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Bis(5-*n*-butylpyridine-2-carboxylato)-copper(II)

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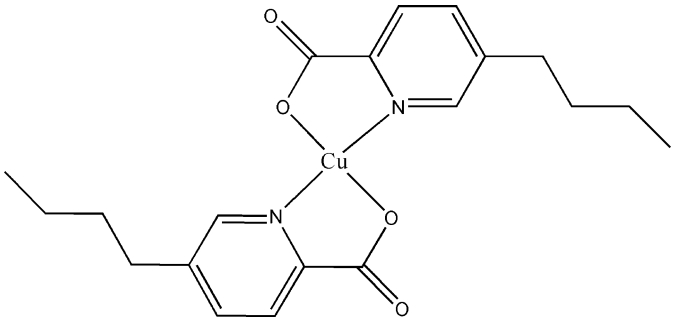
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.107; data-to-parameter ratio = 14.3.

The title complex, $[Cu(C_{10}H_{12}NO_2)_2]$, was obtained by the reaction of 5-butylpyridyl-2-carboxylic acid (fusaric acid), extracted from blasted leaves of *Rhizophora stylosa*, with copper(II) chloride in aqueous solution. The metal atom lies on a center of symmetry. The Cu^{II} atom is coordinated by two carboxylate O atoms and two N atoms from two different fusaric acid ligands, and displays a square-planar geometry.

Related literature

For related literature, see: Okabe, Muranishi & Wada (2002); Okabe, Wada & Muranishi (2002).



Experimental

Crystal data

$[Cu(C_{10}H_{12}NO_2)_2]$
M_r = 419.95
Triclinic, $P\overline{1}$
a = 5.5052 (1) Å
b = 8.0683 (3) Å
c = 11.3008 (5) Å
α = 70.338 (2)°
β = 89.399 (2)°
γ = 78.706 (1)°
V = 462.70 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.21 mm^{-1}
T = 293 (2) K
0.10 × 0.08 × 0.06 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.889, T_{max} = 0.935
3391 measured reflections
1788 independent reflections
1592 reflections with $I > 2\sigma(I)$
R_{int} = 0.103

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
S = 1.03
1788 reflections
125 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9344 (18)	Cu1—N1	1.960 (2)
O1^i—Cu1—O1	180	O1—Cu1—N1	83.97 (8)
O1^i—Cu1—N1	96.03 (8)	N1—Cu1—N1^i	180

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); 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: ZL2030).

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supplementary materials

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Bis(5-*n*-butylpyridine-2-carboxylato)copper(II)

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Comment

Some structures of transition metal complexes containing the 5-butyl-pyridyl-2-carboxylic acid (fusaric acid) ligand have been reported. In the structural investigation of these complexes, it has been found that the fusaric acid functions as a multidentate ligand (Okabe, Muranishi & Wada (2002); Okabe, Wada & Muranishi (2002), with versatile binding and coordination modes. In this paper, we report the crystal structure of the title compound, (I), a new Cu complex obtained by the reaction of fusaric acid extracted from blasted leaves of Rhizophora Stylosa with copper chloride in aqueous solution.

As illustrated in Fig. 1, the Cu^{II} atom lies on a centre of symmetry and has a square planar geometry with the four coordinating atoms being two carboxyl O and two N atoms from two different fusaric acid ligands (Table 1).

Experimental

The title complex was prepared by the addition of a stoichiometric amount of copper chloride (20 mmol) to a hot aqueous solution (25 ml) of 5-butyl-pyridyl-2-carboxylic acid (fusaric acid, 30 mmol) which was extracted from blasted leaves of Rhizophora Stylosa. The pH was then adjusted to 7.0–8.0 with NaOH (30 mmol). The resulting solution was filtered, and blue crystals were obtained at room temperature over several days.

Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93–0.97 Å, and with $U_{iso}(H) = 1.5\ U_{eq}(C_{methyl})$ and $1.2\ U_{eq}(C)$ for all other carbon atoms.

Figures

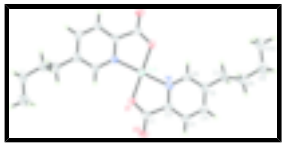

Fig. 1. The structure of (I), showing the atomic numbering scheme. Non-H atoms are shown as 50% probability displacement ellipsoids. Unlabelled atoms are related to the labelled atoms by the symmetry operator ($-x$, $1-y$, $-z$).

