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Bis(acetato-κ^2O,O')bis[4-(dimethylamino)pyridine-κN]copper(II)

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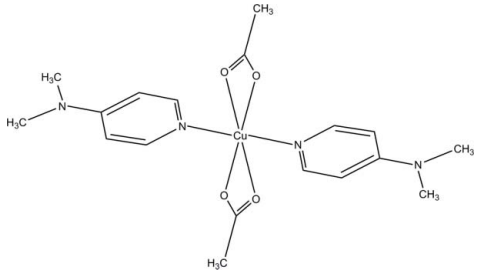
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.002 Å; R factor = 0.027; wR factor = 0.115; data-to-parameter ratio = 19.0.

In the mononuclear title complex, $[Cu(CH_3COO)_2(C_7H_{10}N_2)_2]$, the Cu^{II} ion, located on a crystallographic inversion centre, is six coordinated by two N atoms of two 4-(dimethylamino)pyridine (DMAP) ligands in apical positions and four O atoms from two symmetry-related opposite acetate anions, which are asymmetrically bonded in the equatorial plane. The complex and the crystal packing of the complex are stabilized by intra- and intermolecular C—H···O hydrogen bonds, giving $R_4^2(10)$ rings and generating a layer-like structure.

Related literature

For the importance of copper(II) carboxylate complexes in biology, see: Lippard & Berg (1994). For coordination properties of carboxylates, see: Deacon & Phillips (1980). For a similar structure, see: Li *et al.* (2009). For bond lengths in related copper complexes, see: Cui *et al.* (2009); Zaleski *et al.* (2005). For graph-set motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$[Cu(C_2H_3O_2)_2(C_7H_{10}N_2)_2]$
M_r = 425.98
Triclinic, $P\overline{1}$
a = 7.6930 (2) Å
b = 7.8331 (2) Å
c = 8.2206 (2) Å
α = 90.701 (2)°
β = 96.992 (2)°
γ = 92.949 (2)°
V = 490.95 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 180 K
0.48 × 0.37 × 0.12 mm

Data collection

Agilent Xcalibur Eos Gemini-ultra diffractometer
Absorption correction: multi-scan [ABSPACK in *CrysAlis PRO* (Agilent Technologies, 2010)]
T_{min} = 0.608, T_{max} = 0.872
10140 measured reflections
2362 independent reflections
2307 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.115
S = 1.11
2362 reflections
124 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H81···O4^{i}	0.95	2.51	3.452 (2)	173
C10—H101···O2^{ii}	0.93	2.49	3.381 (2)	161

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

Data collection: *CrysAlis PRO* (Agilent Technologies, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CRYSTALS*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2247).

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supporting information

Acta Cryst. (2011). E**67**, m235 [doi:10.1107/S1600536811002017]

Bis(acetato-κ^2O,O')bis[4-(dimethylamino)pyridine-κN]copper(II)

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S1. Comment

Lewis based coordinated Cu^{II} carboxylate complexes are an important class of coordination compounds due to their relevance as structural and functional models for biologically important metalloenzymes (Lippard & Berg,1994). Anionic carboxylates are highly flexible and versatile O-donor ligands since a range of substituents may be introduced on the alkyl chain to modulate their reactivity and coordination propensity, and result in a variety of coordination modes such as monodentate, bidentate bridging, chelating, monoatomic bridging and chelating bridging (Deacon & Phillips, 1980). The Lewis base 4-Dimethylaminopyridine (DMAP) is a derivative of pyridine that is widely used in hypernucleophilic acylation for a variety of reactions, such as esterifications with anhydrides. We report herein on the molecular structure of a novel compound, namely bis(acetate-κ^2O,O')bis(4-dimethylaminepyridine-κN)] Copper(II).

