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trans-Diaquabis(pyridazine-3-carboxylato-κ^2N^2,O)copper(II)

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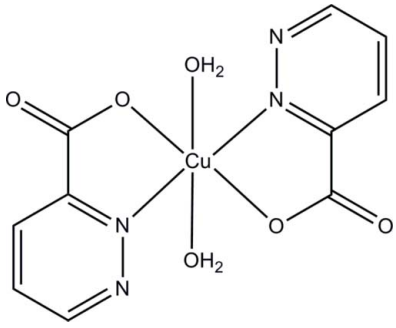
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.065; data-to-parameter ratio = 11.6.

In the title compound, $[Cu(C_5H_3N_2O_2)_2(H_2O)_2]$, the Cu^{II} ion, located on an inversion center, exhibits an octahedral coordination geometry. The equatorial plane is defined by two *trans*-related *N*,*O*-bidentate pyridazine-3-carboxylate ligands and the axial positions are occupied by two water molecules. In the crystal, molecules are connected by O—H···O hydrogen bonds between the water molecules and the noncoordinating carboxylate O atoms, forming layers parallel to the *bc* plane. The layers are stacked along the *a* axis by further O—H···O hydrogen bonds between the water molecules and the coordinating carboxylate O atoms. Weak C—H···O hydrogen bonds are also observed between the pyridazine rings and the water molecules and between the pyridazine rings and the non-coordinating carboxylate O atoms.

Related literature

For the isotypic zinc complex, see: Gryz *et al.* (2004). For a related cobalt(II) complex which contains two non-coordinating water molecules, see: Artetxe *et al.* (2013).



Experimental

Crystal data

$[Cu(C_5H_3N_2O_2)_2(H_2O)_2]$
M_r = 345.76
Monoclinic, $P2_1/c$
a = 5.4014 (1) Å
b = 11.5633 (3) Å
c = 9.6283 (2) Å
β = 101.837 (3)°
V = 588.58 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 100 K
0.19 × 0.09 × 0.06 mm

Data collection

Agilent SuperNova diffractometer
Absorption correction: numerical (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.772, T_{max} = 0.898
2532 measured reflections
1216 independent reflections
1077 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.065
S = 1.06
1216 reflections
105 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.9792 (15)	Cu1—O1*W*	2.4207 (16)
Cu1—N2	1.9822 (18)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1^{i}	0.87 (2)	1.99 (2)	2.865 (2)	175 (2)
O1*W*—H1*WB*···O2^{ii}	0.87 (1)	2.03 (2)	2.878 (2)	165 (3)
C4—H4···O1*W*^{iii}	0.93	2.52	3.403 (3)	158
C6—H6···O2^{iv}	0.93	2.39	3.141 (3)	138

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *OLEX2* (Dolomanov *et al.*, 2009); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

This work was supported financially by Eusko Jaurlaritza/Gobierno Vasco (grant IT477–10). AP also thanks EJ/GV for predoctoral fellowships.

Supporting information for this paper is available from the IUCr electronic archives (Reference: IS5342).

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supplementary materials

Acta Cryst. (2014). E**70**, m114–m115 [doi:10.1107/S1600536814004334]

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1. Comment

The metal ion, the pyridazine ring and carboxylate atoms are coplanar. As expected, the Cu—O and Cu—N distances (Table 1) are similar to the Zn(II) and Co(II) analogue compounds (Gryz *et al.*, 2004; Artetxe *et al.*, 2013). Table 2 summarizes the geometrical parameters of the O—H···O and C—H···O hydrogen bonding interactions.

2. Experimental

To a solution of $CuCl_2.2H_2O$ (34 mg, 0.2 mmol) in water (10 mL) 3-pyridazine carboxylic acid (48 mg, 0.4 mmol) was dropwise added and the resulting solution was stirred for 1 h at 80 °C. Blue prismatic crystals suitable for single-crystal X-ray diffraction were obtained by slow evaporation of the resulting solution after six days.

