# Crystal structure of diaquabis(imidazole-4-carboxylato)copper(II) dihydrate, $Cu(H_2O)_2(C_4H_3N_2O_2)_2 \cdot 2H_2O$

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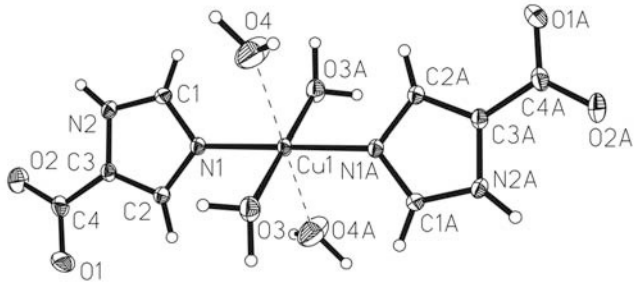


**Abstract**

$C_8H_{14}CuN_4O_8$, monoclinic, $P12_1/c1$ (no. 14), $a$ = 7.6635(2) Å, $b$ = 12.8556(3) Å, $c$ = 6.8608(2) Å, $\beta$ = 101.190(1)°, $V$ = 663.1 Å$^3$, $Z$ = 2, $R_{gf}(F)$ = 0.051, $wR_{ref}(F^2)$ = 0.156, $T$ = 291 K.

## Source of material

All reagents and solvents were used as obtained without further purification. To a solution of imidazole-4-carboxylic acid (224 mg, 2 mmol) in methanol (13 mL) were added a solution of $CuCl_2 \cdot 2H_2O$ (171 mg, 1 mmol) in $H_2O$ (2 mL). The mixture was stirred at room temperature for 1 h to give a clear celeste solution. After keeping the above solution in air for 7 days, blue block-shaped crystals were formed. The crystals were filtered, washed three times with ethanol/water (1/10, *v*/*v*), and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 88 % based on Cu).

## Experimental details

The hydrogen atoms of water were found in the difference Fourier map and refined with $U_{iso}$ = 0.05(2) Å$^2$. The other hydrogen atoms were positioned geometrically with $d$(C—H) = 0.93 Å, and refined as riding with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

## Discussion

Copper is an important life-required element. Due to their biological relevance, many copper complexes with Schiff base have been investigated in recent years [1-4]. In addition, metal complexes with carboxylates are among the most investigated compounds in the field of coordination chemistry [5-8].

The crystal structure of the title complex consists of the mononuclear copper(II) unit $Cu(C_4H_3N_2O_2)_2(H_2O)_2$, and two lattice water molecules. In the mononuclear unit, copper(II) atom is in a square-planar environment, being four-coordinated by two N atoms from two imidazole molecules, and two O atoms from two coordinating water molecules. Interestingly, copper(II) atom of the title complex seems to be in an strongly distorted octahedral environment. N1, N1A, O3 and O3A atoms constitute the basal plane of the octahedron (symmetry code A: –*x*,2–*y*,–*z*). The O4 and O4A atoms occupy the two axial positions. The axial Cu—O4 and Cu—O4A distances are 2.500(6) Å. The Cu—O3 (2.022(5) Å) and Cu—N1 (1.997(4) Å) bond lengths are in normal range. All the molecules participate in intermolecular hydrogen bonds (N2–H2A···O3, O3–H3B···O1, O3–H3B···O2, O3–H3A···N2, O4–H4A···O1, O4–H4B···O2), which further stabilize the 3D framework.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | blue block, size 0.18 × 0.22 × 0.31 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 16.95 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART CCD, $\varphi/\omega$ |
| $2\theta_{max}$: | 54.98° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 5482, 1508 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 1332 |
| $N(param)_{refined}$: | 113 |
| Program: | SHELXTL [9] |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(2A) | 4*e* | 0.1197 | 0.6169 | 0.0126 | 0.036 |
| H(1) | 4*e* | –0.0835 | 0.7578 | –0.0699 | 0.034 |
| H(2) | 4*e* | 0.3759 | 0.8860 | 0.1445 | 0.035 |
| H(3A) | 4*e* | 0.136(7) | 0.974(4) | 0.37(1) | 0.05(2) |
| H(4A) | 4*e* | –0.305(9) | 0.862(2) | 0.16(1) | 0.05 |
| H(3B) | 4*e* | 0.243(4) | 1.063(5) | 0.31(1) | 0.05 |
| H(4B) | 4*e* | –0.323(9) | 0.977(4) | 0.22(1) | 0.05 |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Cu(1) | 2*a* | 0 | 0 | 0 | 0.0279(5) | 0.0170(5) | 0.0302(5) | 0.0043(3) | –0.0004(3) | –0.0007(3) |
| N(1) | 4*e* | 0.1143(6) | 0.8597(3) | 0.0253(6) | 0.029(2) | 0.020(2) | 0.030(2) | 0.002(2) | 0.002(2) | 0.000(2) |

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**Table 3.** Continued.

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| N(2) | 4*e* | 0.1445(6) | 0.6851(3) | 0.0278(7) | 0.035(2) | 0.019(2) | 0.035(2) | 0.000(2) | 0.004(2) | –0.001(2) |
| O(1) | 4*e* | 0.5982(6) | 0.7228(4) | 0.229(1) | 0.036(2) | 0.047(3) | 0.106(5) | 0.008(2) | –0.014(3) | 0.002(3) |
| O(2) | 4*e* | 0.4566(7) | 0.5795(4) | 0.1539(9) | 0.056(3) | 0.029(2) | 0.092(4) | 0.018(2) | 0.010(3) | 0.004(2) |
| O(3) | 4*e* | 0.1148(7) | 1.0309(4) | 0.2850(7) | 0.052(3) | 0.035(2) | 0.044(2) | 0.007(2) | 0.004(2) | 0.001(2) |
| O(4) | 4*e* | –0.254(1) | 0.9328(6) | 0.144(1) | 0.081(5) | 0.058(4) | 0.153(8) | –0.009(3) | 0.057(5) | –0.004(4) |
| C(1) | 4*e* | 0.0368(7) | 0.7654(4) | –0.0154(8) | 0.026(2) | 0.024(3) | 0.035(3) | –0.001(2) | 0.003(2) | –0.001(2) |
| C(2) | 4*e* | 0.2858(7) | 0.8382(4) | 0.1008(8) | 0.029(3) | 0.022(2) | 0.035(3) | 0.002(2) | 0.002(2) | –0.001(2) |
| C(3) | 4*e* | 0.3022(7) | 0.7318(4) | 0.1009(8) | 0.031(2) | 0.024(2) | 0.029(2) | 0.004(2) | 0.004(2) | 0.001(2) |
| C(4) | 4*e* | 0.4600(8) | 0.6750(5) | 0.1647(9) | 0.038(3) | 0.030(3) | 0.047(3) | 0.011(2) | 0.003(2) | 0.002(2) |

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