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Diaquabis(1*H*-1,2,4-triazole-3-carboxylato)copper(II)

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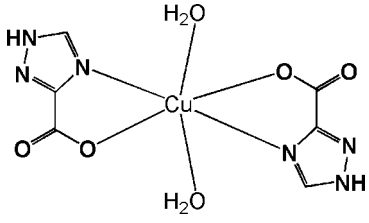
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.021; wR factor = 0.064; data-to-parameter ratio = 11.4.

In the title compound, $[Cu(C_3H_2N_3O_2)_2(H_2O)_2]$, the Cu^{II} atom (site symmetry $\overline{1}$) is coordinated by two *N*,*O*-bidentate 1*H*-1,2,4-triazole-3-carboxyate anions and two water molecules in a distorted *trans*-CuN_2O_4 octahedral arrangement. In the crystal structure, molecules are linked by intermolecular N—H···O and O—H···O hydrogen bonds.

Related literature

For background, see: Costamagna *et al.* (1992).



Experimental

Crystal data

$[Cu(C_3H_2N_3O_2)_2(H_2O)_2]$
M_r = 323.72
Monoclinic, $P2_1/c$
a = 8.6389 (11) Å
b = 9.1819 (12) Å
c = 6.9929 (9) Å
β = 94.212 (2)°
V = 553.19 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.01 mm^{-1}
T = 293 (2) K
0.33 × 0.30 × 0.18 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.455, T_{max} = 0.710
2601 measured reflections
1003 independent reflections
971 reflections with $I > 2\sigma(I)$
R_{int} = 0.007

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.064
S = 1.05
1003 reflections
88 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	1.9886 (15)	Cu1—O3	2.3985 (12)
Cu1—O1	2.0134 (11)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3D···O2^{i}	0.86	1.89	2.7295 (17)	166
O3—H2W···O2^{ii}	0.83	1.99	2.7792 (17)	159
O3—H1W···O1^{iii}	0.82	2.00	2.8067 (16)	166

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2650).

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supplementary materials

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Diaquabis(1*H*-1,2,4-triazole-3-carboxylato)copper(II)

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Comment

Copper coordination chemistry may play a role in catalysis, enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992). We report here the synthesis and structure of the title compound, (I).

The neutral complex is buily up from a central copper(II) ion (site symmetry $\bar{1}$), two bidentate ligands and two coordinated water molecules (Fig. 1). The Cu(II) atom is a distorted octahedral environment (Table 1), doubtless arising from a Jahn-Teller distortion.

A network of N—H···O and O—H···O hydrogen bonds (Table 2) helps to establish the packing.

Experimental

1*H*-1,2,4-triazole-3-carboxylic acid (2 mmol, 226 mg) was dissolved in distilled water (25 ml) and $CuCl_2{\cdot}2H_2O$ (1 mmol, 171 mg) dissoived in 5-ml distilled water was added with stirring at 323 K. The resulting blue solution was allowed to react for three hours and was then filtered. Blue blocks of (I) were obtained by slow evaporation of a water solution over a period of one month (yield 85%). Anal. Calcd (%) for $C_6H_8Cu_N6_O6$: C 22.26; H 2.49; Cu 19.63; N 25.96; O (by difference) 29.66. Found (%): C 22.31; H 2.51; Cu 19.59; N 25.91; O (by difference) 29.62.

Refinement

All the H atoms were placed in geometrically idealized positions (C—H = 0.93 Å, N—H = 0.86 Å, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C, N) or 1.5U_{eq}(O).

Figures

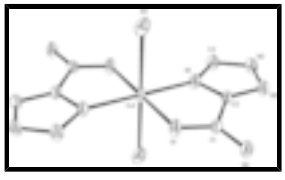

Fig. 1. The molecular structure of (I) showing 50% probability displacement ellipsoids (H atoms omitted for clarity). Unlabelled atoms are generated by the symmetry operation (2 − *x*, −*y*, 1 − *z*).

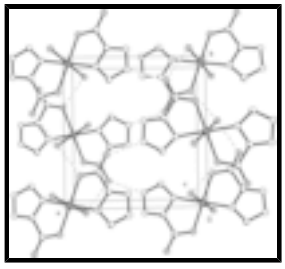

Fig. 2. Crystal packing of (I) showing the donor···acceptor hydrogen bond interactions as dashed lines.

