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Tetra-μ-acetato-$\kappa^8O:O'$-bis[(pyridine-2-carbonitrile-κN^1)copper(II)]

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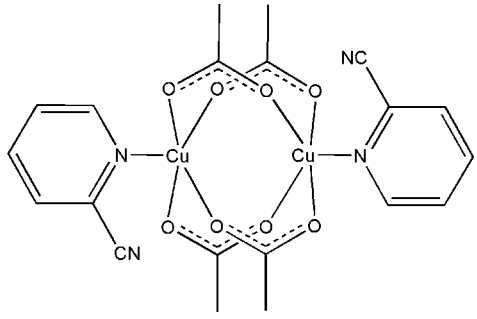
Key indicators: single-crystal X-ray study; T = 140 K; mean σ(C–C) = 0.008 Å; R factor = 0.060; wR factor = 0.159; data-to-parameter ratio = 13.2.

The title binuclear compound, $[Cu_2(CH_3COO)_4(C_6H_4N_2)_2]$, lies about an inversion center, with the Cu^{II} cation bridged by four acetate anions and coordinated by a pyridine N atom in a distorted square-pyramidal geometry. The Cu···Cu distance is 2.5997 (15) Å. In the crystal, molecules are linked by weak C—H···O and C—H···N hydrogen bonds into a three-dimensional supramolecular architecture. The crystal studied was a non-merohedral twin with a minor twin component of 4.1 (1)%.

Related literature

For related binuclear compounds, see: Fairuz *et al.* (2010); Chang *et al.* (2011).



Experimental

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_6H_4N_2)_2]$
M_r = 571.48
Monoclinic, $P2_1/c$
a = 7.929 (5) Å
b = 19.817 (12) Å
c = 8.222 (5) Å
β = 118.83 (2)°
V = 1131.8 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.93 mm^{-1}
T = 140 K
0.32 × 0.12 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.58, T_{max} = 0.89
7361 measured reflections
2077 independent reflections
1792 reflections with $I > 2\sigma(I)$
R_{int} = 0.165

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.159
S = 1.07
2077 reflections
157 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −1.48 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.975 (4)	Cu1—O4	1.952 (4)
Cu1—O2^{i}	1.980 (4)	Cu1—N1	2.235 (4)
Cu1—O3^{i}	1.941 (4)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N2^{ii}	0.93	2.60	3.196 (9)	122
C8—H8B···N2^{iii}	0.96	2.57	3.491 (8)	160
C10—H10A···O4^{iv}	0.96	2.54	3.381 (7)	147

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU5755).

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supporting information

Acta Cryst. (2014). E**70**, m27 [https://doi.org/10.1107/S1600536813034120]

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S1. Comment

The Cu–N complexes have occupied an important position in catalytic processes. In connection with on-going studies into the structural characterization of tetrakisacetatobis[(substituted 2-aminopyridyl)copper] complexes (Fairuz *et al.*, 2010; Chang *et al.* (2011), the title complex, (I), was investigated. The binuclear copper(II) complex, Fig. 1, is situated about a centre of inversion and features two Cu II atoms bridged by four acetate groups. The Cu–O bond distances ranged from 1.941 (4) to 1.980 (4) Å (Table 1). The distorted square-pyramidal coordination environment for the Cu atom is completed by a pyridine-N atom and four carboxyl-O atoms of acetate anions. In the binuclear compound, the Cu ···Cu distance is 2.5997 (15) Å. In the crystal, the molecules are linked by weak C—H···O and C—H···N hydrogen bonds into three dimensional supramolecular architecture.

S2. Experimental

2-Cyanopyridine (23.1233 g, 30 mmol) was added to a THF solution (60 ml) of $Cu(OAc)_2.H_2O$ (1.9972 g, 5 mmol). The reaction mixture was stirred vigorously while refluxing for 48 h. The filtrate was slowly evaporated, the blue single crystals were obtained.

S3. Refinement

H atoms were placed in calculated position with C—H = 0.93 (aromatic) and 0.96 Å (methyl), and refined in a riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms and $1.5U_{eq}(C)$ for methyl H atom.