3. Refinement

H atoms of the water molecules were located in a Fourier difference map and refined isotropically with O—H bond lengths restrained to 0.88 (1) Å. All H atoms of the pyridazine ring were positioned geometrically and refined using a riding model with standard *SHELXL* parameters.

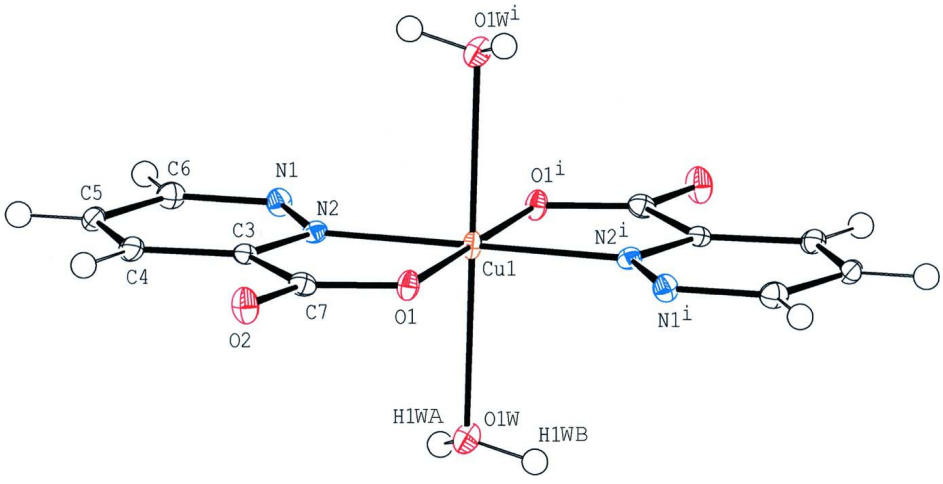

Figure 1

Molecular structure of the title compound, showing atom labelling and 50% probability displacement ellipsoids. [Symmetry code: (i) 1 - *x*, 1 - *y*, 1 - *z*.]

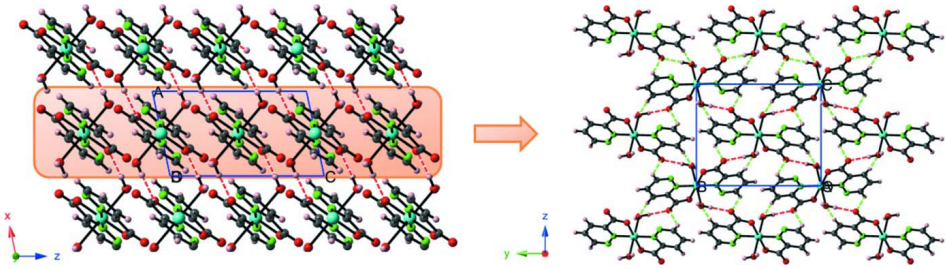

Figure 2

Left: View of the crystal packing along the *b* axis. Right: Projection of a layer along the *a* axis (O—H···O hydrogen bonds represented as dotted red lines and weak C—H···O interactions as dotted green lines).

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Crystal data

$[Cu(C_5H_3N_2O_2)_2(H_2O)_2]$
$M_r = 345.76$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.4014$ (1) Å
$b = 11.5633$ (3) Å
$c = 9.6283$ (2) Å
$\beta = 101.837$ (3)°
$V = 588.58$ (2) Å^3
$Z = 2$
$F(000) = 350$
$D_x = 1.951$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1663 reflections
$\theta = 2.8$–$28.4°$
$\mu = 1.89$ mm^{-1}
$T = 100$ K
Prism, blue
0.19 × 0.09 × 0.06 mm

Data collection

Agilent SuperNova diffractometer
Radiation source: Nova (Mo) X-ray micro-source
Multilayer optics monochromator
Detector resolution: 16.2439 pixels mm^{-1}
ω scans
Absorption correction: numerical (*CrysAlis PRO*; Agilent, 2012)
$T_{min} = 0.772$, $T_{max} = 0.898$
2532 measured reflections
1216 independent reflections
1077 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.8°$
$h = -6 \rightarrow 6$
$k = -13 \rightarrow 14$
$l = -12 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.065$
$S = 1.06$
1216 reflections
105 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2 + 0.6643P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