Diaquabis(1*H*-1,2,4-triazole-3-carboxylato)copper(II)

Crystal data

$[Cu(C_3H_2N_3O_2)_2(H_2O)_2]$	F_{000} = 326
M_r = 323.72	D_x = 1.943 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2439 reflections
a = 8.6389 (11) Å	θ = 3.2–28.3º
b = 9.1819 (12) Å	μ = 2.01 mm^{-1}
c = 6.9929 (9) Å	T = 293 (2) K
β = 94.212 (2)º	Block, blue
V = 553.19 (12) Å^3	0.33 × 0.30 × 0.18 mm
Z = 2	

Data collection

Siemens SMART CCD diffractometer	1003 independent reflections
Radiation source: fine-focus sealed tube	971 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.007
T = 293(2) K	θ_{max} = 25.5º
ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→10
T_{min} = 0.455, T_{max} = 0.710	k = −10→11
2601 measured reflections	l = −8→3

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.021	H-atom parameters constrained
$wR(F^2)$ = 0.064	$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 0.1844P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
1003 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
88 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and *R*-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	1.0000	0.0000	0.5000	0.02470 (15)
O1	0.92210 (12)	0.20569 (11)	0.52024 (16)	0.0270 (3)
O2	0.72248 (12)	0.34931 (12)	0.42677 (17)	0.0288 (3)
O3	0.89522 (14)	−0.07762 (13)	0.79148 (17)	0.0370 (3)
H1W	0.9586	−0.1295	0.8522	0.055*
H2W	0.8583	−0.0138	0.8580	0.055*
N1	0.78961 (17)	−0.03174 (15)	0.3716 (2)	0.0255 (3)
N2	0.56189 (16)	0.08059 (16)	0.2954 (2)	0.0269 (3)
N3	0.55537 (17)	−0.06294 (17)	0.2464 (2)	0.0292 (3)
H3D	0.4746	−0.1055	0.1932	0.035*
C1	0.78598 (17)	0.22851 (16)	0.4437 (2)	0.0217 (3)
C2	0.70511 (17)	0.09383 (17)	0.3694 (2)	0.0215 (3)
C3	0.69045 (19)	−0.12872 (18)	0.2918 (2)	0.0290 (4)
H3A	0.7119	−0.2265	0.2710	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0157 (2)	0.0158 (2)	0.0405 (2)	0.00221 (8)	−0.01208 (13)	−0.00245 (9)
O1	0.0196 (6)	0.0192 (5)	0.0403 (6)	0.0012 (4)	−0.0109 (5)	−0.0031 (4)
O2	0.0213 (6)	0.0191 (6)	0.0447 (6)	0.0037 (4)	−0.0061 (5)	−0.0005 (5)
O3	0.0381 (7)	0.0290 (6)	0.0429 (7)	0.0112 (5)	−0.0027 (5)	0.0045 (5)
N1	0.0193 (7)	0.0187 (6)	0.0371 (7)	0.0003 (6)	−0.0078 (6)	−0.0006 (6)

N2	0.0195 (7)	0.0242 (7)	0.0362 (7)	0.0000 (6)	−0.0050 (5)	0.0004 (6)
N3	0.0196 (7)	0.0251 (8)	0.0416 (7)	−0.0064 (6)	−0.0082 (6)	−0.0032 (6)
C1	0.0182 (7)	0.0201 (7)	0.0263 (7)	0.0011 (6)	−0.0014 (6)	0.0007 (6)
C2	0.0152 (7)	0.0208 (7)	0.0274 (7)	0.0015 (6)	−0.0046 (6)	0.0023 (6)
C3	0.0235 (8)	0.0213 (8)	0.0407 (9)	−0.0011 (6)	−0.0080 (7)	−0.0028 (7)

Geometric parameters (Å, °)