Bis(5-n-butylpyridine-2-carboxylato)copper(II)

Crystal data

$[Cu(C_{10}H_{12}O_2N_1)_2]$	$Z = 1$
$M_r = 419.95$	$F_{000} = 219$
Triclinic, $P\bar{1}$	$D_x = 1.507$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation

	λ = 0.71073 Å
a = 5.50520 (10) Å	Cell parameters from 3400 reflections
b = 8.0683 (3) Å	θ = 1.6–28.0º
c = 11.3008 (5) Å	μ = 1.21 mm^{-1}
α = 70.338 (2)º	*T* = 293 (2) K
β = 89.399 (2)º	Lamellar, blue
γ = 78.7060 (10)º	0.10 × 0.08 × 0.06 mm
V = 462.70 (3) Å^3	

Data collection

Bruker APEX II area-detector diffractometer	1788 independent reflections
Radiation source: fine-focus sealed tube	1592 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.103
T = 293(2) K	θ_{max} = 26.0º
φ and ω scan	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −6→6
T_{min} = 0.889, T_{max} = 0.935	*k* = −8→9
3391 measured reflections	*l* = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.107	$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
1788 reflections	$\Delta\rho_{max}$ = 0.43 e Å^{-3}
125 parameters	$\Delta\rho_{min}$ = −0.57 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.3420 (5)	0.7152 (3)	−0.0530 (3)	0.0335 (6)
C2	0.2087 (5)	0.7509 (3)	0.0571 (2)	0.0283 (5)
C3	0.2515 (5)	0.8740 (4)	0.1089 (3)	0.0347 (6)
H3	0.3761	0.9382	0.0804	0.042*
C4	0.1075 (5)	0.9019 (4)	0.2042 (3)	0.0369 (6)
H4	0.1342	0.9861	0.2395	0.044*
C5	−0.0768 (5)	0.8045 (4)	0.2472 (3)	0.0346 (6)
C6	−0.1070 (5)	0.6822 (4)	0.1910 (3)	0.0340 (6)
H6	−0.2280	0.6144	0.2191	0.041*
C7	−0.2327 (5)	0.8267 (4)	0.3538 (3)	0.0423 (7)
H7A	−0.3602	0.7561	0.3640	0.051*
H7B	−0.3147	0.9518	0.3320	0.051*
C8	−0.0814 (5)	0.7686 (4)	0.4779 (3)	0.0419 (7)
H8A	0.0079	0.6457	0.4962	0.050*
H8B	0.0409	0.8434	0.4677	0.050*
C9	−0.2294 (6)	0.7787 (4)	0.5904 (3)	0.0513 (8)
H9A	−0.1149	0.7486	0.6627	0.062*
H9B	−0.3188	0.9015	0.5727	0.062*
C10	−0.4130 (7)	0.6552 (5)	0.6239 (3)	0.0606 (9)
H10A	−0.5392	0.6931	0.5569	0.091*
H10B	−0.4880	0.6598	0.7001	0.091*
H10C	−0.3282	0.5343	0.6359	0.091*
Cu1	0.0000	0.5000	0.0000	0.0349 (2)
N1	0.0302 (4)	0.6562 (3)	0.0972 (2)	0.0306 (5)
O1	0.2520 (4)	0.6114 (3)	−0.09783 (18)	0.0393 (5)
O2	0.5192 (4)	0.7848 (3)	−0.0923 (2)	0.0468 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0425 (15)	0.0329 (13)	0.0321 (14)	−0.0187 (11)	0.0102 (11)	−0.0141 (12)
C2	0.0325 (12)	0.0285 (12)	0.0269 (13)	−0.0120 (10)	0.0052 (10)	−0.0101 (11)
C3	0.0441 (14)	0.0345 (13)	0.0355 (15)	−0.0229 (11)	0.0094 (11)	−0.0167 (12)
C4	0.0445 (15)	0.0375 (14)	0.0387 (15)	−0.0140 (12)	0.0043 (12)	−0.0226 (13)
C5	0.0341 (13)	0.0410 (14)	0.0335 (14)	−0.0077 (11)	0.0035 (11)	−0.0188 (12)
C6	0.0343 (13)	0.0436 (15)	0.0332 (14)	−0.0174 (11)	0.0090 (11)	−0.0195 (12)
C7	0.0403 (15)	0.0574 (17)	0.0386 (16)	−0.0098 (13)	0.0089 (12)	−0.0287 (14)
C8	0.0450 (15)	0.0478 (16)	0.0412 (16)	−0.0133 (13)	0.0053 (12)	−0.0237 (14)
C9	0.064 (2)	0.0558 (18)	0.0372 (17)	−0.0060 (16)	0.0062 (14)	−0.0233 (15)
C10	0.057 (2)	0.083 (2)	0.0418 (19)	−0.0143 (18)	0.0130 (15)	−0.0211 (18)
Cu1	0.0485 (3)	0.0414 (3)	0.0307 (3)	−0.0303 (2)	0.0160 (2)	−0.0215 (2)
N1	0.0344 (11)	0.0344 (11)	0.0302 (11)	−0.0170 (9)	0.0086 (9)	−0.0151 (10)
O1	0.0533 (11)	0.0479 (11)	0.0355 (10)	−0.0325 (9)	0.0198 (8)	−0.0265 (9)
O2	0.0561 (12)	0.0531 (12)	0.0519 (13)	−0.0392 (10)	0.0278 (10)	−0.0298 (10)