Special details

Experimental. IR (cm^{-1}): 3554(s), 3315(s), 3233(s), 1628(s), 1571(m), 1578(s), 1365(w), 1231(w), 1152(w), 1091(w), 1072(w), 1039(w), 978(m), 851(m), 785(m), 722(m), 669(w), 536(w), 440(w).

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
C3	0.4961 (4)	0.27046 (19)	0.4096 (2)	0.0083 (4)
C4	0.4421 (4)	0.15278 (19)	0.3920 (2)	0.0107 (4)
H4	0.5153	0.1071	0.3318	0.013*
C5	0.2754 (4)	0.10781 (19)	0.4680 (2)	0.0106 (5)
H5	0.2313	0.03	0.4606	0.013*
C6	0.1737 (4)	0.18136 (19)	0.5564 (2)	0.0111 (5)
H6	0.0632	0.1503	0.6089	0.013*
C7	0.6781 (4)	0.33471 (19)	0.3358 (2)	0.0097 (4)
Cu1	0.5	0.5	0.5	0.00820 (13)
N1	0.2267 (3)	0.29375 (16)	0.5696 (2)	0.0101 (4)
N2	0.3890 (3)	0.33637 (16)	0.49462 (18)	0.0084 (4)
O1	0.7022 (3)	0.44303 (13)	0.36438 (16)	0.0100 (3)
O2	0.7873 (3)	0.28108 (13)	0.25561 (17)	0.0135 (4)
O1W	0.1555 (3)	0.53934 (14)	0.30161 (17)	0.0121 (3)
H1WA	0.014 (3)	0.514 (2)	0.321 (3)	0.024 (8)*
H1WB	0.149 (6)	0.6143 (9)	0.292 (4)	0.051 (11)*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C3	0.0088 (10)	0.0095 (11)	0.0063 (10)	0.0001 (8)	0.0005 (8)	0.0003 (8)
C4	0.0128 (11)	0.0094 (11)	0.0094 (10)	0.0035 (9)	0.0014 (9)	−0.0004 (8)
C5	0.0107 (10)	0.0082 (11)	0.0117 (11)	−0.0007 (8)	−0.0007 (9)	0.0019 (8)
C6	0.0106 (10)	0.0125 (11)	0.0106 (11)	−0.0011 (9)	0.0028 (9)	0.0014 (9)
C7	0.0091 (10)	0.0120 (11)	0.0080 (10)	−0.0007 (8)	0.0018 (9)	0.0001 (9)
Cu1	0.0111 (2)	0.0052 (2)	0.0101 (2)	−0.00061 (14)	0.00618 (15)	−0.00061 (14)
N1	0.0107 (9)	0.0099 (9)	0.0104 (9)	−0.0019 (7)	0.0039 (8)	−0.0002 (7)
N2	0.0091 (9)	0.0092 (9)	0.0072 (9)	0.0007 (7)	0.0021 (7)	0.0013 (7)
O1	0.0112 (7)	0.0071 (8)	0.0128 (8)	−0.0012 (6)	0.0052 (6)	0.0004 (6)
O2	0.0158 (8)	0.0120 (8)	0.0152 (8)	−0.0009 (6)	0.0094 (7)	−0.0033 (6)
O1W	0.0101 (8)	0.0105 (8)	0.0161 (8)	0.0006 (6)	0.0037 (7)	0.0023 (7)

Geometric parameters (Å, º)

