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Diaquabis[5-(pyrazin-2-yl)-5*H*-tetrazolato-κ^2N,N']copper(II) monohydrate

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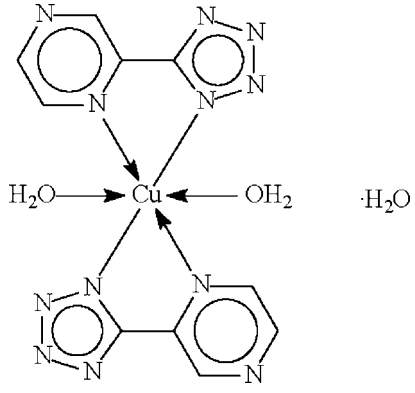
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.027; wR factor = 0.077; data-to-parameter ratio = 11.8.

The Cu^{II} atom in the title compound, $[Cu(C_5H_3N_6)_2(H_2O)_2]\cdot H_2O$, is chelated by two pyrazinyltetrazolate ligands and, in addition, coordinated by two water molecules in a tetragonally elongated octahedral geometry [Cu—N = 1.990 (2) and 2.056 (2) Å, and Cu—O = 2.445 (2) Å]. The Cu^{II} atom lies on a center of inversion. In the crystal structure, molecules are linked by O—H···O and O—H···N hydrogen bonds into a three-dimensional network. The free water molecule is disordered about a twofold axis.

Related literature

There are no crystal structure reports of metal 5-(2-pyrazinyl)-5*H*-tetrazolates (Cambridge Structural Database, Version 5.28; Allen, 2002). For the crystal structure of the hemihydrated organic compound, see: Li *et al.* (2007).



Experimental

Crystal data

$[Cu(C_5H_3N_6)_2(H_2O)_2]\cdot H_2O$
M_r = 411.86
Monoclinic, $C2/c$
a = 13.045 (2) Å
b = 7.341 (1) Å
c = 16.869 (2) Å
β = 101.757 (2)°
V = 1581.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.43 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.18 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.606, T_{max} = 0.784
4287 measured reflections
1603 independent reflections
1375 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.077
S = 1.02
1603 reflections
136 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···N2^{i}	0.84 (1)	2.02 (1)	2.857 (2)	173 (3)
O1w—H12···N4^{ii}	0.85 (1)	2.07 (1)	2.919 (2)	178 (2)
O2*W*—H21···O1*W*	0.86 (1)	1.98 (2)	2.841 (9)	172 (6)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2383).

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supplementary materials

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Diaquabis[5-(pyrazin-2-yl)-5*H*-tetrazolato-κ^2N,N']copper(II) monohydrate

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Comment

The Cambridge Structural Database (Version 5.28, November 2006; Allen, 2002) lists several examples of metal 5-(2-pyridyl)-5*H*-tetrazoles. A second nitrogen donor site in a pyrazine ring group could serve as a donor site, but this is not observed in the copper derivative, which crystallizes as a diaqua monohydrate. The second donor site in the pyrimidyl part of the anion is engaged in hydrogen bonding with the coordinated and lattice water molecules to form a three-dimensional network motif.

Experimental

Copper chloride dihydrate (34 mg, 0.2 mmol) and 2-(1*H*-tetrazol-5-yl)pyrazine (60 mg, 0.4 mmol) were dissolved in 10 ml of a DMF–water (1:1) mixture. The clear solution was filtered; blue crystals were isolated after a month in 30% yield.

Refinement

Carbon-bound H atoms were placed at calculated positions [C—H = 0.93 Å; U(H) = 1.2U_{eq}(C)]. The O2w atom is disordered about a twofold axis, and it was allowed to refine off the symmetry element. The H atoms of the water molecules were located in a difference Fourier map, and were refined with distance restraints of O–H = 0.85±0.01 Å and H···H = 1.39±0.01 Å.

Figures

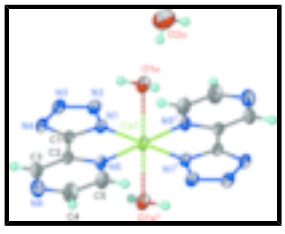

Fig. 1. **Figure 1**. The molecular structure of the title compound with ellipsoids drawn at the 50% probability level. The copper atom lies on a center-of-inversion; dash lines denote the long Cu···O_{water} bonds bonds [symmetry code: (i) -*x* + 1, -*y* + 1, -*z* + 1].