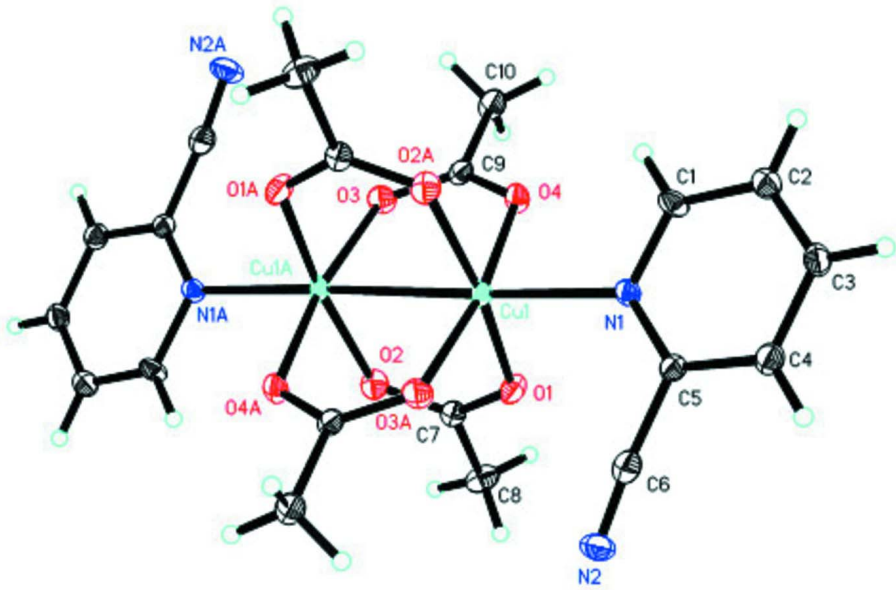

Figure 1

The structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

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Crystal data

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$M_r = 571.48$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.929$ (5) Å
$b = 19.817$ (12) Å
$c = 8.222$ (5) Å
$\beta = 118.83$ (2)°
$V = 1131.8$ (12) Å^3
$Z = 2$
$F(000) = 580$
$D_x = 1.677$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3034 reflections
$\theta = 2.9$–$30.5°$
$\mu = 1.93$ mm^{-1}
$T = 140$ K
Block, blue
0.32 × 0.12 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.58$, $T_{max} = 0.89$
7361 measured reflections
2077 independent reflections
1792 reflections with $I > 2\sigma(I)$
$R_{int} = 0.165$
$\theta_{max} = 25.3°$, $\theta_{min} = 1.0°$
$h = -9 \rightarrow 9$
$k = -23 \rightarrow 23$
$l = -9 \rightarrow 6$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.159$
$S = 1.07$
2077 reflections
157 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
$w = 1/[\sigma^2(F_o^2) + (0.0938P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -1.48$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cu1	0.40864 (8)	0.05361 (2)	0.50591 (7)	0.0184 (3)
N1	0.2510 (5)	0.14273 (19)	0.5328 (6)	0.0199 (8)
N2	0.6530 (7)	0.2387 (2)	0.6344 (9)	0.0436 (14)
O1	0.4618 (6)	0.08980 (17)	0.3114 (5)	0.0295 (8)
O2	0.6269 (6)	−0.00139 (17)	0.3074 (5)	0.0283 (8)
O3	0.3373 (5)	−0.08126 (18)	0.3035 (5)	0.0318 (8)
O4	0.1766 (5)	0.00951 (17)	0.3166 (5)	0.0260 (8)
C1	0.0735 (7)	0.1301 (2)	0.5040 (7)	0.0253 (11)
H1	0.0229	0.0871	0.4645	0.030*
C2	−0.0387 (7)	0.1775 (2)	0.5298 (7)	0.0270 (11)
H2	−0.1624	0.1666	0.5070	0.032*
C3	0.0343 (7)	0.2405 (2)	0.5895 (7)	0.0264 (11)
H3	−0.0394	0.2731	0.6075	0.032*
C4	0.2182 (8)	0.2557 (2)	0.6228 (7)	0.0261 (11)
H4	0.2711	0.2982	0.6643	0.031*
C5	0.3216 (7)	0.2053 (2)	0.5922 (7)	0.0201 (10)
C6	0.5091 (8)	0.2214 (2)	0.6174 (8)	0.0303 (12)
C7	0.5577 (7)	0.0559 (2)	0.2514 (7)	0.0214 (10)
C8	0.5910 (9)	0.0865 (3)	0.1015 (8)	0.0320 (12)
H8A	0.6835	0.0600	0.0860	0.048*
H8B	0.6388	0.1317	0.1362	0.048*
H8C	0.4719	0.0875	−0.0131	0.048*
C9	0.1852 (8)	−0.0478 (2)	0.2547 (7)	0.0228 (10)
C10	0.0014 (8)	−0.0787 (3)	0.1106 (8)	0.0324 (12)
H10A	−0.0097	−0.0723	−0.0099	0.049*
H10B	−0.1056	−0.0575	0.1144	0.049*
H10C	0.0014	−0.1261	0.1349	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0166 (4)	0.0163 (3)	0.0162 (4)	0.0018 (2)	0.0029 (3)	−0.0010 (2)