In the title complex the Cu^{II} cation lies on an inversion centre, as a consequence of which the asymmetric unit comprises one half-molecule (Fig. 1). The Cu^{II} ion is octahedrally coordinated by two (DMAP) ligands and two acetate units. It adopts a Jahn-Teller-distorted *trans*-CuO_4N_2 octahedral coordination similar to our previously reported Cu^{II} compound with the 4-(pyridine-4-yl)pyrimidine-2-sulfonate ligand (Li *et al.*, 2009). The four O atoms [O2, O4, and the symmetry-related atoms, $O2^I$, $O4^I$ (symmetry code: (I) $-x + 1,-y + 1,-z + 1$)] are located in the equatorial plane while the two N atoms of the (DMAP) ligands (N6, $N6^I$) are in the axial positions. The Cu1—N6 bond length of 2.0095 (13) Å agrees well with that reported for related copper complexes (Cui *et al.*, 2009, Zaleski *et al.*, 2005), while the Cu1—O2 and Cu1—O4 bond lengths are 1.9715 (11) and 2.5932 (13) Å, respectively. The dihedral angles formed between the mean planes through the four O atoms and the pyridine ring is 88.59 (1)°.

In the crystal, the packing is consolidated by C—H···O interactions involving aromatic H-atoms (Table 1, Fig 2), in which $R_4^2(10)$ (Bernstein *et al.*,1995) hydrogen-bonded rings are formed, generating a two-dimensional layer-like structure.

S2. Experimental

To a solution of $Cu(CH_3CO_2)_2.H_2O$ (0.2 g, 1 mmol) in methanol (40 cm^3) at room temperature was added solid 4-(Dimethylamino)pyridine (DMAP) (0.122 g, 1 mmol) in small portions under constant stirring. the mixture was then filtered and the filtrate allowed to stand for 20 days, after which small blue block-like crystals of the title complex were obtained. They were filtered and dried under vacuum.

S3. Refinement

All the C-bound H-atoms were located in difference Fourier maps but were treated as riding on their parent atoms: C-H = 0.917 - 0.974 Å with U_{iso}(H) = 1.2U_{eq}(C-aromatic) or U_{iso}(H) = 1.5U_{eq}(C-methyl).

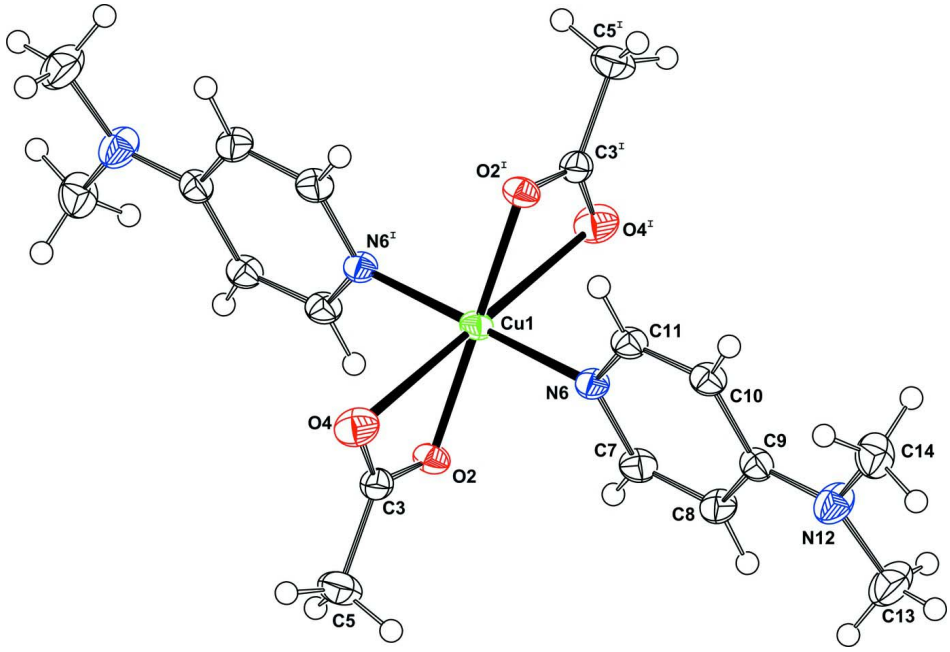

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as spheres of arbitary radius [Symmetry code: (I) = -*x* + 1,-*y* + 1,-*z* + 1].

