{H}_6\text{N}_2)]$
 $M_r = 283.73$

 Monoclinic, $P2_1/n$
 $a = 9.5648$ (3) Å

 $b = 11.1913$ (3) Å
 $c = 10.1910$ (4) Å
 $\beta = 108.284$ (3)°
 $V = 1035.80$ (6) Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 2.11$ mm⁻¹
 $T = 291$ K
 $0.30 \times 0.30 \times 0.08$ mm

Data collection

 KUMA KM4CCD diffractometer
 Absorption correction: multi-scan
 (*CrysAlis RED*; Oxford
 Diffraction, 2006)
 $T_{\text{min}} = 0.578$, $T_{\text{max}} = 0.843$

 12535 measured reflections
 2378 independent reflections
 2267 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.070$
 $S = 1.14$
 2378 reflections

 155 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.60$ e Å⁻³
Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.9605 (11)	Cu1—O4 ⁱⁱ	1.9489 (13)
Cu1—O2	1.9564 (14)	Cu1—N1	2.5150 (18)
Cu1—O3 ⁱ	1.9598 (12)		
O1—Cu1—O2	88.07 (5)	O3 ⁱ —Cu1—O4 ⁱⁱ	93.05 (5)
O1—Cu1—O3 ⁱ	172.89 (6)	O1—Cu1—N1	89.62 (6)
O1—Cu1—O4 ⁱⁱ	90.52 (5)	O2—Cu1—N1	88.95 (6)
O2—Cu1—O3 ⁱ	88.43 (5)	O3 ⁱ —Cu1—N1	96.50 (5)
O2—Cu1—O4 ⁱⁱ	178.42 (5)	O4 ⁱⁱ —Cu1—N1	90.32 (6)

 Symmetry codes: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* (Sheldrick, 2003) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2186).

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supplementary materials

Acta Cryst. (2008). E64, m53 [doi:10.1107/S1600536807063015]

Poly[bis(μ_2 -formate- $\kappa^2O:O'$)(quinoxaline- κN)copper(II)]

L. Sieron

Comment

The structure determination of the title compound was undertaken as a continuation of earlier studies of copper(II) complexes with formic acid (Sieroń, 2003; 2007). A fragment of the title compound structure is shown in Fig. 1.

The Cu^{II} atom has a square-pyramidal environment. The four short equatorial Cu–O bonds, that range from 1.9489 (13) to 1.9605 (11) Å, are formed by the formate anions. The long Cu–N axial bond of 2.515 (2) Å to quinoxaline molecule completes the five coordination geometry around Cu. The degree of trigonality $\tau = 0.092$ [τ is defined by Addison *et al.* (1984); for the regular square-pyramidal (SQP) structure, the trigonality parameter is 0, and for the trigonal-bipyramidal (TBP) structure, it increases to 1] indicates a slightly distorted SQP coordination of the Cu atom.

The O—C distances in both formate groups are approximately equal and range from 1.238 (2) to 1.250 (2) Å, indicating the distinct delocalization of their π electrons (Borthwick, 1980). All the formate anions coordinate in a bidentate *anti-anti* fashion, to result in a two-dimensional framework parallel to (10 $\bar{1}$) plane (Fig. 2). The quinoxaline rings engage in π - π stacking interactions, with distances between ring centroids of 3.6704 (12) Å, and these serve to connect polymeric planes into three-dimensional network.

The closest Cu \cdots Cu distance of 5.6164 (3) Å, corresponds approximately to half the length of the *b* axis. The second-shortest Cu \cdots Cu distance is 5.7924 (4) Å, which is half the length of the diagonal of the *ac* plane.

Experimental

The title complex was prepared by dissolving cupric formate [2 mmol, Cu(HCOO)₂·2H₂O] in 50 ml of water with quinoxaline (2 mmol, C₈H₆N₂). After heating to boiling, the formic acid was added dropwise to clear the solution. The solution was filtered and allowed to cool. After few days, green crystals were obtained.

Refinement

All H atoms were initially located in a difference Fourier synthesis, but were positioned with idealized geometry, with C–H = 0.93 Å, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, and refined using a riding model.

Figures

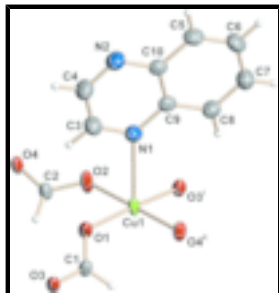


Fig. 1. A view of a fragment of the title compound showing 50% probability displacement ellipsoids. H atoms are shown as spheres of arbitrary radius [symmetry codes: (i) $-x + 3/2, y - 1/2, -z + 1/2$; (ii) $x - 1/2, -y + 3/2, z - 1/2$].

