Crystal structure of [(1,4-di(1-imidazolyl)benzene-κ^2N:N')(μ_2-5-iso nicotinamidoisophthalato-κ^2O^1,O^3)copper(II)], $C_{26}H_{18}CuN_6O_5$

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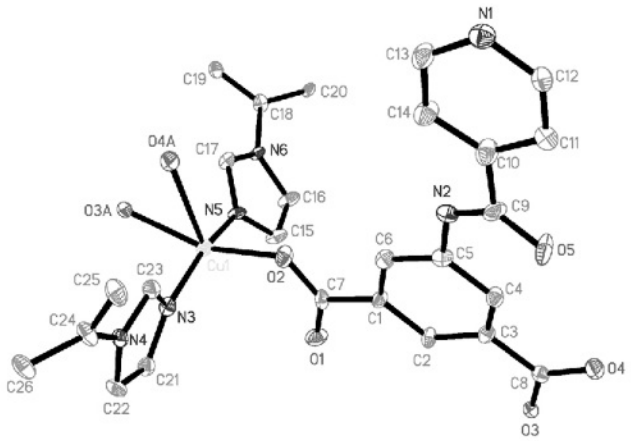

Abstract

$C_{26}H_{18}CuN_6O_5$, triclinic, $P\bar{1}$ (no. 2), a = 7.652(2) Å, b = 10.026(2) Å, c = 16.727(3) Å, α = 72.832(4)°, β = 78.101(3)°, γ = 79.010(4)°, V = 1188.2 Å^3, Z = 2, $R_{gt}(F)$ = 0.0585, $wR_{ref}(F^2)$ = 0.1368, T = 291 K.

Table 1. Data collection and handling.

Crystal:	blue needles, size 0.18×0.20×0.24 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	9.71 cm^{-1}
Diffractometer, scan mode:	Bruker Smart Apex CCD, φ and ω
$2\theta_{max}$:	52°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11106, 4677
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3710
$N(param)_{refined}$:	343
Programs:	SHELX [9]

Source of material

A mixture of $Cu(CH_3CO_2)_2{\cdot}2H_2O$ (0.041 g, 0.1mmol), 5-iso-nicotinamidoisophthalic acid (H_2iaip) (0.029 g, 0.1mmol), NaOH (0.081 g, 0.2mmol), 1,4-di(1-imidazolyl)benzene (dib) (0.021 g, 0.1mmol), CH_3CH_2OH (2 mL) and H_2O (8 mL) was sealed in a 15 ml Teflon-lined stainless steel reactor, which was heated at 393 K for 72 h and then it was cooled to room temperature. Needle blue crystals of the title compound were collected.

Experimental details

H atoms bonded to C atoms were placed geometrically and treated as riding.

Discussion

In recent years, many interest in transition metal complex assembly has been devoted to the development of rational synthetic routes to novel one-, two- and three-dimensional crystal frameworks, due to their potential applications in many areas [1, 2]. Particularly, copper complexes containing heterocycles have been investigated extensively to date [3, 4]. On the other hand, it is well known that carboxylate and pyridine groups have good coordination capacities as well as the amide group, a fascinating functional group with two different types of hydrogen bonding sites: the –NH moiety which acts as an electron acceptor while the –C=O group acts as an electron donor [5-8]. So we have recently prepared a new two-dimensional copper(II) coordination polymer, $[Cu(dib)(iaip)]_n$, (I), with iaip, dib and copper acetate. In the title compound, the central Cu^{II} ion is five-coordinated by two N atoms from dib ligands, three carboxylate O atoms from two iaip ligands in a distorted square-pyramidal geometry (Fig.). Furthermore, two carboxylate groups of the iaip ligand adopt the different coordination mode to connect two Cu(II) atoms, whereas the pyridyl group is free of coordination. Such a coordination mode links (I) into an infinite 1D chain structure. Then, the adjacent chains are interlinked by the rigid dib ligands to form a 2D layer structure.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2)	2*i*	0.8605	0.2732	0.8260	0.029
H(4)	2*i*	0.7625	0.2577	0.6021	0.032
H(6)	2*i*	0.7902	0.6314	0.6400	0.032
H(11)	2*i*	0.7031	0.4398	0.3185	0.043
H(12)	2*i*	0.6468	0.5939	0.1922	0.041
H(13)	2*i*	0.6810	0.9112	0.2694	0.043
H(14)	2*i*	0.7351	0.7655	0.3988	0.043
H(15)	2*i*	0.6496	0.6035	0.9724	0.036
H(16)	2*i*	0.3416	0.6546	1.0460	0.039
H(17)	2*i*	0.4739	1.0000	0.8713	0.025
H(19)	2*i*	0.2447	1.1221	0.9543	0.029
H(20)	2*i*	0.0411	0.7591	1.0165	0.024
H(21)	2*i*	1.2734	0.7109	0.8500	0.029
H(22)	2*i*	1.5230	0.7693	0.7350	0.034
H(23)	2*i*	1.0644	0.9211	0.6460	0.033
H(25)	2*i*	1.2367	0.9109	0.5132	0.043
H(26)	2*i*	1.6234	0.9770	0.6198	0.038
H(2A)	2*i*	0.7169	0.6206	0.5130	0.038

