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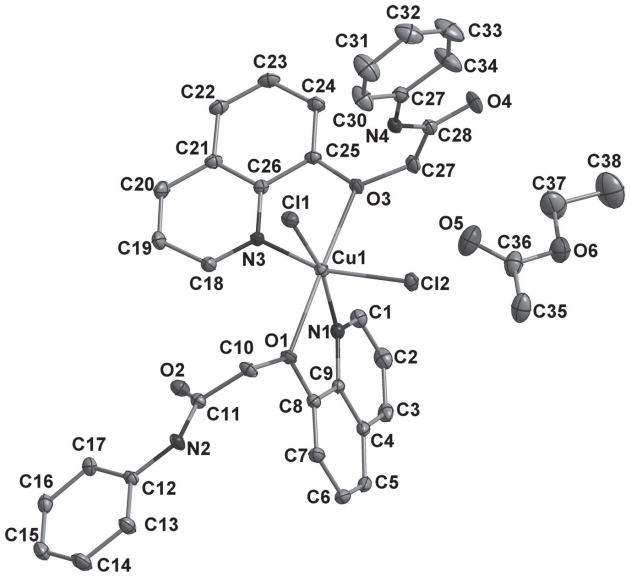
Crystal structure of dichlorido-bis(*N*-benzyl-2-(quinolin-8-yloxy)acetamide-κ²*N*,*O*)copper(II) — ethyl acetate (1/1), $C_{38}H_{36}N_4O_6Cl_2Cu$



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Abstract

$C_{38}H_{36}N_4O_6Cl_2Cu$, triclinic, $P\bar{1}$ (no. 2), $a = 10.749(5)$ Å, $b = 11.074(5)$ Å, $c = 15.951(7)$ Å, $\alpha = 80.471(8)°$, $\beta = 80.987(8)°$, $\gamma = 77.283(8)°$, $V = 1812.3(14)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0465$, $wR_{ref}(F^2) = 0.1279$, $T = 296(2)$ K.

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The asymmetric unit of the title crystal structure 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.

Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.21 × 0.18 × 0.16 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.80 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9637, 6346, 0.024
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4503
$N(param)_{refined}$:	460
Programs:	Bruker [1], SHELX [2]

Source of material

N-Phenyl-2-(quinolin-8-yloxy)acetamide [3] (0.280 g, 1 mmol) was dissolved in ethyl acetate (10 mL), then an ethyl acetate solution (10 mL) containing copper(II) chloride dihydrate (0.179 g, 1 mmol) was added dropwise at room temperature. After stirring for 2 h, the mixture was filtered and set aside to crystallize at room temperature for several days, giving green block crystals.

Experimental details

The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Comment

The structures and luminescent properties of the complexes with amide type ligands bearing quinoline ring have been investigated in our previous work [4–7]. As part of our ongoing work, the title complex was synthesized and characterized.