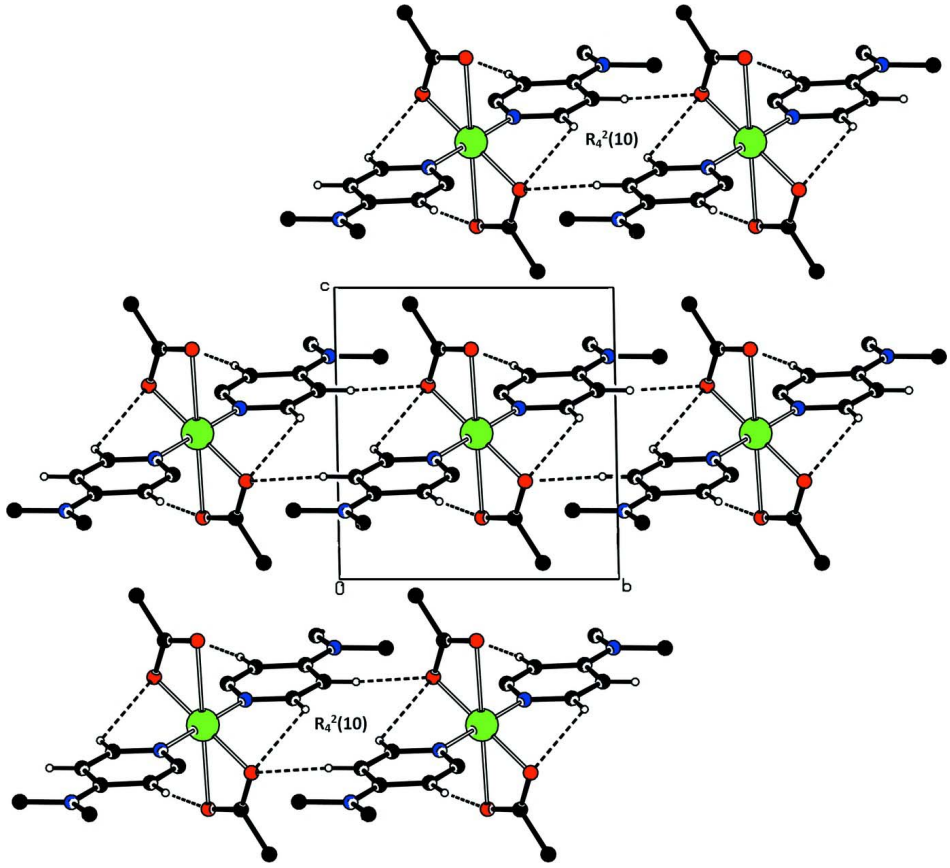

Figure 2

A view along the a-axis of the crystal structure of the title compound showing the formation of $R_4^2(10)$ rings. The C-H···O hydrogen bonds are shown as dashed lines; H-atoms no involved in the C-H..O interactions have been omitted for clarity.

Bis(acetato-κ^2O,O')bis[4-(dimethylamino)pyridine- κN]copper(II)

Crystal data

$[Cu(C_2H_3O_2)_2(C_7H_{10}N_2)_2]$
M_r = 425.98
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.6930 (2) Å
b = 7.8331 (2) Å
c = 8.2206 (2) Å
α = 90.701 (2)°
β = 96.992 (2)°
γ = 92.949 (2)°
V = 490.95 (2) Å^3
Z = 1
$F(000)$ = 223
D_x = 1.441 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 10054 reflections
θ = 3.4–29.0°
μ = 1.14 mm^{-1}
T = 180 K
Plate, blue
0.48 × 0.37 × 0.12 mm

Data collection

Agilent Xcalibur Eos Gemini-ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1978 pixels mm^{-1}
ω scans
Absorption correction: multi-scan [ABSPACK in *CrysAlis PRO* (Agilent Technologies, 2010)]
T_{min} = 0.608, T_{max} = 0.872
10140 measured reflections
2362 independent reflections