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	2*i*	0.8259(5)	0.4663(4)	0.7412(2)	0.027(2)	0.019(2)	0.024(2)	–0.001(2)	–0.004(2)	–0.010(2)
C(2)	2*i*	0.8344(5)	0.3198(4)	0.7720(2)	0.034(2)	0.022(2)	0.021(2)	–0.009(2)	–0.002(2)	–0.010(2)
C(3)	2*i*	0.8022(5)	0.2458(4)	0.7187(2)	0.025(2)	0.021(2)	0.022(2)	–0.003(2)	0.000(2)	–0.008(2)
C(4)	2*i*	0.7770(6)	0.3105(4)	0.6370(2)	0.035(2)	0.025(2)	0.023(2)	–0.006(2)	–0.008(2)	–0.007(2)
C(5)	2*i*	0.7732(6)	0.4577(4)	0.6059(3)	0.033(2)	0.029(2)	0.033(2)	–0.000(2)	–0.012(2)	–0.004(2)
C(6)	2*i*	0.7956(5)	0.5340(4)	0.6595(2)	0.031(2)	0.023(2)	0.023(2)	–0.007(2)	–0.004(2)	0.001(2)
C(7)	2*i*	0.8497(5)	0.5509(4)	0.7979(2)	0.023(2)	0.026(2)	0.027(2)	–0.010(2)	0.003(2)	–0.015(2)
C(8)	2*i*	0.8069(5)	0.0876(4)	0.7503(2)	0.018(2)	0.025(2)	0.022(2)	–0.007(2)	0.001(1)	–0.004(2)
C(9)	2*i*	0.7590(6)	0.4811(4)	0.4550(3)	0.025(2)	0.025(2)	0.043(2)	0.007(2)	–0.002(2)	–0.013(2)
C(10)	2*i*	0.7218(7)	0.5879(5)	0.3727(3)	0.045(3)	0.031(2)	0.032(2)	–0.013(2)	–0.004(2)	–0.005(2)
C(11)	2*i*	0.6974(6)	0.5362(5)	0.3105(3)	0.034(2)	0.035(2)	0.042(3)	–0.005(2)	–0.013(2)	–0.012(2)
C(12)	2*i*	0.6639(6)	0.6307(5)	0.2345(3)	0.039(2)	0.032(2)	0.039(2)	–0.004(2)	–0.015(2)	–0.016(2)
C(13)	2*i*	0.6832(6)	0.8146(5)	0.2792(3)	0.049(3)	0.023(2)	0.034(2)	–0.011(2)	–0.009(2)	–0.001(2)
C(14)	2*i*	0.7165(7)	0.7275(5)	0.3573(3)	0.053(3)	0.028(2)	0.025(2)	–0.006(2)	–0.010(2)	–0.001(2)
C(15)	2*i*	0.5765(6)	0.6903(4)	0.9620(3)	0.027(2)	0.023(2)	0.027(2)	0.005(2)	0.004(2)	0.001(2)
C(16)	2*i*	0.4063(6)	0.7173(4)	1.0028(3)	0.033(2)	0.022(2)	0.028(2)	0.005(2)	0.004(2)	0.003(2)
C(17)	2*i*	0.4806(5)	0.9085(4)	0.9064(2)	0.022(2)	0.019(2)	0.014(2)	–0.006(1)	0.010(1)	0.001(1)
C(18)	2*i*	0.1712(5)	0.9303(4)	0.9839(2)	0.022(2)	0.032(2)	0.022(2)	–0.005(2)	0.006(2)	–0.017(2)
C(19)	2*i*	0.1461(5)	1.0728(4)	0.9731(2)	0.019(2)	0.027(2)	0.024(2)	–0.010(2)	0.003(2)	–0.005(2)
