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Tetra-μ-acetato-κ^8O:O'-bis{[2-(*m*-tolylamino)pyridine-κN]copper(II)}

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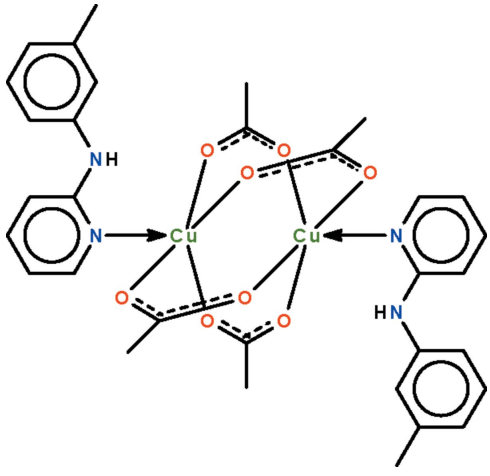
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.098; data-to-parameter ratio = 17.4.

In the crystal structure of the title compound, $[Cu_2(C_2H_3O_2)_4(C_{12}H_{12}N_2)_2]$, the binuclear molecule lies about a center of inversion; the four acetate groups each bridge a pair of Cu^{II} atoms. The coordination of the metal atom is distorted square-pyramidal, with the bonding O atoms comprising a square basal plane and the coordinating N atom of the *N*-heterocycle occupying the apical position. The pyridine ring is twisted with respect to the benzene ring at a dihedral angle of 45.68 (16)°. Intramolecular N—H···O hydrogen bonding is present between the imino and carboxy groups.

Related literature

There are many examples of tetrakisacetatobis[(substituted pyridine)copper] complexes. For examples of 2-aminopyridyl derivatives, see: Barquín *et al.* (2004); Seco *et al.* (2004); Sieroń (2004).



Experimental

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{12}H_{12}N_2)_2]$
M_r = 731.73
Triclinic, $P\overline{1}$
a = 7.7143 (2) Å
b = 10.5625 (3) Å
c = 11.2413 (3) Å
α = 66.531 (2)°
β = 85.740 (2)°
γ = 78.568 (2)°
V = 823.51 (4) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 293 K
0.25 × 0.15 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.730, T_{max} = 0.936
6451 measured reflections
3678 independent reflections
2915 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.098
S = 1.07
3678 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.9762 (19)	Cu1—O4^{i}	1.966 (2)
Cu1—O2^{i}	1.9866 (19)	Cu1—N1	2.197 (2)
Cu1—O3	1.967 (2)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.86	2.17	2.913 (3)	145

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2688).

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supporting information

Acta Cryst. (2009). E**65**, m1690 [doi:10.1107/S1600536809050041]

Tetra-μ-acetato-$\kappa^8O:O'$-bis{[2-(*m*-tolylamino)pyridine-κN]copper(II)}

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S1. Experimental

Copper acetate (0.1 g, 0.5 mmol) was dissolved in acetonitrile (5 ml). The solution was mixed with a solution of 3-tolylamino-2-pyridine (0.2 g, 1.1 mmol) dissolved in acetonitrile (15 ml). The green precipitate that formed was recrystallized from acetonitrile.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93–0.96 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(C). The amino H-atom was similarly treated.

