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Bis(2-bromoacetato- κ^2O,O')(1,10-phenanthroline- κ^2N,N')copper(II)

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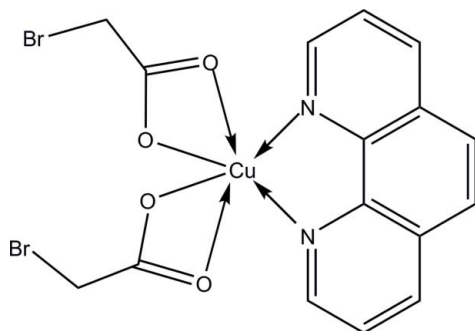
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 Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(C-C) = 0.011$ Å; R factor = 0.057; wR factor = 0.148; data-to-parameter ratio = 13.2.

The two halves of the title compound, $[Cu(C_2H_2BrO_2)_2(C_{12}H_8N_2)]$, are related by twofold symmetry along the b axis through the central Cu^{II} ion. The Cu^{II} ion is coordinated by two symmetry-related N atoms from the 1,10-phenanthroline ligand and four O atoms from two 2-bromoacetate ligands, showing a distorted octahedral geometry. Weak intermolecular $C-H \cdots O$ interactions link neighbouring molecules.

Related literature

For a report on mononuclear, monomeric and polymeric metal complexes, see: Liu *et al.* (2006).



Experimental

Crystal data

 $[Cu(C_2H_2BrO_2)_2(C_{12}H_8N_2)]$
 $M_r = 519.64$
 Monoclinic, $C2/c$
 $a = 10.3898$ (16) Å
 $b = 17.974$ (2) Å
 $c = 10.182$ (3) Å
 $\beta = 116.142$ (19)°

 $V = 1707.0$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 5.99$ mm⁻¹
 $T = 273$ K
 $0.31 \times 0.29 \times 0.27$ mm

Data collection

 Bruker SMART APEX diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.258$, $T_{max} = 0.295$
 (expected range = 0.174–0.199)

 3953 measured reflections
 1505 independent reflections
 984 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.066$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.148$
 $S = 1.00$
 1505 reflections

 114 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 1.11$ e Å⁻³
 $\Delta\rho_{min} = -0.78$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cu1—O2	1.941 (5)	Cu1—O1	2.725 (5)
Cu1—N1	2.016 (6)		

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; 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: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: E22160).

References

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 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
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supporting information

Acta Cryst. (2009). E65, m417 [doi:10.1107/S1600536809009349]

Bis(2-bromoacetato- κ^2O,O')(1,10-phenanthroline- κ^2N,N')copper(II)**Guofang He, Junshan Sun, Rengao Zhao and Jikun Li****S1. Comment**

Metal complexes with carboxylates are among the most investigated complexes in the field of coordination chemistry. Due to their versatile bonding modes with metal ions, they have been used in the synthesis of mononuclear, monomeric and polymeric complexes (Liu *et al.*, 2006). In order to develop new topological structures, we have studied the reaction of the copper(II) ion and 2-bromoacetic acid with the presence of 1,10-phenanthroline.

The molecular structure and a unit cell of the title complex are shown in Figs. 1 and 2. The Cu atom exhibits a six-coordinated distorted octahedral geometry. The two strongly bound carboxyl O atoms (Cu—O 1.941 (5) Å) and the two N atoms (Cu—N 2.016 (6) Å) occupy the equatorial positions. The two weakly bound O atoms (Cu1—O1 2.725 (5) Å) lie in the apical positions. Weak intermolecular C—H \cdots O hydrogen bonds link the molecules into a one-dimensional chain structure along the *c* axis.

S2. Experimental

The reaction was carried out by the solvothermal method. 2-bromoacetic acid (0.104 g, 2 mmol) and cupric acetate (0.199 g, 1 mmol) and 1,10-phenanthroline (0.180 g, 1 mmol) were added to the airtight vessel with 20 ml water. The resulting green solution was filtered. The filtrate was placed for several days yielding blue block-shaped crystals. Yield: 78%. Elemental analysis: calc. for C₁₆H₁₂CuBr₂N₂O₄: C 36.98, H 2.33, N 5.39; found: C 36.75, H 2.49, N 5.22. The elemental analyses were performed with PERKIN ELMER model 2400 series II.