Cu1—N1	1.9886 (15)	O3—H2W	0.8265
Cu1—N1^{i}	1.9886 (15)	N1—C3	1.330 (2)
Cu1—O1^{i}	2.0134 (11)	N1—C2	1.364 (2)
Cu1—O1	2.0134 (11)	N2—C2	1.311 (2)
Cu1—O3^{i}	2.3985 (12)	N2—N3	1.362 (2)
Cu1—O3	2.3985 (12)	N3—C3	1.332 (2)
O1—C1	1.2732 (19)	N3—H3D	0.8600
O2—C1	1.2392 (19)	C1—C2	1.495 (2)
O3—H1W	0.8200	C3—H3A	0.9300
N1—Cu1—N1^{i}	180.0	H1W—O3—H2W	113.0
N1—Cu1—O1^{i}	97.47 (5)	C3—N1—C2	103.50 (14)
N1^{i}—Cu1—O1^{i}	82.53 (5)	C3—N1—Cu1	145.78 (12)
N1—Cu1—O1	82.53 (5)	C2—N1—Cu1	110.60 (11)
N1^{i}—Cu1—O1	97.47 (5)	C2—N2—N3	102.09 (13)
O1^{i}—Cu1—O1	180.0	C3—N3—N2	111.09 (13)
N1—Cu1—O3^{i}	92.83 (5)	C3—N3—H3D	124.5
N1^{i}—Cu1—O3^{i}	87.16 (5)	N2—N3—H3D	124.5
O1^{i}—Cu1—O3^{i}	94.01 (4)	O2—C1—O1	125.18 (14)
O1—Cu1—O3^{i}	85.99 (4)	O2—C1—C2	121.00 (13)
N1—Cu1—O3	87.17 (5)	O1—C1—C2	113.81 (12)
N1^{i}—Cu1—O3	92.84 (5)	N2—C2—N1	114.50 (14)
O1^{i}—Cu1—O3	85.99 (4)	N2—C2—C1	128.12 (14)
O1—Cu1—O3	94.01 (4)	N1—C2—C1	117.34 (13)
O3^{i}—Cu1—O3	180.0	N1—C3—N3	108.82 (15)
C1—O1—Cu1	115.34 (9)	N1—C3—H3A	125.6
Cu1—O3—H1W	109.5	N3—C3—H3A	125.6
Cu1—O3—H2W	116.9		
N1—Cu1—O1—C1	−2.24 (11)	Cu1—O1—C1—C2	5.40 (15)
N1^{i}—Cu1—O1—C1	177.76 (11)	N3—N2—C2—N1	−0.33 (17)
O3^{i}—Cu1—O1—C1	91.15 (10)	N3—N2—C2—C1	177.42 (15)
O3—Cu1—O1—C1	−88.85 (10)	C3—N1—C2—N2	0.38 (19)
O1^{i}—Cu1—N1—C3	3.0 (2)	Cu1—N1—C2—N2	−176.85 (11)
O1—Cu1—N1—C3	−177.0 (2)	C3—N1—C2—C1	−177.63 (13)
O3^{i}—Cu1—N1—C3	97.4 (2)	Cu1—N1—C2—C1	5.14 (17)
O3—Cu1—N1—C3	−82.6 (2)	O2—C1—C2—N2	−5.8 (2)
O1^{i}—Cu1—N1—C2	178.22 (11)	O1—C1—C2—N2	175.09 (15)
O1—Cu1—N1—C2	−1.78 (11)	O2—C1—C2—N1	171.92 (14)

O3^{i}—Cu1—N1—C2	−87.35 (11)	O1—C1—C2—N1	−7.21 (19)
O3—Cu1—N1—C2	92.65 (11)	C2—N1—C3—N3	−0.25 (18)
C2—N2—N3—C3	0.15 (17)	Cu1—N1—C3—N3	175.13 (16)
Cu1—O1—C1—O2	−173.69 (12)	N2—N3—C3—N1	0.07 (19)

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3D···O2^{ii}	0.86	1.89	2.7295 (17)	166
O3—H2W···O2^{iii}	0.83	1.99	2.7792 (17)	159
O3—H1W···O1^{iv}	0.82	2.00	2.8067 (16)	166

Symmetry codes: (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) *x*, −*y*+1/2, *z*+1/2; (iv) −*x*+2, *y*−1/2, −*z*+3/2.

Fig. 1

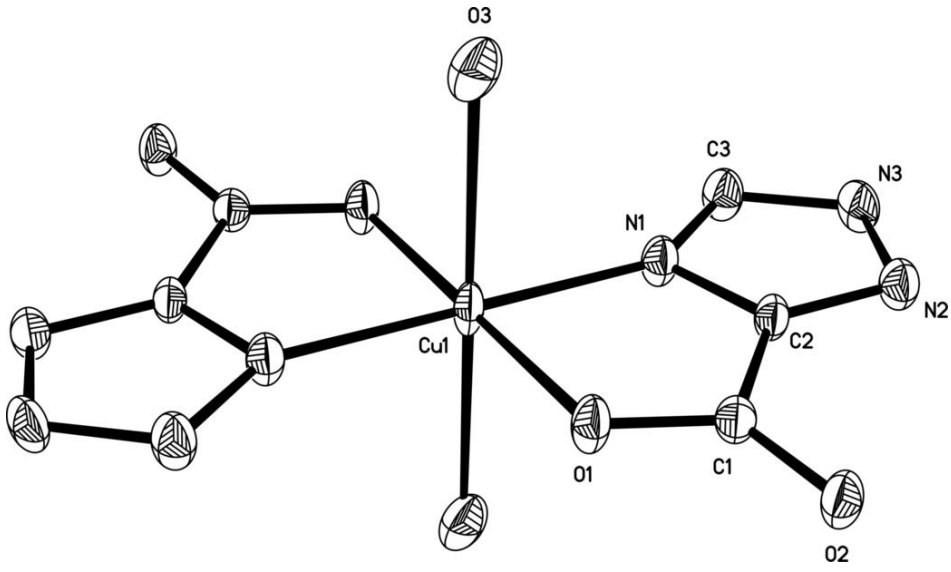

Fig. 2