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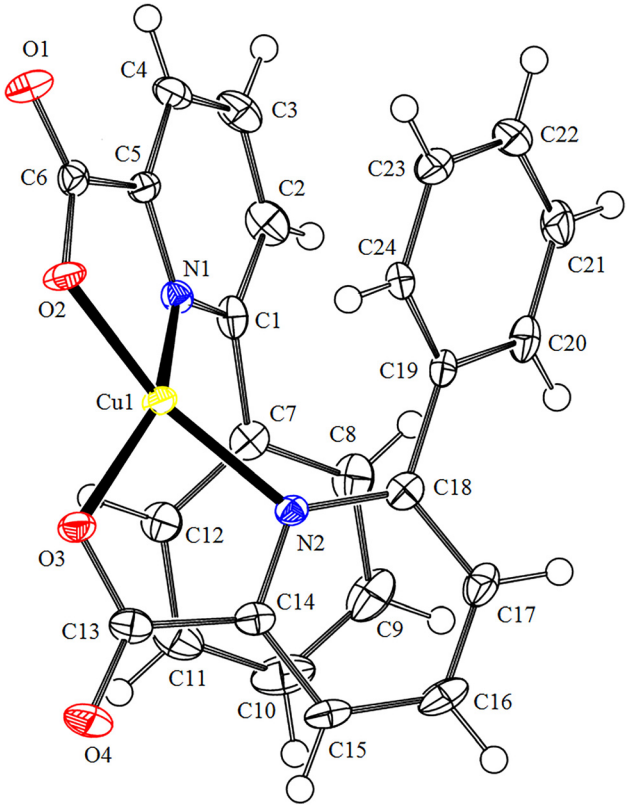
The crystal structure of bis(6-phenylpyridine-2-carboxylato-κ^2*N*,*O*)copper(II), $C_{24}H_{16}N_2O_4Cu$



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Abstract

$C_{24}H_{16}N_2O_4Cu$, triclinic, $P\bar{1}$ (no. 2), a = 11.2454(6) Å, b = 13.5960(7) Å, c = 14.0076(8) Å, V = 1958.9(2) Å^3, α = 79.019(5)°, β = 71.729(5)°, γ = 76.126(5)°, Z = 4, $R_{gt}(F)$ = 0.0438, $wR_{ref}(F^2)$ = 0.1030, T = 150 K.

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Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.12 × 0.11 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.15 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12,959, 6850, 0.037
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 5525
$N(param)_{refined}$:	559
Programs:	Bruker [1], Olex2 [2], SHELX [3], Diamond [4]

One of the two crystallographically independent Cu(II) complexes is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

About 0.5 mmol (0.0996 g) of 6-phenylpyridine-2-carboxylic acid, 0.5 mmol (0.020 g) of NaOH and 0.25 mmol of (0.0499 g) copper(II) acetate monohydrate were added to 20 ml of water-ethanol (v:v = 1:1) at room temperature. After 10 min, precipitation appeared in the solution. The mixture was continuously stirred for 4.5 h at 85 °C. The solution was cooled to room temperature and filtered. After 16 days, the green crystals of the title compound were obtained from the filtrate.

Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93 Å). Their U_{iso} values were set to 1.2U_{eq} of the parent atoms.

Comment

Some copper complexes with ligands containing a pyridine-carboxylate moiety exhibit novel coordination compounds [5]