Diaquabis[5-(pyrazin-2-yl)-5*H*-tetrazolato-κ^2*N*,*N*']copper(II) monohydrate

Crystal data

$[Cu(C_5H_3N_6)_2(H_2O)_2]\cdot H_2O$	F_{000} = 836
M_r = 411.86	D_x = 1.730 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2454 reflections
a = 13.045 (2) Å	θ = 3.2–26.3°

b = 7.341 (1) Å	μ = 1.43 mm^{-1}
c = 16.869 (2) Å	T = 294 (2) K
β = 101.757 (2)º	Block, blue
V = 1581.5 (4) Å^3	0.24 × 0.22 × 0.18 mm
Z = 4	

Data collection

Bruker APEX area-detector diffractometer	1603 independent reflections
Radiation source: fine-focus sealed tube	1375 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 294(2) K	θ_{max} = 26.3º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	h = −15→16
T_{min} = 0.606, T_{max} = 0.784	k = −9→9
4287 measured reflections	l = −14→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.027	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.077	$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 1.3231P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
1603 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
136 parameters	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
18 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.5000	0.5000	0.5000	0.02729 (14)	
O1W	0.60924 (12)	0.6371 (2)	0.41419 (10)	0.0387 (4)	
H11	0.6673 (11)	0.582 (3)	0.4237 (16)	0.046*	
H12	0.6171 (17)	0.7461 (16)	0.4309 (15)	0.046*	
O2W	0.5303 (4)	0.6846 (6)	0.2457 (5)	0.0821 (19)	0.50
H21	0.556 (5)	0.660 (7)	0.2958 (15)	0.099*	0.50
H22	0.508 (7)	0.583 (5)	0.223 (3)	0.099*	0.50
N1	0.40820 (12)	0.7190 (2)	0.48450 (10)	0.0267 (4)	
N2	0.32571 (13)	0.7878 (2)	0.43186 (11)	0.0322 (4)	
N3	0.30323 (14)	0.9464 (3)	0.45989 (12)	0.0337 (4)	

N4	0.36960 (15)	0.9853 (2)	0.53077 (12)	0.0318 (4)
N5	0.57264 (12)	0.6487 (2)	0.59883 (10)	0.0281 (4)
N6	0.64382 (16)	0.8787 (3)	0.72971 (12)	0.0460 (5)
C1	0.43250 (14)	0.8413 (2)	0.54351 (12)	0.0251 (4)
C2	0.52281 (15)	0.8057 (3)	0.60846 (12)	0.0261 (4)
C3	0.55893 (18)	0.9186 (3)	0.67355 (14)	0.0364 (5)
H3	0.5230	1.0261	0.6784	0.044*
C4	0.6933 (2)	0.7251 (3)	0.71873 (15)	0.0474 (6)
H4	0.7536	0.6941	0.7561	0.057*
C5	0.65859 (17)	0.6091 (3)	0.65368 (14)	0.0384 (5)
H5	0.6956	0.5031	0.6484	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0274 (2)	0.0203 (2)	0.0296 (2)	0.00697 (13)	−0.00475 (14)	−0.00489 (14)
O1W	0.0332 (8)	0.0308 (8)	0.0497 (10)	0.0062 (6)	0.0030 (7)	−0.0004 (7)
O2W	0.100 (5)	0.073 (3)	0.064 (3)	−0.024 (3)	−0.006 (4)	0.005 (3)
N1	0.0247 (8)	0.0226 (8)	0.0306 (9)	0.0042 (6)	0.0005 (7)	0.0001 (7)
N2	0.0278 (8)	0.0293 (9)	0.0368 (10)	0.0066 (7)	0.0003 (7)	0.0029 (8)
N3	0.0300 (9)	0.0277 (9)	0.0425 (10)	0.0070 (7)	0.0051 (8)	0.0039 (8)
N4	0.0310 (9)	0.0233 (9)	0.0416 (10)	0.0048 (7)	0.0089 (8)	0.0007 (7)
N5	0.0274 (8)	0.0234 (8)	0.0310 (9)	0.0018 (7)	−0.0001 (7)	−0.0036 (7)
N6	0.0512 (12)	0.0410 (12)	0.0397 (11)	−0.0005 (9)	−0.0054 (9)	−0.0108 (9)
C1	0.0246 (9)	0.0203 (9)	0.0315 (10)	0.0020 (7)	0.0080 (8)	−0.0003 (8)
C2	0.0267 (9)	0.0222 (10)	0.0298 (10)	−0.0013 (7)	0.0064 (8)	−0.0014 (8)
C3	0.0414 (12)	0.0305 (12)	0.0366 (12)	0.0019 (10)	0.0066 (10)	−0.0067 (10)
C4	0.0448 (13)	0.0423 (14)	0.0449 (14)	0.0044 (11)	−0.0149 (11)	−0.0082 (11)
C5	0.0357 (12)	0.0320 (12)	0.0412 (13)	0.0057 (9)	−0.0068 (10)	−0.0035 (10)

Geometric parameters (Å, °)

