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trans-Bis[2,3-diamino-(*R*,*S*)-propionato-*N*,*N*′]diaquacopper(II) dihydrate

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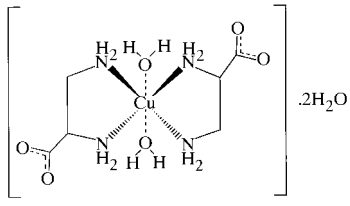
The title copper complex, $[Cu(DL\text{-}DAP)_2(H_2O)_2]\cdot 2H_2O$ or $[Cu(C_3H_7N_2O_2)_2(H_2O)_2]\cdot 2H_2O$, prepared from the non-protein amino acid DL-2,3-diaminopropionic acid (DL-HDAP), has a center of symmetry and a distorted octahedral coordination, with four N atoms in equatorial positions and two water molecules in apical sites. The water molecule of crystallization is hydrogen bonded to the deprotonated carboxylate group of the ligand.

Comment

The crystal structure of the title compound, (I), consists of discrete molecules of $[Cu(DL\text{-}DAP)_2(H_2O)_2]$ (DL-DAP is DL-2,3-diaminopropionate), with one molecule per unit cell along with two molecules of water of crystallization. The molecular structure consists of a central Cu atom in a distorted octahedral geometry coordinating to two bidentate DAP ligands



(I)

through their N atoms in equatorial positions in a *trans*-coplanar configuration. The geometry about copper is completed by coordination of two water molecules bonding *via* their O atoms in the apical sites. The other two water molecules within the unit cell do not coordinate to the copper but are hydrogen bonded to the deprotonated carboxylate groups. The Cu—N bond lengths are 2.009 (3) and 2.022 (3) Å, which are comparable to the Cu—N bond distances seen in other copper–amino acid complexes (Freeman *et al.*, 1964). The Cu—O bond length is 2.613 (3) Å.

Experimental

The complex $[Cu(DL\text{-}DAP)_2(H_2O)_2]\cdot 2H_2O$ was prepared by the stoichiometric reaction of DL-2,3-diaminoproprionic acid (DL-HDAP; 0.141 g, 1 mmol) with copper perchlorate hexahydrate (0.123 g, 0.5 mmol) in deionized water (5 ml). The pH was adjusted to 10 using a concentrated KOH solution. The deep-royal-blue aqueous solution was filtered and allowed to evaporate over several days to yield well formed prism-shaped crystals. Analysis calculated: C 21.1, H 6.4, N 16.4%; found: C 21.1, H 6.4, N 16.3% [m.p. 484 K (decomposition)].

Crystal data

$[Cu(C_3H_7N_2O_2)_2(H_2O)_2]\cdot 2H_2O$
M_r = 341.82
Triclinic, $P\overline{1}$
a = 6.5070 (10) Å
b = 7.448 (2) Å
c = 7.735 (2) Å
α = 109.25 (4)°
β = 95.11 (4)°
γ = 109.52 (5)°
V = 325.10 (13) Å^3
Z = 1
D_x = 1.746 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 11.04–13.69°
μ = 1.723 mm^{-1}
T = 180 (2) K
Prism, violet
0.2 × 0.2 × 0.1 mm

Data collection

Enraf—Nonius CAD-4 diffractometer
Non-profiled $\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.712, T_{max} = 0.842
1527 measured reflections
1417 independent reflections
1265 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 26.93°
$h = -8 \rightarrow 7$
$k = 0 \rightarrow 9$
$l = -9 \rightarrow 9$
2 standard reflections
frequency: 60 min
intensity decay: 26%

Refinement

Refinement on F^2
$R(F)$ = 0.039
$wR(F^2)$ = 0.106
S = 1.054
1417 reflections
133 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0680P)^2 + 0.2597P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.009 (3)	Cu1—O3	2.613 (3)
Cu1—N2	2.022 (3)		
N1—Cu1—N2	84.36 (11)	N2—Cu1—O3	90.75 (11)
N1—Cu1—O3	92.66 (12)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···O2^{i}	0.77 (5)	2.27 (5)	3.033 (5)	168 (4)
N2—H2···O1^{ii}	0.84 (4)	2.34 (4)	2.991 (4)	134 (3)
N1—H6···O4^{iii}	0.80 (6)	2.16 (6)	2.941 (4)	166 (6)
N1—H7···O4	0.79 (5)	2.40 (5)	2.999 (4)	134 (4)
O3—H8···O1^{iv}	0.78 (3)	1.93 (3)	2.704 (3)	175 (6)
O3—H9···O2^{v}	0.78 (3)	2.02 (3)	2.779 (4)	165 (5)
O4—H10···O2^{v}	0.78 (3)	2.02 (3)	2.774 (4)	162 (4)
O4—H11···O3^{vi}	0.77 (3)	2.08 (3)	2.797 (3)	157 (5)

Symmetry codes: (i) $-x, -y, -1-z$; (ii) $x-1, y, z$; (iii) $1-x, -y, -z$; (iv) $1-x, 1-y, -z$; (v) $x, y, 1+z$; (vi) $1+x, y, z$.

H-atom positional parameters were determined from difference electron-density maps, and refined isotropically [N—H 0.77 (5)–0.84 (4), O—H 0.77 (3)–0.78 (3) and C—H 0.98 (4)–1.13 (6) Å]. The H atoms of the water molecules were constrained using the *DFIX* (O—H = 0.82 Å) command of *SHELXL*97 (Sheldrick, 1997).

Data collection and cell refinement: *CAD*-4-*PC* (Enraf—Nonius, 1992); data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *DIRDIF*96 (Beurskens *et al.*, 1996); program(s) used to refine structure: *SHELXL*97 software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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