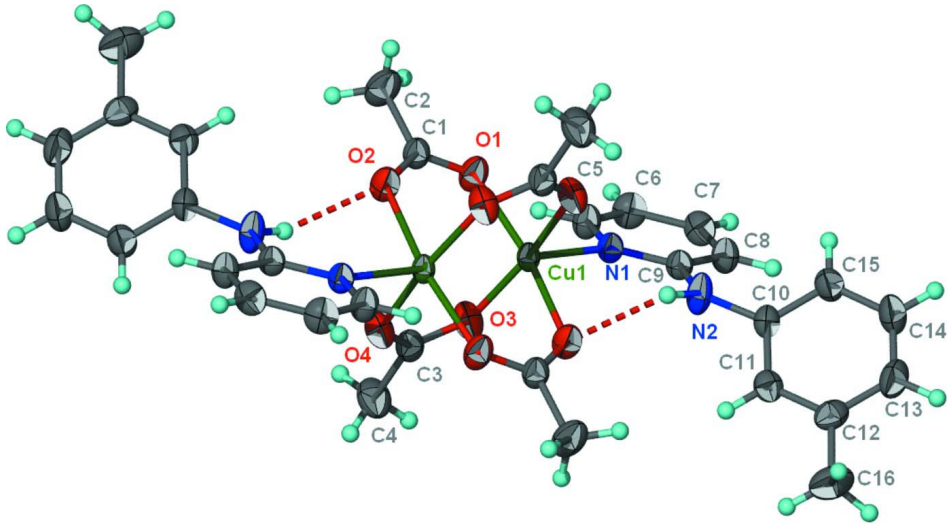

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $Cu_2(C_2H_3O_2)_4(C_{12}H_{12}N_2)_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. Dashed lines indicate the hydrogen bonding.

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γ = 78.568 (2)°
V = 823.51 (4) Å^3
Z = 1
F(000) = 378
D_x = 1.475 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2561 reflections

θ = 2.3–27.6°
μ = 1.35 mm^{-1}
T = 293 K

Prism, green
0.25 × 0.15 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.730, T_{max} = 0.936

6451 measured reflections
3678 independent reflections
2915 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 2.0°
h = −10→9
k = −13→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.098
S = 1.07
3678 reflections
211 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
$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.4239P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.58894 (4)	0.46743 (4)	0.60797 (3)	0.03044 (12)
O1	0.6955 (3)	0.6324 (2)	0.50147 (18)	0.0439 (5)
O2	0.5505 (3)	0.6857 (2)	0.31997 (18)	0.0419 (5)
O3	0.7582 (3)	0.3494 (2)	0.53769 (19)	0.0460 (5)
O4	0.6100 (3)	0.4052 (2)	0.35536 (19)	0.0436 (5)
N1	0.7506 (3)	0.4120 (2)	0.7806 (2)	0.0304 (5)
N2	0.5409 (3)	0.3175 (3)	0.9254 (2)	0.0446 (6)
H2	0.4771	0.3436	0.8573	0.053*
C1	0.6579 (4)	0.7076 (3)	0.3856 (3)	0.0342 (6)
C2	0.7467 (5)	0.8317 (4)	0.3197 (3)	0.0570 (9)
H2A	0.8448	0.8237	0.3717	0.085*
H2B	0.6637	0.9162	0.3091	0.085*
H2C	0.7885	0.8346	0.2363	0.085*
C3	0.7354 (4)	0.3375 (3)	0.4329 (3)	0.0378 (6)
C4	0.8709 (5)	0.2335 (4)	0.4000 (3)	0.0578 (9)
H4A	0.9175	0.1573	0.4784	0.087*
H4B	0.9652	0.2787	0.3520	0.087*
H4C	0.8169	0.1979	0.3485	0.087*
C5	0.9143 (4)	0.4436 (3)	0.7539 (3)	0.0389 (7)
H5	0.9471	0.4835	0.6675	0.047*
C6	1.0348 (4)	0.4198 (3)	0.8479 (3)	0.0438 (7)
H6	1.1454	0.4446	0.8259	0.053*