N1	0.0151 (18)	0.0218 (18)	0.018 (2)	0.0014 (16)	0.0041 (16)	−0.0018 (16)
N2	0.029 (3)	0.028 (2)	0.079 (4)	−0.007 (2)	0.031 (3)	−0.014 (2)
O1	0.038 (2)	0.0219 (16)	0.031 (2)	0.0029 (16)	0.0185 (18)	0.0034 (15)
O2	0.034 (2)	0.0291 (18)	0.0237 (19)	0.0055 (16)	0.0161 (17)	0.0009 (15)
O3	0.0231 (18)	0.0252 (17)	0.034 (2)	−0.0019 (17)	0.0034 (17)	−0.0079 (16)
O4	0.0175 (17)	0.0260 (17)	0.0216 (19)	0.0029 (14)	−0.0010 (15)	−0.0027 (14)
C1	0.019 (2)	0.024 (2)	0.025 (3)	−0.005 (2)	0.005 (2)	−0.003 (2)
C2	0.019 (2)	0.028 (2)	0.031 (3)	0.000 (2)	0.010 (2)	0.001 (2)
C3	0.023 (3)	0.024 (2)	0.029 (3)	0.006 (2)	0.010 (2)	0.001 (2)
C4	0.028 (3)	0.020 (2)	0.029 (3)	0.003 (2)	0.013 (2)	0.000 (2)
C5	0.020 (2)	0.018 (2)	0.019 (2)	0.0016 (19)	0.007 (2)	0.0021 (18)
C6	0.034 (3)	0.018 (2)	0.042 (3)	0.004 (2)	0.021 (3)	−0.002 (2)
C7	0.019 (2)	0.022 (2)	0.016 (2)	−0.003 (2)	0.004 (2)	−0.0023 (18)
C8	0.040 (3)	0.030 (3)	0.023 (3)	−0.006 (2)	0.013 (2)	0.001 (2)
C9	0.022 (3)	0.022 (2)	0.014 (2)	−0.003 (2)	0.001 (2)	0.0004 (19)
C10	0.024 (3)	0.029 (3)	0.026 (3)	−0.005 (2)	−0.003 (2)	0.001 (2)

Geometric parameters (Å, º)

Cu1—O1	1.975 (4)	C1—H1	0.9300
Cu1—O2^{i}	1.980 (4)	C2—C3	1.366 (7)
Cu1—O3^{i}	1.941 (4)	C2—H2	0.9300
Cu1—O4	1.952 (4)	C3—C4	1.380 (7)
Cu1—N1	2.235 (4)	C3—H3	0.9300
Cu1—Cu1^{i}	2.5997 (15)	C4—C5	1.389 (7)
N1—C1	1.334 (6)	C4—H4	0.9300
N1—C5	1.352 (6)	C5—C6	1.435 (7)
N2—C6	1.133 (7)	C7—C8	1.507 (7)
O1—C7	1.279 (6)	C8—H8A	0.9600
O2—C7	1.248 (6)	C8—H8B	0.9600
O2—Cu1^{i}	1.980 (4)	C8—H8C	0.9600
O3—C9	1.261 (7)	C9—C10	1.496 (7)
O3—Cu1^{i}	1.941 (4)	C10—H10A	0.9600
O4—C9	1.259 (6)	C10—H10B	0.9600
C1—C2	1.379 (7)	C10—H10C	0.9600
O3^{i}—Cu1—O4	169.17 (14)	C2—C3—C4	119.6 (5)
O3^{i}—Cu1—O1	90.43 (17)	C2—C3—H3	120.2
O4—Cu1—O1	90.23 (16)	C4—C3—H3	120.2
O3^{i}—Cu1—O2^{i}	90.11 (17)	C3—C4—C5	117.9 (5)
O4—Cu1—O2^{i}	87.28 (16)	C3—C4—H4	121.1
O1—Cu1—O2^{i}	169.40 (14)	C5—C4—H4	121.1
O3^{i}—Cu1—N1	96.27 (15)	N1—C5—C4	123.2 (4)
O4—Cu1—N1	94.34 (15)	N1—C5—C6	118.4 (4)
O1—Cu1—N1	98.10 (15)	C4—C5—C6	118.4 (4)
O2^{i}—Cu1—N1	92.35 (14)	N2—C6—C5	175.1 (6)
O3^{i}—Cu1—Cu1^{i}	83.16 (11)	O2—C7—O1	125.0 (4)
O4—Cu1—Cu1^{i}	86.12 (11)	O2—C7—C8	116.7 (4)

O1—Cu1—Cu1^{i}	85.76 (11)	O1—C7—C8	118.3 (4)
O2^{i}—Cu1—Cu1^{i}	83.80 (10)	C7—C8—H8A	109.5
N1—Cu1—Cu1^{i}	176.10 (10)	C7—C8—H8B	109.5
C1—N1—C5	117.0 (4)	H8A—C8—H8B	109.5
C1—N1—Cu1	115.2 (3)	C7—C8—H8C	109.5
C5—N1—Cu1	127.4 (3)	H8A—C8—H8C	109.5
C7—O1—Cu1	121.3 (3)	H8B—C8—H8C	109.5
C7—O2—Cu1^{i}	124.0 (3)	O4—C9—O3	125.1 (5)
C9—O3—Cu1^{i}	124.7 (3)	O4—C9—C10	117.9 (5)
C9—O4—Cu1	120.8 (3)	O3—C9—C10	117.0 (4)
N1—C1—C2	123.3 (5)	C9—C10—H10A	109.5
N1—C1—H1	118.4	C9—C10—H10B	109.5
C2—C1—H1	118.4	H10A—C10—H10B	109.5
C3—C2—C1	119.1 (4)	C9—C10—H10C	109.5
C3—C2—H2	120.5	H10A—C10—H10C	109.5
C1—C2—H2	120.5	H10B—C10—H10C	109.5

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N2^{ii}	0.93	2.60	3.196 (9)	122
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