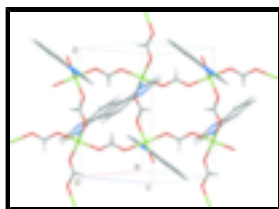


Fig. 2. The packing diagram showing two-dimensional polymeric framework parallel to $(10\bar{1})$ plane.

(I)

Crystal data

$[\text{Cu}(\text{CHO}_2)_2(\text{C}_8\text{H}_6\text{N}_2)]$

$M_r = 283.73$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 9.5648\ (3)\ \text{\AA}$

$b = 11.1913\ (3)\ \text{\AA}$

$c = 10.1910\ (4)\ \text{\AA}$

$\beta = 108.284\ (3)^\circ$

$V = 1035.80\ (6)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 572$

$D_x = 1.819\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 7748 reflections

$\theta = 2.8\text{--}32.3^\circ$

$\mu = 2.11\ \text{mm}^{-1}$

$T = 291\ \text{K}$

Prism, green

$0.30 \times 0.30 \times 0.08\ \text{mm}$

Data collection

KUMA KM4CCD diffractometer

Monochromator: graphite

Detector resolution: $8.2356\ \text{pixels mm}^{-1}$

$T = 291\ \text{K}$

ω scans

Absorption correction: multi-scan
(CrysAlis RED; Oxford Diffraction, 2006)

$T_{\min} = 0.578, T_{\max} = 0.843$

12535 measured reflections

2378 independent reflections

2267 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\max} = 27.5^\circ$

$\theta_{\min} = 3.1^\circ$

$h = -12 \rightarrow 12$

$k = -14 \rightarrow 14$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.027$	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2 + 0.4837P]$
$wR(F^2) = 0.070$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{\max} = 0.001$
2378 reflections	$\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$
155 parameters	$\Delta\rho_{\min} = -0.60 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: shelxl, $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0054 (8)

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.72396 (2)	0.74628 (2)	0.24693 (2)	0.0231 (1)
O1	0.75356 (15)	0.89959 (10)	0.34492 (12)	0.0276 (4)
O2	0.88757 (15)	0.68234 (11)	0.39838 (14)	0.0349 (4)
O3	0.78057 (14)	1.09526 (10)	0.35166 (12)	0.0257 (3)
O4	1.05990 (14)	0.68686 (11)	0.59961 (12)	0.0275 (3)
N1	0.55057 (18)	0.68333 (15)	0.37545 (17)	0.0316 (5)
N2	0.3759 (2)	0.66292 (17)	0.55363 (17)	0.0376 (6)
C1	0.75006 (19)	0.99809 (14)	0.28872 (19)	0.0240 (5)
C2	0.9877 (2)	0.73484 (16)	0.48872 (18)	0.0243 (5)
C3	0.5850 (3)	0.73576 (19)	0.4970 (2)	0.0376 (7)
C4	0.4972 (3)	0.7260 (2)	0.5847 (2)	0.0411 (7)
C5	0.2092 (2)	0.53257 (19)	0.3880 (2)	0.0357 (6)
C6	0.1703 (2)	0.4739 (2)	0.2637 (2)	0.0404 (7)
C7	0.2566 (3)	0.4848 (2)	0.1746 (2)	0.0400 (7)
C8	0.3807 (2)	0.55395 (19)	0.2109 (2)	0.0340 (6)
C9	0.4245 (2)	0.61503 (16)	0.33862 (19)	0.0280 (5)

