

μ -4,4'-Bipyridine- $\kappa^2N:N'$ -bis[aqua(4,4'-bipyridine- κN)(L-valinato- κ^2N,O)-copper(II)] dinitrate dihydrate

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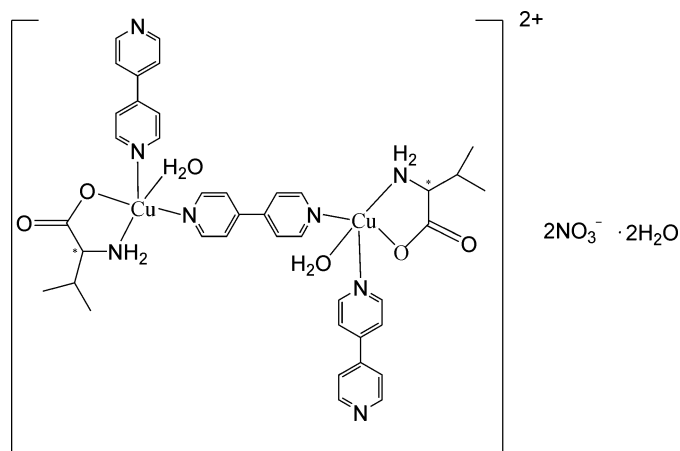
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.008$ Å; R factor = 0.035; wR factor = 0.087; data-to-parameter ratio = 11.3.

In the title dinuclear complex, $[Cu_2(C_5H_{10}NO_2)_2(C_{10}H_8N_2)_3 \cdot (H_2O)_2](NO_3)_2 \cdot 2H_2O$, each of the two L-valinate anions chelates a Cu^{II} center through the amino N and carboxylate O atom, forming a five-membered ring. A 4,4'-bipyridine molecule bridges two water-coordinated Cu atoms, each of which is connected to another 4,4'-bipyridine, giving rise to a square-pyramidal coordination geometry for the Cu^{II} centers. The dinuclear dications, nitrate anions and uncoordinated water molecules are linked into a two-dimensional structure.

Related literature

For background, see: Yamauchi *et al.* (2002).



Experimental

Crystal data

$[Cu_2(C_5H_{10}NO_2)_2(C_{10}H_8N_2)_3 \cdot (H_2O)_2](NO_3)_2 \cdot 2H_2O$

$M_r = 1024.00$
Triclinic, $P1$

$a = 8.9675$ (14) Å
 $b = 9.6545$ (16) Å
 $c = 13.9421$ (15) Å
 $\alpha = 91.533$ (5)°
 $\beta = 100.384$ (4)°
 $\gamma = 105.393$ (8)°

$V = 1141.2$ (3) Å³
 $Z = 1$
Mo $K\alpha$ radiation
 $\mu = 1.01$ mm⁻¹
 $T = 293$ (2) K
 $0.20 \times 0.15 \times 0.13$ mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
 $T_{min} = 0.824$, $T_{max} = 0.880$

8898 measured reflections
6761 independent reflections
5710 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.086$
 $S = 1.02$
6761 reflections
599 parameters
3 restraints

H-atom parameters constrained
 $\Delta\rho_{max} = 0.38$ e Å⁻³
 $\Delta\rho_{min} = -0.34$ e Å⁻³
Absolute structure: Flack (1983),
1599 Friedel pairs
Flack parameter: 0.006 (12)

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.937 (5)	Cu2—O4	1.944 (5)
Cu1—N4	1.993 (5)	Cu2—N2	1.967 (5)
Cu1—N1	2.011 (5)	Cu2—N3	2.001 (5)
Cu1—N5	2.031 (5)	Cu2—N7	2.028 (5)
Cu1—O3	2.275 (4)	Cu2—O6	2.308 (4)
O1—Cu1—N4	172.71 (19)	O4—Cu2—N2	84.0 (2)
O1—Cu1—N1	83.15 (19)	O4—Cu2—N3	171.74 (19)
N4—Cu1—N1	95.7 (2)	N2—Cu2—N3	95.2 (2)
O1—Cu1—N5	88.54 (19)	O4—Cu2—N7	89.66 (19)
N4—Cu1—N5	90.7 (2)	N2—Cu2—N7	165.8 (2)
N1—Cu1—N5	162.53 (18)	N3—Cu2—N7	89.2 (2)
O1—Cu1—O3	92.32 (18)	O4—Cu2—O6	92.17 (18)
N4—Cu1—O3	94.97 (18)	N2—Cu2—O6	95.07 (18)
N1—Cu1—O3	98.71 (17)	N3—Cu2—O6	96.10 (18)
N5—Cu1—O3	96.94 (17)	N7—Cu2—O6	97.82 (17)

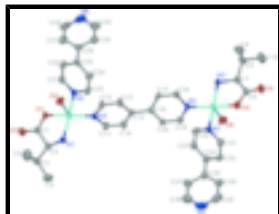
Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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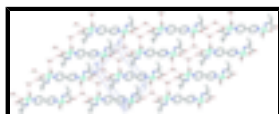
Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2423).

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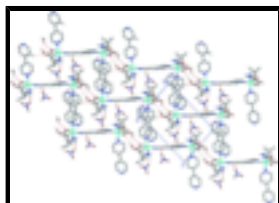
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