C3—N2	1.334 (3)	C7—C3	1.520 (3)
C3—C4	1.395 (3)	Cu1—O1^{i}	1.9792 (15)
C3—C7	1.520 (3)	Cu1—O1	1.9792 (15)
C4—C5	1.374 (3)	Cu1—N2	1.9822 (18)
C4—H4	0.93	Cu1—N2^{i}	1.9822 (18)
C5—C6	1.393 (3)	Cu1—O1W	2.4207 (16)
C5—H5	0.93	Cu1—O1W^{i}	2.4207 (16)
C6—N1	1.331 (3)	N1—N2	1.339 (3)
C6—H6	0.93	O1W—H1WA	0.872 (10)
C7—O2	1.231 (3)	O1W—H1WB	0.872 (10)
C7—O1	1.283 (3)		
N2—C3—C4	121.7 (2)	O1^{i}—Cu1—N2^{i}	82.52 (7)
N2—C3—C7	114.28 (19)	N2—Cu1—N2^{i}	180
C4—C3—C7	124.0 (2)	O1—Cu1—O1W	88.90 (6)
C5—C4—C3	116.6 (2)	O1^{i}—Cu1—O1W	91.10 (6)
C5—C4—H4	121.7	N2—Cu1—O1W	88.82 (6)
C3—C4—H4	121.7	N2^{i}—Cu1—O1W	91.18 (6)
C4—C5—C6	118.6 (2)	O1—Cu1—O1W^{i}	91.10 (6)
C4—C5—H5	120.7	O1^{i}—Cu1—O1W^{i}	88.90 (6)
C6—C5—H5	120.7	N2—Cu1—O1W^{i}	91.18 (6)
N1—C6—C5	123.4 (2)	N2^{i}—Cu1—O1W^{i}	88.82 (6)
N1—C6—H6	118.3	O1W—Cu1—O1W^{i}	180
C5—C6—H6	118.3	C6—N1—N2	117.37 (19)
O2—C7—O1	125.8 (2)	C3—N2—N1	122.33 (19)
O2—C7—C3	119.1 (2)	C3—N2—Cu1	113.24 (15)
O1—C7—C3	115.06 (19)	N1—N2—Cu1	124.43 (14)
O1^{i}—Cu1—O1	180	C7—O1—Cu1	114.89 (13)
O1—Cu1—N2	82.52 (7)	Cu1—O1W—H1WA	109.8 (19)
O1^{i}—Cu1—N2	97.48 (7)	Cu1—O1W—H1WB	106 (2)
O1—Cu1—N2^{i}	97.48 (7)	H1WA—O1W—H1WB	109 (2)
N2—C3—C4—C5	−0.8 (3)	O1W—Cu1—N2—C3	89.46 (15)
C7—C3—C4—C5	179.22 (19)	O1W^{i}—Cu1—N2—C3	−90.54 (15)
C3—C4—C5—C6	−0.2 (3)	O1—Cu1—N2—N1	179.32 (17)
C4—C5—C6—N1	1.1 (3)	O1^{i}—Cu1—N2—N1	−0.68 (17)
C5—C6—N1—N2	−0.9 (3)	O1W—Cu1—N2—N1	−91.63 (16)
C4—C3—N2—N1	1.0 (3)	O1W^{i}—Cu1—N2—N1	88.37 (16)
C7—C3—N2—N1	−179.04 (18)	O2—C7—O1—Cu1	−179.34 (18)
C4—C3—N2—Cu1	179.92 (16)	C3—C7—O1—Cu1	0.8 (2)
C7—C3—N2—Cu1	−0.1 (2)	N2—Cu1—O1^{i}—C7^{i}	−179.30 (15)
C6—N1—N2—C3	−0.1 (3)	N2—Cu1—O1—C7	−0.70 (15)
C6—N1—N2—Cu1	−178.91 (15)	O1W—Cu1—O1—C7	−89.65 (15)
O1—Cu1—N2—C3	0.41 (14)	O1W^{i}—Cu1—O1—C7	90.35 (15)
O1^{i}—Cu1—N2—C3	−179.59 (14)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1^{ii}	0.87 (2)	1.99 (2)	2.865 (2)	175 (2)
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C6—H6···O2^{v}	0.93	2.39	3.141 (3)	138

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