In the title complex, there exist one complex and one crystal ethyl acetate molecule. The six-coordinated Cu atom is in a distorted octahedral geometry coordinated by two O atoms and two N atoms from two independent ligands, and two chlorido ligands. In the crystal, a pair of intermolecular N—H···Cl hydrogen bonds between two complex molecules create a centrosymmetric dimer.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.60611(4)	0.37282(4)	0.29338(2)	0.04625(15)
O1	0.4715(2)	0.3647(2)	0.42825(14)	0.0539(6)
O2	0.2351(2)	0.3063(2)	0.42852(16)	0.0642(7)
O3	0.7468(2)	0.3616(2)	0.15939(14)	0.0568(6)
O4	1.0215(3)	0.5015(3)	0.0964(2)	0.0994(11)
O5	1.0138(5)	0.0845(4)	0.2071(3)	0.1529(18)
O6	1.2116(4)	0.0257(4)	0.2350(3)	0.1226(13)
N1	0.6389(2)	0.1930(3)	0.34953(18)	0.0475(7)
N2	0.1637(3)	0.4015(3)	0.54707(18)	0.0530(7)
H2A	0.1830	0.4518	0.5764	0.064*
N3	0.5059(3)	0.3329(3)	0.20803(17)	0.0488(7)
N4	0.8138(3)	0.5916(3)	0.13613(19)	0.0617(8)
H4A	0.7401	0.5730	0.1557	0.074*
C1	0.7159(4)	0.1060(4)	0.3095(3)	0.0634(10)
H1A	0.7379	0.1234	0.2507	0.076*
C2	0.7667(4)	−0.0120(4)	0.3508(4)	0.0798(13)
H2B	0.8205	−0.0714	0.3197	0.096*
C3	0.7372(4)	−0.0385(4)	0.4357(3)	0.0771(13)
H3A	0.7717	−0.1162	0.4640	0.093*
C4	0.6546(3)	0.0504(4)	0.4816(3)	0.0612(10)
C5	0.6195(4)	0.0307(5)	0.5709(3)	0.0780(13)
H5A	0.6516	−0.0454	0.6022	0.094*
C6	0.5404(4)	0.1205(5)	0.6113(3)	0.0795(14)
H6A	0.5194	0.1063	0.6704	0.095*
C7	0.4887(4)	0.2356(4)	0.5658(2)	0.0664(11)
H7A	0.4341	0.2970	0.5949	0.080*
C8	0.5182(3)	0.2575(3)	0.4798(2)	0.0505(9)
C9	0.6049(3)	0.1665(3)	0.4357(2)	0.0473(8)
C10	0.3570(3)	0.4451(3)	0.4602(2)	0.0591(10)
H10A	0.3380	0.5192	0.4188	0.071*
H10B	0.3693	0.4710	0.5130	0.071*
C11	0.2453(3)	0.3764(3)	0.4766(2)	0.0504(8)
C12	0.0501(3)	0.3563(3)	0.5795(2)	0.0496(8)
C13	0.0026(4)	0.3685(5)	0.6630(3)	0.0822(14)
H13A	0.0453	0.4037	0.6961	0.099*
C14	−0.1102(5)	0.3278(6)	0.6979(3)	0.1067(18)
H14A	−0.1440	0.3376	0.7543	0.128*
C15	−0.1715(4)	0.2739(5)	0.6505(4)	0.0894(15)
H15A	−0.2457	0.2447	0.6748	0.107*
C16	−0.1248(4)	0.2628(4)	0.5684(3)	0.0756(12)
H16A	−0.1676	0.2266	0.5360	0.091*
C17	−0.0144(3)	0.3042(3)	0.5315(3)	0.0603(10)
H17A	0.0165	0.2969	0.4744	0.072*
C18	0.3868(4)	0.3214(4)	0.2319(2)	0.0651(10)
H18A	0.3562	0.3164	0.2900	0.078*
C19	0.3026(4)	0.3163(4)	0.1739(3)	0.0774(13)
H19A	0.2177	0.3102	0.1934	0.093*
C20	0.3464(4)	0.3201(4)	0.0900(3)	0.0765(12)
H20A	0.2921	0.3159	0.0510	0.092*
C21	0.4741(4)	0.3306(3)	0.0615(2)	0.0584(9)
C22	0.5243(5)	0.3402(4)	−0.0258(3)	0.0704(11)
H22A	0.4743	0.3334	−0.0668	0.084*
C23	0.6451(5)	0.3593(4)	−0.0497(3)	0.0764(12)
H23A	0.6770	0.3666	−0.1076	0.092*
C24	0.7234(4)	0.3684(4)	0.0097(2)	0.0643(10)
H24A	0.8058	0.3833	−0.0087	0.077*
C25	0.6793(3)	0.3556(3)	0.0946(2)	0.0492(8)
C26	0.5520(3)	0.3382(3)	0.1227(2)	0.0480(8)
C27	0.8804(3)	0.3661(4)	0.1417(3)	0.0677(11)
H27A	0.9175	0.3212	0.0935	0.081*
H27B	0.9222	0.3224	0.1909	0.081*
C28	0.9104(4)	0.4945(4)	0.1219(2)	0.0647(10)
C29	0.8170(4)	0.7186(4)	0.1234(2)	0.0647(10)
C30	0.7116(6)	0.8039(5)	0.1427(4)	0.114(2)
H30A	0.6359	0.7769	0.1659	0.137*
C31	0.7108(7)	0.9296(6)	0.1296(5)	0.134(2)
H31A	0.6348	0.9854	0.1436	0.161*
C32	0.8159(8)	0.9732(6)	0.0975(4)	0.124(2)
H32A	0.8141	1.0587	0.0875	0.149*
C33	0.9230(9)	0.8923(8)	0.0802(6)	0.181(4)
H33A	0.9972	0.9225	0.0576	0.218*
C34	0.9300(5)	0.7672(6)	0.0937(5)	0.146(3)
H34A	1.0087	0.7132	0.0836	0.176*
C35	1.0649(5)	0.1060(6)	0.3441(4)	0.126(2)
H35A	1.1432	0.0849	0.3699	0.188*
H35B	1.0319	0.1943	0.3412	0.188*
H35C	1.0029	0.0616	0.3779	0.188*
C36	1.0908(6)	0.0710(5)	0.2572(5)	0.1075(18)
C37	1.2403(7)	−0.0079(9)	0.1474(5)	0.181(3)
H37A	1.1998	−0.0764	0.1432	0.217*
H37B	1.2086	0.0630	0.1065	0.217*
C38	1.3799(8)	−0.0448(9)	0.1300(6)	0.226(5)
H38A	1.4028	−0.0675	0.0733	0.338*
H38B	1.4187	0.0237	0.1344	0.338*
H38C	1.4100	−0.1150	0.1709	0.338*
Cl1	0.52520(9)	0.57859(9)	0.25784(6)	0.0611(3)
Cl2	0.77810(9)	0.39807(9)	0.35042(6)	0.0622(3)

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