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C10	0.3373 (2)	0.60485 (17)	0.42837 (19)	0.0292 (5)
H1	0.72280	0.99990	0.19270	0.0290*
H2	1.00950	0.81340	0.47250	0.0290*
H3	0.67060	0.78110	0.52620	0.0450*
H4	0.52680	0.76630	0.66870	0.0490*
H5	0.15140	0.52490	0.44590	0.0430*
H6	0.08630	0.42650	0.23790	0.0480*
H7	0.22870	0.44470	0.09040	0.0480*
H8	0.43650	0.56080	0.15120	0.0410*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0250 (2)	0.0143 (1)	0.0206 (1)	0.0024 (1)	-0.0063 (1)	-0.0023 (1)
O1	0.0403 (8)	0.0154 (5)	0.0213 (6)	-0.0021 (5)	0.0015 (5)	-0.0004 (4)
O2	0.0341 (7)	0.0218 (6)	0.0316 (7)	0.0032 (5)	-0.0142 (6)	-0.0024 (5)
O3	0.0340 (7)	0.0157 (5)	0.0215 (6)	-0.0028 (5)	0.0002 (5)	0.0003 (4)
O4	0.0267 (6)	0.0233 (6)	0.0233 (6)	-0.0048 (5)	-0.0052 (5)	0.0009 (5)
N1	0.0287 (8)	0.0350 (9)	0.0303 (8)	-0.0032 (7)	0.0082 (7)	0.0034 (7)
N2	0.0380 (10)	0.0450 (10)	0.0316 (9)	-0.0026 (8)	0.0134 (7)	0.0008 (7)
C1	0.0300 (9)	0.0186 (8)	0.0187 (7)	0.0009 (7)	0.0008 (6)	0.0002 (6)
C2	0.0243 (9)	0.0191 (8)	0.0238 (9)	-0.0003 (6)	-0.0007 (7)	-0.0011 (6)
C3	0.0331 (11)	0.0429 (12)	0.0358 (11)	-0.0087 (9)	0.0094 (9)	-0.0020 (8)
C4	0.0442 (13)	0.0482 (12)	0.0309 (10)	-0.0072 (10)	0.0119 (9)	-0.0050 (9)
C5	0.0323 (10)	0.0386 (10)	0.0381 (11)	-0.0022 (8)	0.0140 (8)	0.0059 (9)
C6	0.0348 (11)	0.0400 (11)	0.0447 (12)	-0.0105 (9)	0.0102 (9)	0.0004 (9)
C7	0.0428 (12)	0.0412 (11)	0.0337 (11)	-0.0062 (9)	0.0089 (9)	-0.0041 (9)
C8	0.0342 (10)	0.0378 (10)	0.0305 (9)	-0.0014 (8)	0.0107 (8)	0.0027 (8)
C9	0.0274 (9)	0.0270 (9)	0.0278 (9)	0.0025 (7)	0.0063 (7)	0.0073 (7)
C10	0.0295 (10)	0.0284 (9)	0.0289 (9)	0.0022 (7)	0.0080 (7)	0.0067 (7)

Geometric parameters (\AA , $^\circ$)

Cu1—O1	1.9605 (11)	C5—C6	1.371 (3)
Cu1—O2	1.9564 (14)	C5—C10	1.417 (3)
Cu1—O3 ⁱ	1.9598 (12)	C6—C7	1.411 (3)
Cu1—O4 ⁱⁱ	1.9489 (13)	C7—C8	1.367 (3)
Cu1—N1	2.5150 (18)	C8—C9	1.412 (3)
O1—C1	1.238 (2)	C9—C10	1.423 (3)
O2—C2	1.248 (2)	C1—H1	0.93
O3—C1	1.250 (2)	C2—H2	0.93
O4—C2	1.246 (2)	C3—H3	0.93
N1—C3	1.316 (3)	C4—H4	0.93
N1—C9	1.377 (3)	C5—H5	0.93
N2—C4	1.309 (3)	C6—H6	0.93
N2—C10	1.376 (3)	C7—H7	0.93
C3—C4	1.410 (4)	C8—H8	0.93
O1—Cu1—O2	88.07 (5)	C6—C7—C8	120.55 (19)

