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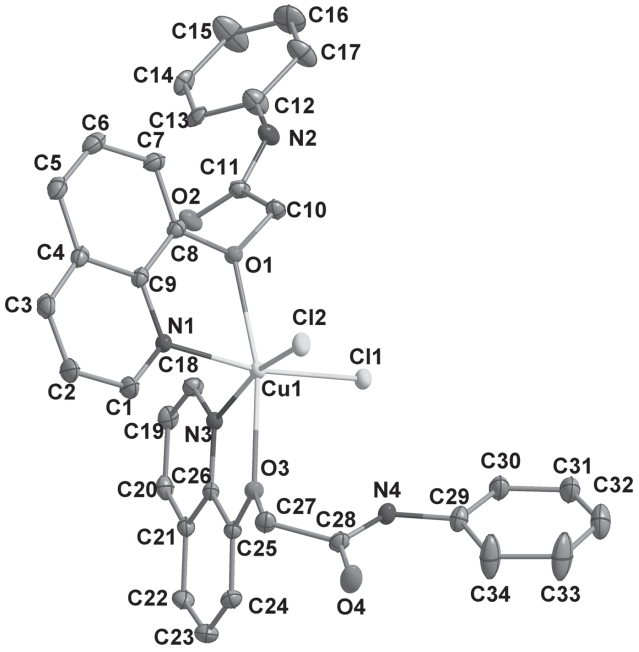
Crystal structure of dichlorido-bis(*N*-phenyl-2-(quinolin-8-yloxy)acetamide-κ²*N*,*O*) – acetone (2/1), $C_{35.5}H_{31}N_4O_{4.5}Cl_2Cu$



https://doi.org/10.1515/ncrs-2017-0275
Received November 4, 2017; accepted January 19, 2018; available online February 9, 2018

Abstract

$C_{35.5}H_{31}N_4O_{4.5}Cl_2Cu$, monoclinic, $P2_1/c$ (no. 14), $a = 14.8239(3)$ Å, $b = 16.2169(2)$ Å, $c = 15.6515(3)$ Å, $\beta = 109.889(1)°$, $V = 3538.16(11)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0499$, $wR_{ref}(F^2) = 0.1577$, $T = 296(2)$ K.

CCDC no.: 1818050

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.20 × 0.16 × 0.15 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.81 mm^{-1}
Diffractometer, scan mode:	Bruker SAINT, φ and ω-scans
θ_{max}, completeness:	28.3°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	33725, 8761, 0.053
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 5076
$N(param)_{refined}$:	473
Programs:	Bruker programs [1], SHELX [2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.40306(2)	0.48936(2)	0.76574(2)	0.04791(14)
Cl1	0.35000(6)	0.40030(4)	0.85050(5)	0.0583(2)
Cl2	0.34912(7)	0.60267(5)	0.81912(6)	0.0683(2)
O1	0.56855(15)	0.49165(12)	0.86627(14)	0.0574(5)
O2	0.70179(18)	0.37310(17)	0.87689(16)	0.0839(8)
O3	0.25566(15)	0.48294(12)	0.63831(14)	0.0561(5)
O4	0.02723(19)	0.5655(2)	0.6188(2)	0.1063(10)
N1	0.47628(18)	0.56683(15)	0.71062(17)	0.0562(6)
N2	0.7509(2)	0.37025(18)	1.03045(19)	0.0746(8)
H2A[a]	0.7375	0.3927	1.0745	0.090*
H2B[b]	0.7353	0.3869	1.0757	0.090*
N3	0.41638(17)	0.39525(14)	0.68547(16)	0.0491(6)
N4	0.1223(2)	0.47925(17)	0.72320(19)	0.0636(7)
H4	0.1768	0.4545	0.7388	0.076*
C1	0.4298(3)	0.6030(2)	0.6333(3)	0.0796(11)
H1	0.3679	0.5854	0.6009	0.096*
C2	0.4692(3)	0.6672(3)	0.5970(3)	0.0901(12)
H2	0.4337	0.6917	0.5421	0.108*
C3	0.5584(3)	0.6925(2)	0.6426(3)	0.0820(11)
H3	0.5851	0.7351	0.6194	0.098*
C4	0.6120(2)	0.6552(2)	0.7249(2)	0.0667(9)
C5	0.7064(3)	0.6788(2)	0.7758(3)	0.0827(11)
H5	0.7368	0.7203	0.7548	0.099*
C6	0.7526(3)	0.6403(3)	0.8557(3)	0.0876(12)
H6	0.8148	0.6567	0.8889	0.105*
C7	0.7104(2)	0.5765(2)	0.8907(3)	0.0725(10)
H7	0.7439	0.5515	0.9459	0.087*
C8	0.6186(2)	0.55238(19)	0.8413(2)	0.0565(7)
C9	0.5678(2)	0.59097(18)	0.7579(2)	0.0551(7)