2307 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 29.1°$, $\theta_{min} = 3.4°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.115$
$S = 1.11$
2362 reflections
124 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.1P)^2 + 0.0P]$, where $P = p(6)*\max(F_o^2,0) + (1-p(6))F_c^2$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.5000	0.5000	0.0192
O2	0.44954 (15)	0.32890 (15)	0.66419 (14)	0.0229
C3	0.5609 (2)	0.3691 (2)	0.79019 (19)	0.0222
O4	0.67659 (17)	0.48560 (17)	0.78860 (16)	0.0321
C5	0.5412 (3)	0.2708 (3)	0.9440 (2)	0.0328
N6	0.32934 (17)	0.65325 (17)	0.58644 (16)	0.0204
C7	0.1803 (2)	0.5914 (2)	0.6416 (2)	0.0244
C8	0.0597 (2)	0.6918 (2)	0.6986 (2)	0.0247
C9	0.0888 (2)	0.8714 (2)	0.70624 (18)	0.0217
C10	0.2452 (2)	0.9354 (2)	0.64866 (19)	0.0226
C11	0.3565 (2)	0.8244 (2)	0.59137 (19)	0.0228
N12	−0.0240 (2)	0.9759 (2)	0.7651 (2)	0.0320
C13	−0.1935 (3)	0.9125 (3)	0.8063 (3)	0.0419
C14	0.0055 (3)	1.1609 (2)	0.7637 (2)	0.0338
H51	0.6487	0.2899	1.0188	0.0450*
H53	0.4473	0.3138	0.9949	0.0447*
H52	0.5228	0.1509	0.9233	0.0442*
H71	0.1609	0.4749	0.6399	0.0287*
H81	−0.0432	0.6385	0.7331	0.0283*
H101	0.2738	1.0521	0.6478	0.0252*
H111	0.4575	0.8681	0.5535	0.0258*
H132	−0.2467	0.9992	0.8633	0.0610*
H131	−0.1792	0.8177	0.8754	0.0606*
H133	−0.2691	0.8797	0.7128	0.0611*
H142	−0.0664	1.2144	0.8370	0.0514*
H141	0.1245	1.1930	0.8012	0.0513*
H143	−0.0217	1.1993	0.6517	0.0513*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02144 (19)	0.01507 (18)	0.02130 (19)	−0.00171 (11)	0.00403 (11)	0.00410 (11)

O2	0.0263 (6)	0.0200 (5)	0.0222 (5)	−0.0024 (4)	0.0037 (4)	0.0049 (4)
C3	0.0243 (7)	0.0201 (7)	0.0236 (7)	0.0039 (6)	0.0072 (5)	0.0023 (6)
O4	0.0290 (6)	0.0317 (7)	0.0348 (7)	−0.0083 (5)	0.0055 (5)	−0.0006 (5)
C5	0.0434 (10)	0.0332 (10)	0.0233 (8)	0.0038 (8)	0.0085 (7)	0.0068 (7)
N6	0.0203 (6)	0.0167 (6)	0.0245 (6)	−0.0022 (5)	0.0047 (5)	0.0027 (5)
C7	0.0250 (8)	0.0176 (7)	0.0305 (8)	−0.0049 (6)	0.0043 (6)	0.0045 (6)
C8	0.0206 (7)	0.0203 (7)	0.0331 (8)	−0.0051 (5)	0.0053 (6)	0.0035 (6)
C9	0.0213 (7)	0.0203 (7)	0.0226 (7)	−0.0017 (5)	0.0001 (5)	0.0024 (6)
C10	0.0243 (7)	0.0170 (7)	0.0258 (7)	−0.0040 (5)	0.0030 (6)	0.0019 (6)
C11	0.0225 (7)	0.0196 (8)	0.0259 (8)	−0.0049 (6)	0.0035 (6)	0.0037 (6)
N12	0.0270 (7)	0.0237 (7)	0.0470 (9)	−0.0012 (6)	0.0119 (6)	0.0003 (7)
C13	0.0266 (9)	0.0430 (11)	0.0583 (12)	−0.0011 (8)	0.0158 (8)	0.0032 (9)
C14	0.0341 (9)	0.0229 (8)	0.0446 (10)	0.0044 (7)	0.0050 (7)	0.0000 (7)

Geometric parameters (Å, º)