S3. Refinement

All the H atoms were found in Fourier map, but placed in idealized positions (C—H 0.93–0.97 Å, O—H 0.85 Å), with the $U_{\text{iso}}(\text{H})$ values set at $1.2U_{\text{eq}}(\text{C},\text{O})$ of the parent atoms.

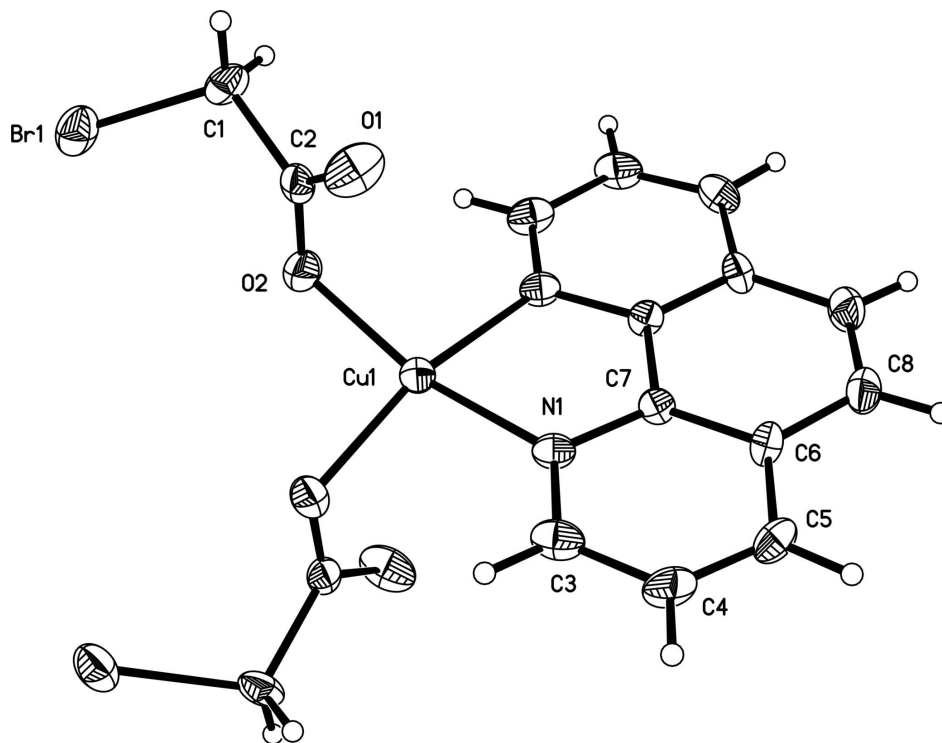


Figure 1

The molecular structure of title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

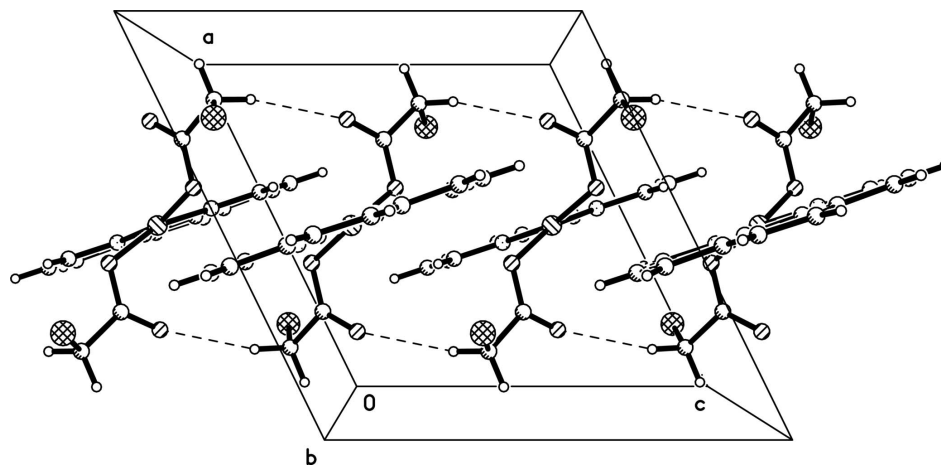


Figure 2

The stacking of the title compound into one-dimensional chains along the *c* axis. C—H...O interactions are indicated by dashed lines.