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

Atom	x	y	z	U_{iso}*/U_{eq}
Cu1	0.47135 (4)	0.36703 (3)	−0.00940 (3)	0.01507 (12)
O1	0.8121 (2)	0.38318 (17)	−0.00452 (18)	0.0234 (6)
O2	0.6290 (2)	0.41365 (17)	−0.04643 (17)	0.0198 (5)
O3	0.4163 (2)	0.43253 (17)	−0.12634 (16)	0.0183 (5)
O4	0.2494 (2)	0.4538 (2)	−0.18717 (18)	0.0298 (6)
N1	0.5682 (2)	0.24241 (19)	0.05580 (19)	0.0140 (6)
N2	0.2892 (2)	0.36682 (19)	0.05673 (19)	0.0134 (6)
C1	0.5310 (3)	0.1537 (2)	0.1029 (2)	0.0176 (7)
C2	0.5941 (3)	0.0918 (3)	0.1708 (3)	0.0236 (8)
H2	0.565617	0.033002	0.207054	0.028*
C3	0.6980 (4)	0.1174 (3)	0.1840 (3)	0.0249 (8)
H3	0.738621	0.077277	0.230657	0.030*
C4	0.7423 (3)	0.2033 (3)	0.1278 (2)	0.0189 (8)
H4	0.816359	0.218867	0.132232	0.023*
C5	0.6743 (3)	0.2651 (2)	0.0650 (2)	0.0144 (7)
C6	0.7116 (3)	0.3618 (2)	0.0008 (2)	0.0162 (7)
C7	0.4264 (3)	0.1268 (2)	0.0767 (3)	0.0174 (7)
C8	0.3309 (3)	0.0833 (3)	0.1505 (3)	0.0247 (8)
H8	0.336002	0.066381	0.216851	0.030*
C9	0.2291 (4)	0.0650 (3)	0.1260 (3)	0.0307 (9)
H9	0.164233	0.038210	0.176016	0.037*
C10	0.2241 (4)	0.0870 (3)	0.0265 (3)	0.0355 (10)
H10	0.155572	0.074778	0.009917	0.043*
C11	0.3197 (4)	0.1267 (3)	−0.0482 (3)	0.0274 (9)
H11	0.316553	0.139810	−0.115079	0.033*
C12	0.4203 (3)	0.1470 (3)	−0.0233 (3)	0.0209 (8)
H12	0.484474	0.174284	−0.073585	0.025*
C13	0.2995 (3)	0.4290 (2)	−0.1177 (3)	0.0193 (8)
C14	0.2240 (3)	0.3922 (2)	−0.0132 (2)	0.0158 (7)
C15	0.0965 (3)	0.3869 (2)	0.0119 (3)	0.0197 (8)
H15	0.053908	0.400949	−0.037827	0.024*
C16	0.0334 (3)	0.3603 (3)	0.1119 (3)	0.0259 (9)
H16	−0.052350	0.355959	0.130661	0.031*
C17	0.0993 (3)	0.3405 (3)	0.1832 (3)	0.0222 (8)
H17	0.056855	0.325009	0.251158	0.027*
C18	0.2283 (3)	0.3432 (2)	0.1553 (2)	0.0166 (7)
C19	0.3021 (3)	0.3258 (2)	0.2304 (2)	0.0163 (7)
C20	0.2830 (3)	0.2501 (3)	0.3139 (2)	0.0216 (8)
H20	0.221951	0.210798	0.323719	0.026*
C21	0.3546 (3)	0.2334 (3)	0.3819 (3)	0.0272 (9)
H21	0.343072	0.181918	0.436272	0.033*
C22	0.4434 (3)	0.2934 (3)	0.3690 (3)	0.0283 (9)
H22	0.491755	0.282182	0.414472	0.034*
C23	0.4601 (3)	0.3703 (3)	0.2880 (3)	0.0221 (8)
H23	0.519048	0.411157	0.279836	0.026*
C24	0.3898 (3)	0.3866 (3)	0.2196 (2)	0.0176 (7)
H24	0.401320	0.438634	0.165839	0.021*
Cu2	1.00839 (4)	0.13203 (3)	−0.47829 (3)	0.01778 (12)
O5	0.9162 (2)	0.11547 (18)	−0.72097 (17)	0.0250 (6)
O6	1.0172 (2)	0.08432 (18)	−0.60066 (17)	0.0220 (6)
O7	1.1771 (2)	0.07280 (17)	−0.46650 (16)	0.0192 (5)
O8	1.2948 (2)	0.0688 (2)	−0.36298 (19)	0.0321 (6)
N3	0.9029 (2)	0.2582 (2)	−0.53186 (19)	0.0151 (6)
N4	0.9638 (3)	0.1379 (2)	−0.3318 (2)	0.0168 (6)
C25	0.8637 (3)	0.2375 (3)	−0.6061 (2)	0.0186 (8)
C26	0.9351 (3)	0.1376 (3)	−0.6471 (2)	0.0199 (8)
C27	0.7712 (3)	0.3043 (3)	−0.6439 (3)	0.0233 (8)
H27	0.745555	0.288584	−0.695283	0.028*
C28	0.7174 (4)	0.3956 (3)	−0.6033 (3)	0.0283 (9)