C7	0.9871 (4)	0.3582 (3)	0.9752 (3)	0.0403 (7)
H7	1.0662	0.3400	1.0411	0.048*
C8	0.8228 (4)	0.3236 (3)	1.0051 (3)	0.0395 (7)
H8	0.7896	0.2817	1.0912	0.047*
C9	0.7059 (3)	0.3518 (3)	0.9053 (2)	0.0309 (6)
C10	0.4629 (4)	0.2444 (3)	1.0447 (2)	0.0339 (6)
C11	0.3760 (4)	0.1388 (3)	1.0512 (3)	0.0365 (6)
H11	0.3785	0.1149	0.9799	0.044*
C12	0.2858 (4)	0.0682 (3)	1.1613 (3)	0.0417 (7)
C13	0.2886 (5)	0.1024 (4)	1.2678 (3)	0.0513 (8)
H13	0.2327	0.0539	1.3440	0.062*
C14	0.3736 (5)	0.2078 (4)	1.2618 (3)	0.0522 (8)
H14	0.3734	0.2302	1.3339	0.063*
C15	0.4592 (4)	0.2808 (3)	1.1506 (3)	0.0420 (7)
H15	0.5137	0.3533	1.1468	0.050*
C16	0.1823 (5)	−0.0390 (4)	1.1628 (4)	0.0658 (10)
H16A	0.2210	−0.0685	1.0932	0.099*
H16B	0.0587	0.0016	1.1522	0.099*
H16C	0.2012	−0.1187	1.2440	0.099*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02917 (19)	0.0399 (2)	0.02439 (17)	−0.01136 (14)	0.00032 (12)	−0.01252 (14)
O1	0.0492 (13)	0.0523 (13)	0.0312 (10)	−0.0263 (10)	−0.0027 (9)	−0.0090 (9)
O2	0.0452 (12)	0.0516 (13)	0.0325 (10)	−0.0246 (10)	−0.0018 (9)	−0.0125 (9)
O3	0.0414 (12)	0.0601 (14)	0.0384 (11)	−0.0004 (10)	−0.0021 (9)	−0.0250 (10)
O4	0.0412 (12)	0.0558 (13)	0.0376 (11)	−0.0023 (10)	−0.0020 (9)	−0.0251 (10)
N1	0.0282 (12)	0.0365 (13)	0.0277 (11)	−0.0101 (10)	−0.0003 (9)	−0.0118 (10)
N2	0.0374 (14)	0.0714 (18)	0.0249 (11)	−0.0241 (13)	−0.0002 (10)	−0.0123 (12)
C1	0.0330 (15)	0.0411 (16)	0.0309 (14)	−0.0141 (12)	0.0046 (11)	−0.0138 (12)
C2	0.065 (2)	0.058 (2)	0.0484 (19)	−0.0362 (19)	−0.0014 (16)	−0.0094 (16)
C3	0.0370 (16)	0.0418 (17)	0.0353 (15)	−0.0110 (13)	0.0082 (12)	−0.0154 (13)
C4	0.058 (2)	0.062 (2)	0.051 (2)	0.0063 (18)	0.0032 (16)	−0.0289 (18)
C5	0.0349 (16)	0.0487 (18)	0.0323 (14)	−0.0123 (14)	0.0022 (12)	−0.0133 (13)
C6	0.0298 (15)	0.0532 (19)	0.0489 (18)	−0.0094 (14)	−0.0038 (13)	−0.0191 (15)
C7	0.0344 (16)	0.0476 (18)	0.0387 (16)	−0.0007 (13)	−0.0117 (12)	−0.0179 (14)
C8	0.0398 (17)	0.0489 (18)	0.0277 (14)	−0.0074 (14)	−0.0039 (12)	−0.0125 (13)
C9	0.0293 (14)	0.0353 (15)	0.0289 (13)	−0.0068 (11)	−0.0014 (10)	−0.0129 (11)
C10	0.0299 (14)	0.0421 (16)	0.0272 (13)	−0.0056 (12)	0.0013 (10)	−0.0117 (12)
C11	0.0327 (15)	0.0406 (16)	0.0362 (15)	−0.0027 (12)	0.0003 (11)	−0.0171 (13)
C12	0.0366 (16)	0.0317 (16)	0.0494 (18)	−0.0040 (13)	0.0041 (13)	−0.0100 (13)
C13	0.052 (2)	0.055 (2)	0.0358 (16)	−0.0099 (16)	0.0131 (14)	−0.0090 (15)
C14	0.058 (2)	0.068 (2)	0.0357 (16)	−0.0142 (18)	0.0102 (14)	−0.0261 (16)
C15	0.0450 (18)	0.0476 (18)	0.0385 (16)	−0.0129 (15)	0.0054 (13)	−0.0210 (14)
C16	0.065 (3)	0.047 (2)	0.080 (3)	−0.0220 (19)	0.006 (2)	−0.0163 (19)