Bis(2-bromoacetato- κ^2O,O')(1,10-phenanthroline- κ^2N,N')copper(II)

Crystal data

[Cu(C₂H₂BrO₂)₂(C₁₂H₈N₂)]
M_r = 519.64

Monoclinic, *C2/c*
a = 10.3898 (16) Å

$b = 17.974$ (2) Å
 $c = 10.182$ (3) Å
 $\beta = 116.142$ (19)°
 $V = 1707.0$ (7) Å³
 $Z = 4$
 $F(000) = 1012$
 $D_x = 2.022$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 1329 reflections
 $\theta = 2.5$ – 25.5 °
 $\mu = 5.99$ mm⁻¹
 $T = 273$ K
 Block, blue
 $0.31 \times 0.29 \times 0.27$ mm

Data collection

Bruker SMART APEX
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.258$, $T_{\max} = 0.295$

3953 measured reflections
 1505 independent reflections
 984 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.066$
 $\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.5$ °
 $h = -12 \rightarrow 12$
 $k = -14 \rightarrow 21$
 $l = -11 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.148$
 $S = 1.00$
 1505 reflections
 114 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
 $w = 1/[\sigma^2(F_o^2) + (0.08P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.11$ e Å⁻³
 $\Delta\rho_{\min} = -0.78$ e Å⁻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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	1.0000	0.05952 (7)	0.2500	0.0345 (4)
N1	1.0486 (6)	0.1441 (3)	0.3940 (6)	0.0344 (14)
O1	0.7140 (6)	0.0296 (3)	0.1339 (6)	0.0598 (17)
O2	0.8977 (6)	-0.0134 (3)	0.0992 (6)	0.0486 (14)
Br1	0.72014 (9)	-0.15682 (5)	-0.05512 (9)	0.0529 (4)
C1	0.6633 (8)	-0.0541 (4)	-0.0643 (8)	0.0418 (19)
H1A	0.6604	-0.0315	-0.1522	0.050*
H1B	0.5675	-0.0517	-0.0705	0.050*
C2	0.7655 (8)	-0.0101 (4)	0.0685 (7)	0.0344 (17)
C3	1.0941 (7)	0.1419 (5)	0.5403 (8)	0.042 (2)

H3	1.1074	0.0960	0.5866	0.051*
C4	1.1215 (8)	0.2065 (5)	0.6232 (8)	0.045 (2)
H4	1.1530	0.2031	0.7238	0.054*
C5	1.1031 (7)	0.2740 (5)	0.5597 (8)	0.0416 (19)
H5	1.1242	0.3170	0.6162	0.050*
C6	1.0505 (7)	0.2786 (4)	0.4043 (8)	0.0336 (17)
C7	1.0261 (7)	0.2126 (4)	0.3290 (7)	0.0277 (15)
C8	1.0229 (9)	0.3460 (4)	0.3253 (9)	0.045 (2)
H8	1.0354	0.3910	0.3746	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0365 (7)	0.0306 (8)	0.0303 (7)	0.000	0.0092 (6)	0.000
N1	0.038 (3)	0.042 (4)	0.020 (3)	0.001 (3)	0.010 (3)	0.002 (3)
O1	0.065 (4)	0.081 (5)	0.042 (3)	-0.013 (3)	0.031 (3)	-0.026 (3)
O2	0.044 (3)	0.036 (3)	0.055 (4)	0.000 (2)	0.012 (3)	-0.012 (3)
Br1	0.0681 (7)	0.0460 (6)	0.0436 (6)	-0.0113 (4)	0.0236 (5)	-0.0127 (4)
C1	0.048 (4)	0.050 (5)	0.022 (4)	-0.013 (4)	0.010 (3)	-0.009 (4)
C2	0.049 (5)	0.028 (4)	0.023 (4)	0.000 (3)	0.012 (4)	0.004 (3)
C3	0.039 (4)	0.060 (6)	0.030 (4)	0.001 (4)	0.017 (4)	0.012 (4)
C4	0.048 (5)	0.063 (6)	0.021 (4)	0.000 (4)	0.012 (4)	-0.011 (4)
C5	0.049 (5)	0.044 (5)	0.032 (4)	-0.008 (4)	0.018 (4)	-0.017 (4)
C6	0.044 (4)	0.025 (4)	0.037 (4)	-0.006 (3)	0.022 (4)	-0.006 (3)
C7	0.036 (4)	0.031 (4)	0.019 (3)	0.003 (3)	0.015 (3)	0.000 (3)
C8	0.056 (5)	0.030 (5)	0.046 (5)	0.001 (4)	0.020 (4)	-0.007 (4)