O1—Cu1—O3 ⁱ	172.89 (6)	C7—C8—C9	120.31 (19)
O1—Cu1—O4 ⁱⁱ	90.52 (5)	N1—C9—C8	120.08 (18)
O2—Cu1—O3 ⁱ	88.43 (5)	N1—C9—C10	120.61 (17)
O2—Cu1—O4 ⁱⁱ	178.42 (5)	C8—C9—C10	119.31 (18)
O3 ⁱ —Cu1—O4 ⁱⁱ	93.05 (5)	N2—C10—C5	119.66 (18)
O1—Cu1—N1	89.62 (6)	N2—C10—C9	121.20 (18)
O2—Cu1—N1	88.95 (6)	C5—C10—C9	119.14 (17)
O3 ⁱ —Cu1—N1	96.50 (5)	O1—C1—H1	118
O4 ⁱⁱ —Cu1—N1	90.32 (6)	O3—C1—H1	118
Cu1—O1—C1	124.40 (11)	O2—C2—H2	118
Cu1—O2—C2	130.44 (12)	O4—C2—H2	118
Cu1 ⁱⁱⁱ —O3—C1	121.55 (11)	N1—C3—H3	119
Cu1 ^{iv} —O4—C2	128.06 (12)	C4—C3—H3	119
Cu1—N1—C3	110.74 (15)	N2—C4—H4	118
Cu1—N1—C9	132.68 (13)	C3—C4—H4	118
C3—N1—C9	116.32 (19)	C6—C5—H5	120
C4—N2—C10	116.02 (18)	C10—C5—H5	120
O1—C1—O3	124.71 (17)	C5—C6—H6	120
O2—C2—O4	123.02 (17)	C7—C6—H6	120
N1—C3—C4	122.7 (2)	C6—C7—H7	120
N2—C4—C3	123.19 (19)	C8—C7—H7	120
C6—C5—C10	120.07 (18)	C7—C8—H8	120
C5—C6—C7	120.6 (2)	C9—C8—H8	120

Symmetry codes: (i) $-x+3/2, y-1/2, -z+1/2$; (ii) $x-1/2, -y+3/2, z-1/2$; (iii) $-x+3/2, y+1/2, -z+1/2$; (iv) $x+1/2, -y+3/2, z+1/2$.

Fig. 1

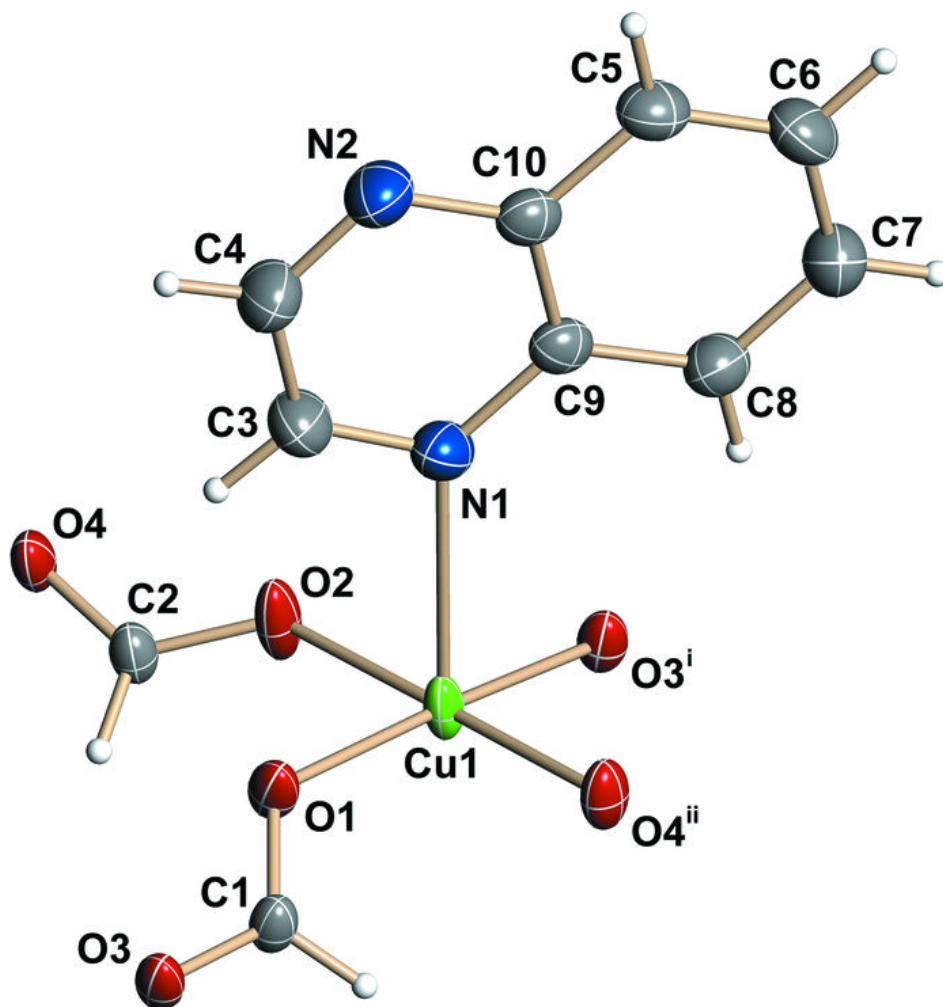


Fig. 2