H28	0.652838	0.441333	−0.625788	0.034*
C29	0.7603 (3)	0.4182 (3)	−0.5294 (3)	0.0242 (8)
H29	0.724771	0.479233	−0.501804	0.029*
C30	0.8567 (3)	0.3495 (3)	−0.4962 (2)	0.0187 (8)
C31	0.9184 (3)	0.3733 (2)	−0.4269 (2)	0.0184 (8)
C32	1.0510 (3)	0.3503 (3)	−0.4491 (3)	0.0226 (8)
H32	1.099580	0.322956	−0.508520	0.027*
C33	1.1108 (4)	0.3680 (3)	−0.3831 (3)	0.0287 (9)
H33	1.199345	0.352157	−0.398076	0.034*
C34	1.0390 (4)	0.4094 (3)	−0.2945 (3)	0.0343 (10)
H34	1.079088	0.420635	−0.249784	0.041*
C35	0.9079 (4)	0.4339 (3)	−0.2732 (3)	0.0302 (9)
H35	0.859501	0.461271	−0.213801	0.036*
C36	0.8481 (3)	0.4178 (2)	−0.3397 (3)	0.0238 (8)
H36	0.759896	0.437046	−0.325909	0.029*
C37	1.1925 (3)	0.0842 (3)	−0.3819 (3)	0.0208 (8)
C38	1.0703 (3)	0.1178 (2)	−0.3015 (3)	0.0183 (7)
C39	1.0671 (4)	0.1298 (3)	−0.2052 (3)	0.0247 (8)
H39	1.141907	0.117809	−0.186041	0.030*
C40	0.9499 (4)	0.1601 (3)	−0.1378 (3)	0.0320 (10)
H40	0.944929	0.169499	−0.072553	0.038*
C41	0.8409 (4)	0.1761 (3)	−0.1674 (3)	0.0264 (9)
H41	0.761823	0.194825	−0.121485	0.032*
C42	0.8480 (3)	0.1647 (2)	−0.2657 (2)	0.0190 (8)
C43	0.7331 (3)	0.1776 (2)	−0.3004 (2)	0.0186 (7)
C44	0.6271 (3)	0.2538 (3)	−0.2698 (3)	0.0243 (8)
H44	0.628896	0.298754	−0.228092	0.029*
C45	0.5194 (3)	0.2635 (3)	−0.3006 (3)	0.0287 (9)
H45	0.449866	0.315749	−0.281008	0.034*
C46	0.5146 (4)	0.1952 (3)	−0.3609 (3)	0.0307 (9)
H46	0.441200	0.200751	−0.380364	0.037*
C47	0.6193 (3)	0.1189 (3)	−0.3921 (3)	0.0274 (9)
H47	0.616644	0.074029	−0.433531	0.033*
C48	0.7275 (3)	0.1094 (3)	−0.3619 (2)	0.0222 (8)
H48	0.797163	0.057487	−0.382312	0.027*

and excellent properties in many ways such as non-linear optical (NLO) property, antitumor activity, electrical conductance property, magnetic property [6–9]. Therefore, studies on structure and property of copper complexes have been one of the hot topics. In our previous work, some metal complexes with ligands containing pyridine-carboxylate moieties have been synthesized and structural characterized [10–12]. In order to further enrich the structure of the copper complexes with ligands such, a new Cu(II) complex was synthesized using 6-phenylpyridine-2-carboxylic acid, NaOH and cupric acetate monohydrate as raw materials.

The asymmetric unit of Cu(II) complex contains two Cu(II) ion and four bidentate 6-phenylpyridine-2-carboxylate

ligands. Each Cu(II) ion is four-coordinated with two O atoms and two N atoms from two different 6-phenylpyridine-2-carboxylate ligands. The sum of bond angles around Cu1, for example is 372.47°, showing that the O2, N1, N2, O3 is almost coplanar. The complex molecules form a 1D chained structure by the π-π stacking of phenyl and pyridine rings.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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