Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Diaquabis(propane-1,2-diamine-κ^2N,N')-copper(II) terephthalate dihydrate

Zhi-Dong Lin,[a]* Li-Ming Liu,[a,b] Jin-Yu Lu[a] and Xiang-Gao Meng[c]

[a]School of Materials Science and Technology, Wuhan Institute of Chemical Technology, Wuhan 430073, People's Republic of China, [b]School of Electronic Information and Control Engineering, Beijing Polytechnic University, Beijing 100022, People's Republic of China, and [c]Central China Normal University Wuhan, Wuhan 430073, People's Republic of China

Correspondence e-mail:
xianggao_meng@126.com

Received 30 November 2004
Accepted 26 January 2005
Online 26 February 2005

The title compound, $[Cu(C_3H_{10}N_2)_2(H_2O)_2](C_8H_4O_4)\cdot 2H_2O$, is a mononuclear complex. The Cu^{II} atom is coordinated by four N atoms from two 1,2-propanediamine ligands and two O atoms from two water molecules, to form a distorted octahedral geometry. All the N atoms of the 1,2-propanediamine ligands, and all the O atoms in the water molecules and terephthalate anions, contribute to the formation of a hydrogen-bonded three-dimensional network.

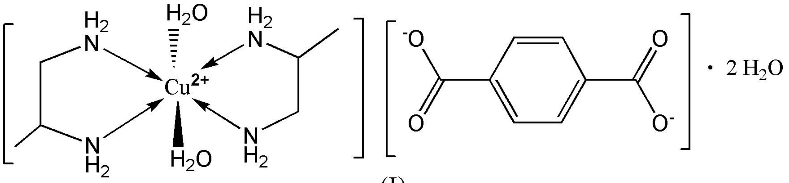
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.047
wR factor = 0.141
Data-to-parameter ratio = 17.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Amine complexes with transition metal carboxylates represent an important branch in the field of coordination chemistry. Diamine complexes have higher stability than monoamine complexes. We report here the crystal structure of the title compound, (I), a new Cu^{II} diamine complex.



(I)

The molecular structure of (I) is shown in Fig. 1. The asymmetric unit is composed of a Cu^{II} ion, two half-terephthalate anions, two propane-1,2-diamine ligands, two coordinated water molecules and two uncoordinated water molecules. The Cu^{II} ion is six-coordinate, and the coordination geometry can best be described as distorted octahedral. The square equatorial plane is defined by four N atoms from two propane-1,2-diamine ligands, each propane-1,2-diamine

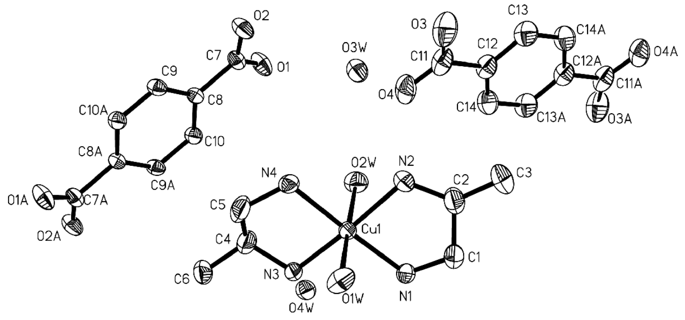


Figure 1
The molecular components of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms and the minor component of the disordered propane-1,2-diamine ligand have been omitted for clarity. Atoms with the suffix A are generated by the symmetry code ($\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$) in one of the terephthalate anions (O1) and ($1 - x, -x, 1 - z$) in the other.

© 2005 International Union of Crystallography
Printed in Great Britain – all rights reserved

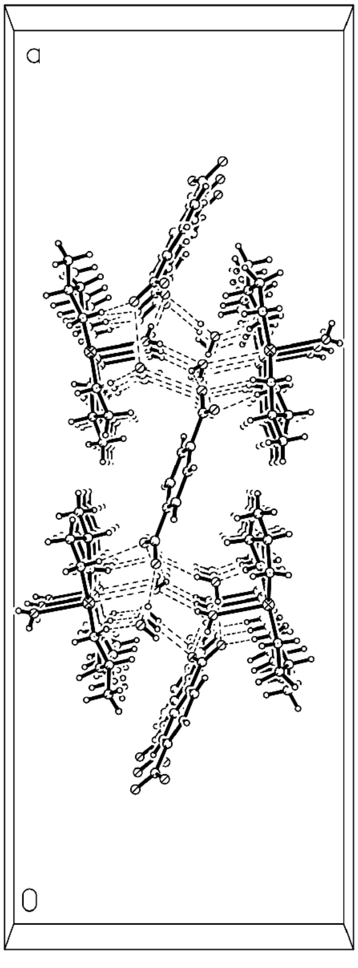


Figure 2
The crystal packing of (I) viewing along the *b* axis. The O—H···O and N—H···O hydrogen-bonding interactions are shown as dashed lines.

coordinating to the central Cu^{II} ion as a bidentate ligand. The two water molecules occupy the axial positions. The Cu—N distances, ranging from 2.000 (2) to 2.018 (2) Å, show normal values. In similar complexes, the Cu—N bond lengths lie in the range 2.00–2.05 Å (Li *et al.*, 1999; Procter *et al.*, 1968). The Cu—O1*W* distance of 2.377 (2) Å is consistent with other copper(II) complexes with water (Amirov *et al.*, 2003), but the Cu—O2*W* distance of 2.895 (3) Å is longer than the normal value and indicates weak coordination. N—H···O and O—H···O hydrogen bonds (Fig. 2) link the complex cations and anions of (I) into a three-dimensional network.