Geometric parameters (Å, °)

Cu1—O2	1.941 (5)	C1—H1B	0.9700
Cu1—O2 ⁱ	1.941 (5)	C3—C4	1.389 (11)
Cu1—N1	2.016 (6)	C3—H3	0.9300
Cu1—N1 ⁱ	2.016 (6)	C4—C5	1.348 (11)
Cu1—O1	2.725 (5)	C4—H4	0.9300
N1—C3	1.350 (9)	C5—C6	1.431 (10)
N1—C7	1.368 (8)	C5—H5	0.9300
O1—C2	1.246 (8)	C6—C7	1.374 (9)
O2—C2	1.268 (8)	C6—C8	1.412 (10)
Br1—C1	1.929 (7)	C7—C7 ⁱ	1.455 (12)
C1—C2	1.521 (10)	C8—C8 ⁱ	1.392 (16)
C1—H1A	0.9700	C8—H8	0.9300
O2—Cu1—O2 ⁱ	95.1 (3)	O1—C2—O2	124.6 (7)
O2—Cu1—N1	163.5 (2)	O1—C2—C1	118.5 (7)
O2 ⁱ —Cu1—N1	93.4 (2)	O2—C2—C1	116.8 (6)
O2—Cu1—N1 ⁱ	93.4 (2)	N1—C3—C4	121.6 (7)
O2 ⁱ —Cu1—N1 ⁱ	163.5 (2)	N1—C3—H3	119.2
N1—Cu1—N1 ⁱ	82.1 (3)	C4—C3—H3	119.2

O2—Cu1—O1	53.88 (19)	C5—C4—C3	120.9 (7)
O2 ⁱ —Cu1—O1	108.8 (2)	C5—C4—H4	119.6
N1—Cu1—O1	109.9 (2)	C3—C4—H4	119.6
N1 ⁱ —Cu1—O1	87.6 (2)	C4—C5—C6	119.1 (7)
C3—N1—C7	117.5 (6)	C4—C5—H5	120.5
C3—N1—Cu1	129.3 (5)	C6—C5—H5	120.5
C7—N1—Cu1	113.1 (4)	C7—C6—C8	118.8 (6)
C2—O1—Cu1	72.7 (4)	C7—C6—C5	117.0 (6)
C2—O2—Cu1	108.7 (5)	C8—C6—C5	124.2 (7)
C2—C1—Br1	112.0 (5)	N1—C7—C6	123.9 (5)
C2—C1—H1A	109.2	N1—C7—C7 ⁱ	115.8 (3)
Br1—C1—H1A	109.2	C6—C7—C7 ⁱ	120.3 (4)
C2—C1—H1B	109.2	C8 ⁱ —C8—C6	120.8 (4)
Br1—C1—H1B	109.2	C8 ⁱ —C8—H8	119.6
H1A—C1—H1B	107.9	C6—C8—H8	119.6

Symmetry code: (i) $-x+2, y, -z+1/2$.