Geometric parameters (Å, °)

C1—O2	1.225 (3)	C7—H7B	0.9700
C1—O1	1.288 (3)	C8—C9	1.520 (4)
C1—C2	1.519 (4)	C8—H8A	0.9700
C2—N1	1.344 (3)	C8—H8B	0.9700
C2—C3	1.367 (4)	C9—C10	1.514 (5)
C3—C4	1.383 (4)	C9—H9A	0.9700
C3—H3	0.9300	C9—H9B	0.9700
C4—C5	1.389 (4)	C10—H10A	0.9600
C4—H4	0.9300	C10—H10B	0.9600
C5—C6	1.375 (4)	C10—H10C	0.9600
C5—C7	1.511 (4)	Cu1—O1^{i}	1.9344 (18)
C6—N1	1.345 (3)	Cu1—O1	1.9344 (18)
C6—H6	0.9300	Cu1—N1	1.960 (2)
C7—C8	1.520 (4)	Cu1—N1^{i}	1.960 (2)
C7—H7A	0.9700		
O2—C1—O1	125.5 (3)	C7—C8—H8A	108.4
O2—C1—C2	119.8 (2)	C9—C8—H8B	108.4
O1—C1—C2	114.7 (2)	C7—C8—H8B	108.4
N1—C2—C3	121.3 (2)	H8A—C8—H8B	107.5
N1—C2—C1	113.9 (2)	C10—C9—C8	113.9 (3)
C3—C2—C1	124.7 (2)	C10—C9—H9A	108.8
C2—C3—C4	119.3 (2)	C8—C9—H9A	108.8
C2—C3—H3	120.4	C10—C9—H9B	108.8
C4—C3—H3	120.4	C8—C9—H9B	108.8
C3—C4—C5	120.1 (3)	H9A—C9—H9B	107.7
C3—C4—H4	119.9	C9—C10—H10A	109.5
C5—C4—H4	119.9	C9—C10—H10B	109.5
C6—C5—C4	117.1 (2)	H10A—C10—H10B	109.5
C6—C5—C7	121.1 (2)	C9—C10—H10C	109.5
C4—C5—C7	121.8 (3)	H10A—C10—H10C	109.5
N1—C6—C5	123.1 (2)	H10B—C10—H10C	109.5
N1—C6—H6	118.5	O1^{i}—Cu1—O1	180.00 (11)
C5—C6—H6	118.5	O1^{i}—Cu1—N1	96.03 (8)
C5—C7—C8	112.8 (2)	O1—Cu1—N1	83.97 (8)
C5—C7—H7A	109.0	O1^{i}—Cu1—N1^{i}	83.97 (8)
C8—C7—H7A	109.0	O1—Cu1—N1^{i}	96.03 (8)
C5—C7—H7B	109.0	N1—Cu1—N1^{i}	180.00 (8)
C8—C7—H7B	109.0	C2—N1—C6	119.1 (2)
H7A—C7—H7B	107.8	C2—N1—Cu1	112.24 (17)
C9—C8—C7	115.4 (2)	C6—N1—Cu1	128.59 (18)
C9—C8—H8A	108.4	C1—O1—Cu1	114.62 (17)

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

Fig. 1