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
C10	0.6124(2)	0.4506(2)	0.9515(2)	0.0610(8)
H10A	0.5644	0.4185	0.9662	0.073*
H10B	0.6380	0.4913	0.9991	0.073*
C11	0.6932(2)	0.3938(2)	0.9476(2)	0.0608(8)
C12[a]	0.8278(10)	0.3165(9)	1.0579(10)	0.093(10)
C13[a]	0.8695(12)	0.2867(12)	0.9967(9)	0.061(5)
H13[a]	0.8451	0.3023	0.9360	0.073*
C14[a]	0.9475(13)	0.2335(11)	1.0264(12)	0.066(5)
H14[a]	0.9753	0.2135	0.9854	0.080*
C15[a]	0.9838(13)	0.2100(12)	1.1171(13)	0.161(13)
H15[a]	1.0360	0.1744	1.1369	0.194*
C16[a]	0.942(2)	0.2398(18)	1.1783(9)	0.136(9)
H16[a]	0.9665	0.2241	1.2390	0.163*
C17[a]	0.8642(19)	0.2930(16)	1.1487(9)	0.107(8)
H17[a]	0.8363	0.3130	1.1896	0.128*
C12A[b]	0.8342(5)	0.3212(4)	1.0515(6)	0.062(4)
C13A[b]	0.8535(7)	0.2665(7)	0.9915(5)	0.059(3)
H13A[b]	0.8102	0.2610	0.9326	0.071*
C14A[b]	0.9372(7)	0.2201(7)	1.0194(7)	0.093(5)
H14A[b]	0.9501	0.1835	0.9793	0.112*
C15A[b]	1.0018(6)	0.2283(6)	1.1074(7)	0.107(4)
H15A[b]	1.0579	0.1972	1.1260	0.128*
C16A[b]	0.9826(7)	0.2830(9)	1.1674(7)	0.111(5)
H16A[b]	1.0258	0.2885	1.2262	0.133*
C17A[b]	0.8988(7)	0.3295(8)	1.1394(7)	0.093(3)
H17A[b]	0.8859	0.3661	1.1796	0.112*
C18	0.4966(2)	0.3527(2)	0.7069(2)	0.0618(8)
H18	0.5482	0.3702	0.7566	0.074*
C19	0.5090(3)	0.2832(2)	0.6600(2)	0.0685(9)
H19	0.5672	0.2551	0.6784	0.082*
C20	0.4347(3)	0.2572(2)	0.5867(2)	0.0676(9)
H20	0.4416	0.2107	0.5546	0.081*
C21	0.3474(2)	0.30074(19)	0.5595(2)	0.0583(8)
C22	0.2677(3)	0.2781(2)	0.4837(2)	0.0757(10)
H22	0.2714	0.2333	0.4480	0.091*
C23	0.1851(3)	0.3225(3)	0.4635(3)	0.0878(12)
H23	0.1321	0.3067	0.4142	0.105*
C24	0.1776(2)	0.3904(2)	0.5139(2)	0.0694(9)
H24	0.1201	0.4192	0.4987	0.083*
C25	0.2533(2)	0.41484(19)	0.5849(2)	0.0533(7)
C26	0.3407(2)	0.37029(17)	0.61094(18)	0.0481(6)
C27	0.1788(2)	0.5415(2)	0.6098(2)	0.0646(9)
H27A	0.1499	0.5393	0.5441	0.078*
H27B	0.2049	0.5964	0.6260	0.078*
C28	0.1020(2)	0.5272(2)	0.6508(2)	0.0631(8)
C29	0.0661(2)	0.4635(2)	0.7782(3)	0.0722(9)
C30	0.0987(3)	0.4098(3)	0.8476(3)	0.0944(13)
H30	0.1567	0.3830	0.8570	0.113*
C31	0.0481(4)	0.3935(4)	0.9049(3)	0.1155(17)
H31	0.0716	0.3553	0.9515	0.139*
C32	−0.0351(5)	0.4326(4)	0.8938(5)	0.134(2)
H32	−0.0665	0.4249	0.9354	0.161*
C33	−0.0725(6)	0.4828(5)	0.8221(7)	0.186(4)
H33	−0.1323	0.5067	0.8125	0.224*

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
C34	−0.0238(3)	0.5001(4)	0.7616(5)	0.163(3)
H34	−0.0502	0.5348	0.7120	0.196*
C35[c]	0.3354(11)	0.5227(8)	0.3873(12)	0.193(6)
H35B[c]	0.3362	0.5087	0.3280	0.290*
H35A[c]	0.3149	0.4759	0.4134	0.290*
H35C[c]	0.3987	0.5387	0.4254	0.290*
C36[c]	0.2694(6)	0.5909(5)	0.3800(6)	0.105(3)
C37[c]	0.2383(8)	0.6584(7)	0.3140(7)	0.140(4)
H37A[c]	0.2633	0.7096	0.3432	0.210*
H37B[c]	0.1695	0.6607	0.2910	0.210*
H37C[c]	0.2618	0.6489	0.2647	0.210*
O5[c]	0.2586(6)	0.5890(5)	0.4491(6)	0.162(3)

Occupancies: [a] = 0.36(3), [b] = 0.64(3), [c] = 0.5

Source of material

N-phenyl-2-(quinolin-8-yloxy)acetamide [1] (0.280 g, 1 mmol) was dissolved in acetone (10 mL), then an acetone solution (10 mL) of copper(II) chloride dihydrate (0.179 g, 1 mmol) was added 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.

Discussion

Structures and luminescent properties of the complexes with amide type ligands bearing quinoline ring have been investigated in our previous work [3–6]. As part of our ongoing work, the title complex was synthesized and characterized.

In the asymmetric unit there is one complex and a half of a acetone molecule. The six-coordinated Cu atom is in a distorted octahedral geometry with the donor centers of two O atoms and two N atom from two organic and two chlorido ligands. In the crystal, a pair of intermolecular N—H···Cl hydrogen bonds between two complexes create a centrosymmetric dimer.

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