C(20)	2*i*	0.0245(5)	0.8557(4)	1.0102(2)	0.020(2)	0.013(2)	0.024(2)	–0.003(1)	0.002(1)	–0.001(1)
C(21)	2*i*	1.2621(5)	0.7610(4)	0.7944(2)	0.026(2)	0.023(2)	0.025(2)	–0.003(2)	–0.000(2)	–0.011(2)
C(22)	2*i*	1.4008(5)	0.7921(4)	0.7313(3)	0.015(2)	0.037(2)	0.031(2)	–0.003(2)	–0.003(2)	–0.006(2)
C(23)	2*i*	1.1463(5)	0.8758(4)	0.6828(3)	0.025(2)	0.026(2)	0.030(2)	–0.006(2)	–0.006(2)	–0.004(2)
C(24)	2*i*	1.4178(5)	0.9298(5)	0.5788(2)	0.020(2)	0.047(3)	0.021(2)	–0.014(2)	0.006(2)	–0.011(2)
C(25)	2*i*	1.3437(6)	0.9462(5)	0.5078(3)	0.030(2)	0.048(3)	0.030(2)	–0.018(2)	0.001(2)	–0.007(2)
C(26)	2*i*	1.5742(5)	0.9854(5)	0.5718(3)	0.019(2)	0.051(3)	0.028(2)	–0.009(2)	0.003(2)	–0.017(2)
Cu(1)	2*i*	0.84655(6)	0.82708(5)	0.81954(3)	0.0226(3)	0.0189(2)	0.0252(3)	–0.0031(2)	0.0021(2)	–0.0049(2)
N(1)	2*i*	0.6542(5)	0.7667(4)	0.2173(2)	0.034(2)	0.033(2)	0.029(2)	–0.005(2)	–0.005(2)	–0.003(2)
N(2)	2*i*	0.7461(5)	0.5308(4)	0.5221(2)	0.033(2)	0.030(2)	0.034(2)	–0.000(2)	–0.017(2)	–0.005(2)
N(3)	2*i*	1.1010(4)	0.8142(3)	0.7648(2)	0.020(2)	0.023(2)	0.022(2)	–0.007(1)	0.008(1)	–0.006(1)
N(4)	2*i*	1.3260(4)	0.8638(3)	0.6605(2)	0.020(2)	0.022(2)	0.025(2)	–0.008(1)	–0.002(1)	0.000(1)
N(5)	2*i*	0.6230(4)	0.8094(3)	0.9039(2)	0.023(2)	0.018(2)	0.018(2)	0.004(1)	–0.004(1)	0.002(1)
N(6)	2*i*	0.3499(4)	0.8568(3)	0.9666(2)	0.018(2)	0.013(1)	0.021(2)	0.001(1)	0.002(1)	–0.002(1)
O(1)	2*i*	0.8971(4)	0.4898(3)	0.8664(2)	0.045(2)	0.030(2)	0.031(2)	0.005(1)	–0.016(1)	–0.006(1)
O(2)	2*i*	0.8084(4)	0.6830(3)	0.7714(2)	0.044(2)	0.029(2)	0.025(2)	–0.008(1)	–0.008(1)	–0.013(1)
O(3)	2*i*	0.8466(3)	0.0253(3)	0.8222(2)	0.024(1)	0.023(1)	0.026(1)	–0.002(1)	–0.011(1)	–0.009(1)
O(4)	2*i*	0.7694(4)	0.0246(3)	0.7033(2)	0.039(2)	0.030(2)	0.039(2)	–0.006(1)	–0.017(1)	–0.007(1)
O(5)	2*i*	0.7893(5)	0.3580(3)	0.4594(2)	0.075(2)	0.024(2)	0.038(2)	–0.021(2)	–0.015(2)	–0.007(1)

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