Cu1—N1	1.990 (2)	N3—N4	1.356 (3)
Cu1—N1^{i}	1.990 (2)	N4—C1	1.328 (2)
Cu1—N5	2.056 (2)	N5—C5	1.332 (3)
Cu1—N5^{i}	2.056 (2)	N5—C2	1.349 (2)
Cu1—O1w	2.445 (2)	N6—C4	1.331 (3)
O1W—H11	0.84 (1)	N6—C3	1.335 (3)
O1W—H12	0.85 (1)	C1—C2	1.460 (3)
O2W—H21	0.86 (1)	C2—C3	1.380 (3)
O2W—H22	0.86 (1)	C3—H3	0.9300
N1—C1	1.330 (2)	C4—C5	1.390 (3)
N1—N2	1.346 (2)	C4—H4	0.9300
N2—N3	1.312 (3)	C5—H5	0.9300
N1^{i}—Cu1—N1	180.000 (1)	C5—N5—C2	117.45 (18)
N1^{i}—Cu1—N5^{i}	80.97 (6)	C5—N5—Cu1	129.11 (14)
N1—Cu1—N5^{i}	99.03 (6)	C2—N5—Cu1	113.42 (13)

N1^{i}—Cu1—N5	99.03 (6)	C4—N6—C3	116.3 (2)
N1—Cu1—N5	80.97 (6)	N4—C1—N1	111.76 (17)
N5^{i}—Cu1—N5	180.0	N4—C1—C2	129.91 (18)
N1^{i}—Cu1—O1W	90.14 (6)	N1—C1—C2	118.27 (16)
N1—Cu1—O1W	89.86 (6)	N5—C2—C3	120.95 (18)
N5^{i}—Cu1—O1W	88.07 (6)	N5—C2—C1	113.44 (17)
N5—Cu1—O1W	91.93 (6)	C3—C2—C1	125.58 (18)
Cu1—O1W—H11	107.4 (18)	N6—C3—C2	122.1 (2)
Cu1—O1W—H12	103.7 (17)	N6—C3—H3	118.9
H11—O1W—H12	110.1 (15)	C2—C3—H3	118.9
H21—O2W—H22	106.4 (17)	N6—C4—C5	122.6 (2)
C1—N1—N2	106.08 (15)	N6—C4—H4	118.7
C1—N1—Cu1	113.68 (12)	C5—C4—H4	118.7
N2—N1—Cu1	140.23 (13)	N5—C5—C4	120.5 (2)
N3—N2—N1	107.61 (16)	N5—C5—H5	119.8
N2—N3—N4	110.81 (16)	C4—C5—H5	119.8
C1—N4—N3	103.74 (16)		
N5^{i}—Cu1—N1—C1	176.48 (13)	Cu1—N1—C1—N4	179.87 (13)
N5—Cu1—N1—C1	−3.52 (13)	N2—N1—C1—C2	−177.69 (17)
O1W—Cu1—N1—C1	−95.49 (14)	Cu1—N1—C1—C2	2.4 (2)
N5^{i}—Cu1—N1—N2	−3.3 (2)	C5—N5—C2—C3	−1.1 (3)
N5—Cu1—N1—N2	176.7 (2)	Cu1—N5—C2—C3	177.58 (16)
O1W—Cu1—N1—N2	84.7 (2)	C5—N5—C2—C1	177.32 (18)
C1—N1—N2—N3	0.1 (2)	Cu1—N5—C2—C1	−4.0 (2)
Cu1—N1—N2—N3	179.95 (16)	N4—C1—C2—N5	−175.75 (19)
N1—N2—N3—N4	0.0 (2)	N1—C1—C2—N5	1.1 (3)
N2—N3—N4—C1	−0.2 (2)	N4—C1—C2—C3	2.6 (3)
N1^{i}—Cu1—N5—C5	2.7 (2)	N1—C1—C2—C3	179.5 (2)
N1—Cu1—N5—C5	−177.3 (2)	C4—N6—C3—C2	1.3 (4)
O1W—Cu1—N5—C5	−87.79 (19)	N5—C2—C3—N6	−0.2 (3)
N1^{i}—Cu1—N5—C2	−175.81 (14)	C1—C2—C3—N6	−178.4 (2)
N1—Cu1—N5—C2	4.19 (14)	C3—N6—C4—C5	−1.3 (4)
O1W—Cu1—N5—C2	93.74 (14)	C2—N5—C5—C4	1.1 (3)
N3—N4—C1—N1	0.3 (2)	Cu1—N5—C5—C4	−177.28 (18)
N3—N4—C1—C2	177.32 (19)	N6—C4—C5—N5	0.0 (4)
N2—N1—C1—N4	−0.3 (2)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···N3^{ii}	0.84 (1)	2.02 (1)	2.857 (2)	173 (3)
O1w—H12···N4^{iii}	0.85 (1)	2.07 (1)	2.919 (2)	178 (2)
O2w—H21···O1w	0.86 (1)	1.98 (2)	2.841 (9)	172 (6)

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

Fig. 1