Geometric parameters (Å, º)

Cu1—O1	1.9762 (19)	C4—H4C	0.9600
Cu1—O2^{i}	1.9866 (19)	C5—C6	1.372 (4)
Cu1—O3	1.967 (2)	C5—H5	0.9300
Cu1—O4^{i}	1.966 (2)	C6—C7	1.372 (4)
Cu1—N1	2.197 (2)	C6—H6	0.9300
Cu1—Cu1^{i}	2.6532 (6)	C7—C8	1.370 (4)
O1—C1	1.246 (3)	C7—H7	0.9300
O2—C1	1.259 (3)	C8—C9	1.393 (4)
O2—Cu1^{i}	1.9866 (19)	C8—H8	0.9300
O3—C3	1.261 (3)	C10—C11	1.387 (4)
O4—C3	1.250 (4)	C10—C15	1.385 (4)
O4—Cu1^{i}	1.966 (2)	C11—C12	1.384 (4)
N1—C9	1.339 (3)	C11—H11	0.9300
N1—C5	1.352 (3)	C12—C13	1.385 (4)
N2—C9	1.370 (3)	C12—C16	1.503 (4)
N2—C10	1.413 (3)	C13—C14	1.377 (5)
N2—H2	0.8600	C13—H13	0.9300
C1—C2	1.498 (4)	C14—C15	1.380 (4)
C2—H2A	0.9600	C14—H14	0.9300
C2—H2B	0.9600	C15—H15	0.9300
C2—H2C	0.9600	C16—H16A	0.9600
C3—C4	1.500 (4)	C16—H16B	0.9600
C4—H4A	0.9600	C16—H16C	0.9600
C4—H4B	0.9600		

O4^{i}—Cu1—O3	167.64 (8)	H4A—C4—H4C	109.5
O4^{i}—Cu1—O1	88.77 (9)	H4B—C4—H4C	109.5
O3—Cu1—O1	90.33 (9)	N1—C5—C6	123.4 (3)
O4^{i}—Cu1—O2^{i}	89.16 (9)	N1—C5—H5	118.3
O3—Cu1—O2^{i}	89.01 (9)	C6—C5—H5	118.3
O1—Cu1—O2^{i}	167.27 (8)	C5—C6—C7	118.1 (3)
O4^{i}—Cu1—N1	98.40 (8)	C5—C6—H6	121.0
O3—Cu1—N1	93.96 (8)	C7—C6—H6	121.0
O1—Cu1—N1	94.60 (8)	C8—C7—C6	119.8 (3)
O2^{i}—Cu1—N1	98.13 (8)	C8—C7—H7	120.1
O4^{i}—Cu1—Cu1^{i}	84.47 (6)	C6—C7—H7	120.1
O3—Cu1—Cu1^{i}	83.19 (6)	C7—C8—C9	119.3 (3)
O1—Cu1—Cu1^{i}	83.69 (6)	C7—C8—H8	120.3
O2^{i}—Cu1—Cu1^{i}	83.61 (6)	C9—C8—H8	120.3
N1—Cu1—Cu1^{i}	176.65 (6)	N1—C9—N2	115.0 (2)
C1—O1—Cu1	124.57 (18)	N1—C9—C8	121.4 (2)
C1—O2—Cu1^{i}	123.80 (18)	N2—C9—C8	123.6 (2)
C3—O3—Cu1	124.0 (2)	C11—C10—C15	119.4 (3)
C3—O4—Cu1^{i}	122.82 (18)	C11—C10—N2	117.7 (2)
C9—N1—C5	118.0 (2)	C15—C10—N2	122.7 (3)
C9—N1—Cu1	127.85 (17)	C10—C11—C12	121.6 (3)