Cu1—O2	1.9715 (11)	C7—H71	0.917
Cu1—C3	2.6076 (16)	C8—C9	1.413 (2)
Cu1—O4	2.5932 (13)	C8—H81	0.951
Cu1—N6	2.0095 (13)	C9—C10	1.416 (2)
Cu1—O4^{i}	2.5932 (13)	C9—N12	1.350 (2)
Cu1—C3^{i}	2.6076 (16)	C10—C11	1.370 (2)
Cu1—N6^{i}	2.0095 (13)	C10—H101	0.929
Cu1—O2^{i}	1.9715 (11)	C11—H111	0.923
O2—C3	1.286 (2)	N12—C13	1.451 (2)
C3—O4	1.243 (2)	N12—C14	1.455 (2)
C3—C5	1.507 (2)	C13—H132	0.958
C5—H51	0.972	C13—H131	0.943
C5—H53	0.951	C13—H133	0.931
C5—H52	0.953	C14—H142	0.972
N6—C7	1.353 (2)	C14—H141	0.950
N6—C11	1.3452 (19)	C14—H143	0.974
C7—C8	1.367 (2)		
O4^{i}—Cu1—C3^{i}	27.66 (5)	H51—C5—H53	108.3
O4^{i}—Cu1—N6^{i}	91.06 (5)	C3—C5—H52	112.4
C3^{i}—Cu1—N6^{i}	89.28 (5)	H51—C5—H52	108.0
O4^{i}—Cu1—O2^{i}	56.16 (4)	H53—C5—H52	110.7
C3^{i}—Cu1—O2^{i}	28.54 (5)	Cu1—N6—C7	122.31 (11)
N6^{i}—Cu1—O2^{i}	89.50 (5)	Cu1—N6—C11	121.62 (10)
O4^{i}—Cu1—O2	123.84 (4)	C7—N6—C11	116.07 (13)
C3^{i}—Cu1—O2	151.46 (5)	N6—C7—C8	123.95 (14)
N6^{i}—Cu1—O2	90.50 (5)	N6—C7—H71	116.8
O2^{i}—Cu1—O2	179.994	C8—C7—H71	119.2
O4^{i}—Cu1—C3	152.34 (5)	C7—C8—C9	120.21 (14)
C3^{i}—Cu1—C3	179.996	C7—C8—H81	118.9
N6^{i}—Cu1—C3	90.72 (5)	C9—C8—H81	120.9
O2^{i}—Cu1—C3	151.46 (5)	C8—C9—C10	115.59 (14)

O2—Cu1—C3	28.54 (5)	C8—C9—N12	122.54 (14)
O4^{i}—Cu1—O4	179.996	C10—C9—N12	121.87 (14)
C3^{i}—Cu1—O4	152.34 (5)	C9—C10—C11	119.82 (14)
N6^{i}—Cu1—O4	88.94 (5)	C9—C10—H101	121.3
O2^{i}—Cu1—O4	123.84 (4)	C11—C10—H101	118.9
O2—Cu1—O4	56.16 (4)	C10—C11—N6	124.35 (14)
O4^{i}—Cu1—N6	88.94 (5)	C10—C11—H111	118.8
C3^{i}—Cu1—N6	90.72 (5)	N6—C11—H111	116.8
N6^{i}—Cu1—N6	179.994	C9—N12—C13	121.83 (16)
O2^{i}—Cu1—N6	90.50 (5)	C9—N12—C14	121.12 (15)
O2—Cu1—N6	89.50 (5)	C13—N12—C14	116.23 (16)
C3—Cu1—O4	27.66 (5)	N12—C13—H132	110.3
C3—Cu1—N6	89.28 (5)	N12—C13—H131	109.8
O4—Cu1—N6	91.06 (5)	H132—C13—H131	108.1
Cu1—O2—C3	104.37 (9)	N12—C13—H133	111.4
Cu1—C3—O2	47.09 (7)	H132—C13—H133	108.3
Cu1—C3—O4	75.53 (10)	H131—C13—H133	109.0
O2—C3—O4	122.50 (15)	N12—C14—H142	110.0
Cu1—C3—C5	162.83 (12)	N12—C14—H141	110.5
O2—C3—C5	116.55 (14)	H142—C14—H141	107.5
O4—C3—C5	120.92 (15)	N12—C14—H143	108.7
Cu1—O4—C3	76.82 (9)	H142—C14—H143	111.3
C3—C5—H51	108.2	H141—C14—H143	108.8
C3—C5—H53	109.2		

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*
C8—H81···O4^{ii}	0.95	2.51	3.452 (2)	173
C10—H101···O2^{iii}	0.93	2.49	3.381 (2)	161
C11—H111···O2^{i}	0.92	2.54	2.9946 (19)	111

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*−1, *y*, *z*; (iii) *x*, *y*+1, *z*.