C5—N1—Cu1	114.18 (17)	C10—C11—H11	119.2
C9—N2—C10	127.9 (2)	C12—C11—H11	119.2
C9—N2—H2	116.1	C13—C12—C11	118.2 (3)
C10—N2—H2	116.1	C13—C12—C16	121.2 (3)
O1—C1—O2	124.3 (2)	C11—C12—C16	120.6 (3)
O1—C1—C2	117.9 (2)	C14—C13—C12	120.5 (3)
O2—C1—C2	117.8 (3)	C14—C13—H13	119.8
C1—C2—H2A	109.5	C12—C13—H13	119.8
C1—C2—H2B	109.5	C13—C14—C15	121.2 (3)
H2A—C2—H2B	109.5	C13—C14—H14	119.4
C1—C2—H2C	109.5	C15—C14—H14	119.4
H2A—C2—H2C	109.5	C14—C15—C10	119.1 (3)
H2B—C2—H2C	109.5	C14—C15—H15	120.5
O4—C3—O3	125.3 (3)	C10—C15—H15	120.5
O4—C3—C4	118.0 (3)	C12—C16—H16A	109.5
O3—C3—C4	116.7 (3)	C12—C16—H16B	109.5
C3—C4—H4A	109.5	H16A—C16—H16B	109.5
C3—C4—H4B	109.5	C12—C16—H16C	109.5
H4A—C4—H4B	109.5	H16A—C16—H16C	109.5
C3—C4—H4C	109.5	H16B—C16—H16C	109.5

O4^{i}—Cu1—O1—C1	−84.3 (2)	C9—N1—C5—C6	−1.4 (4)
O3—Cu1—O1—C1	83.4 (2)	Cu1—N1—C5—C6	178.8 (2)
O2^{i}—Cu1—O1—C1	−3.6 (6)	N1—C5—C6—C7	1.3 (5)
N1—Cu1—O1—C1	177.4 (2)	C5—C6—C7—C8	−0.5 (5)
Cu1^{i}—Cu1—O1—C1	0.3 (2)	C6—C7—C8—C9	−0.1 (5)
O4^{i}—Cu1—O3—C3	0.2 (6)	C5—N1—C9—N2	−177.5 (3)
O1—Cu1—O3—C3	−85.6 (2)	Cu1—N1—C9—N2	2.2 (4)
O2^{i}—Cu1—O3—C3	81.7 (2)	C5—N1—C9—C8	0.7 (4)
N1—Cu1—O3—C3	179.8 (2)	Cu1—N1—C9—C8	−179.6 (2)
Cu1^{i}—Cu1—O3—C3	−2.0 (2)	C10—N2—C9—N1	175.0 (3)
O4^{i}—Cu1—N1—C9	58.8 (2)	C10—N2—C9—C8	−3.2 (5)
O3—Cu1—N1—C9	−121.1 (2)	C7—C8—C9—N1	0.0 (4)
O1—Cu1—N1—C9	148.2 (2)	C7—C8—C9—N2	178.1 (3)
O2^{i}—Cu1—N1—C9	−31.6 (2)	C9—N2—C10—C11	−134.6 (3)
O4^{i}—Cu1—N1—C5	−121.5 (2)	C9—N2—C10—C15	50.2 (5)
O3—Cu1—N1—C5	58.6 (2)	C15—C10—C11—C12	−0.2 (4)
O1—Cu1—N1—C5	−32.0 (2)	N2—C10—C11—C12	−175.6 (3)
O2^{i}—Cu1—N1—C5	148.2 (2)	C10—C11—C12—C13	−2.0 (4)
Cu1—O1—C1—O2	−2.2 (4)	C10—C11—C12—C16	175.8 (3)
Cu1—O1—C1—C2	178.1 (2)	C11—C12—C13—C14	2.4 (5)
Cu1^{i}—O2—C1—O1	3.4 (4)	C16—C12—C13—C14	−175.4 (3)
Cu1^{i}—O2—C1—C2	−176.9 (2)	C12—C13—C14—C15	−0.6 (5)
Cu1^{i}—O4—C3—O3	−5.7 (4)	C13—C14—C15—C10	−1.6 (5)
Cu1^{i}—O4—C3—C4	174.4 (2)	C11—C10—C15—C14	2.0 (4)

Cu1—O3—C3—O4	5.2 (4)	N2—C10—C15—C14	177.2 (3)
Cu1—O3—C3—C4	−175.0 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.86	2.17	2.913 (3)	145

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