Experimental

CuO (1 mmol, 80 mg), terephthalic acid (2 mmol, 332 mg) and propane-1,2-diamine (2 mmol, 148 mg) were dissolved in aqueous ammonia (30 ml, 30%) and the mixture was stirred for 30 min at room temperature. The resulting clear blue solution was kept in air and after slow evaporation of the solvent over a period of a week, blue crystals of (I) were formed at the bottom of the vessel. The crystals were isolated and washed three times with water and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 38%). Analysis calculated for $C_{14}H_{30}CuN_4O_7$: C 39.11, H 7.03, N 13.03%; found: C 39.36, H 7.28, N 13.31%.

Crystal data

$[Cu(C_3H_{10}N_2)_2(H_2O)_2]$-$(C_8H_4O_4)\cdot 2H_2O$
$M_r = 447.98$
Monoclinic, $C2/c$
$a = 40.922$ (6) Å
$b = 6.8025$ (9) Å
$c = 15.151$ (2) Å
$\beta = 90.000$ (2)°
$V = 4217.7$ (10) Å^3
$Z = 8$
$D_x = 1.411$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 1200 reflections
$\theta = 2.3$–26.5°
$\mu = 1.08$ mm^{-1}
$T = 295$ (2) K
Block, blue
0.39 × 0.34 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.663$, $T_{max} = 0.748$
12723 measured reflections
4892 independent reflections
3976 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 28.3°$
$h = -53 \rightarrow 48$
$k = -8 \rightarrow 8$
$l = -19 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.141$
$S = 1.10$
4892 reflections
278 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0763P)^2 + 3.3497P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.97$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	2.000 (2)	Cu1—N2	2.018 (2)
Cu1—N4	2.009 (2)	Cu1—O1*W*	2.377 (2)
Cu1—N1	2.013 (2)	Cu1—O2*W*	2.895 (3)
N3—Cu1—N4	84.61 (9)	N1—Cu1—O1*W*	91.44 (9)
N3—Cu1—N1	96.55 (10)	N2—Cu1—O1*W*	96.38 (10)
N4—Cu1—N1	177.84 (9)	N3—Cu1—O2*W*	86.19 (9)
N3—Cu1—N2	171.85 (10)	N4—Cu1—O2*W*	92.57 (9)
N4—Cu1—N2	94.75 (10)	N1—Cu1—O2*W*	85.70 (9)
N1—Cu1—N2	83.84 (10)	N2—Cu1—O2*W*	85.72 (9)
N3—Cu1—O1*W*	91.75 (10)	O1*W*—Cu1—O2*W*	176.26 (8)
N4—Cu1—O1*W*	90.34 (9)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2*W*^{i}	0.83 (3)	2.15 (3)	2.932 (4)	156 (3)
N1—H1*A*···O3*W*^{i}	0.90	2.05	2.945 (4)	175
N1—H1*B*···O3^{ii}	0.90	2.15	3.039 (4)	167
O1*W*—H1*WB*···O2^{iii}	0.84 (3)	1.89 (4)	2.732 (4)	176 (4)
N2—H2*A*···O4	0.90	2.27	3.114 (4)	157
N2—H2*B*···O3*W*^{iii}	0.90	2.10	2.996 (4)	173
O2*W*—H2*WA*···O3^{ii}	0.85 (3)	2.01 (3)	2.813 (4)	158 (4)
N3—H3*A*···O4*W*	0.90	2.04	2.909 (3)	163
N3—H3*B*···O1^{i}	0.90	2.17	3.017 (3)	156
O2*W*—H2*WB*···O4	0.85 (4)	2.45 (3)	3.122 (4)	136 (4)
N4—H4*A*···O1^{iii}	0.90	2.22	3.115 (3)	177
N4—H4*B*···O4*W*^{iv}	0.90	2.08	2.924 (3)	155
O3*W*—H3*WA*···O4	0.83 (2)	2.06 (3)	2.814 (4)	150 (4)
O3*W*—H3*WB*···O1	0.83 (1)	1.91 (1)	2.741 (3)	175 (5)
O4*W*—H4*WA*···O2^{ii}	0.84 (3)	1.99 (3)	2.826 (3)	176 (2)
O4*W*—H4*WB*···O4^{ii}	0.83 (2)	1.90 (2)	2.706 (4)	163 (4)

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

Acta Cryst. (2005). E**61**, m590–m592 Lin *et al.* • $[Cu(C_3H_{10}N_2)_2(H_2O)_2](C_8H_4O_4)\cdot 2H_2O$ **m591**

One of the propane-1,2-diamine ligands was found to be disordered over two orientations related by a 180° rotation. The occupancies of the disordered positions C3 and C3′ were refined to 0.528 (9) and 0.472 (9), respectively. H atoms of the water molecules were located in a difference map and their positional parameters were refined with the O—H and H···H distances restrained to 0.84 (2) and 1.37 (2), respectively. The remaining H atoms were positioned geometrically and refined using a riding model, with N—H = 0.90 Å and C—H distances in the range 0.93–0.98 Å. The isotropic displacement parameters were set equal to $1.5U_{\rm eq}$(parent atom) for water and methyl H atoms and $1.2U_{\rm eq}$(parent atom) for remaining H atoms. The monoclinic β angle is very close to 90°. Cell refinement and data reduction were also carried out under orthorhombic symmetry, but no suitable orthorhombic space group was found.

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*.

The authors thank the Education Office of Hubei Province, People's Republic of China, for research grant No. 2004D007.

References

Amirov, R. R., Litvinov, I. A. Gubaidullin, A. T. & Matyugicheva, U. V. (2003). *Russ. J. Gen. Chem.* **73**, 1860–1865.

Li, B.-L., Xu, Z., Cao, Z.-B., Zhu, L.-M. & Yu, K.-B. (1999). *Transition Met. Chem.* **24**, 622–627.

Procter, I. M., Hathaway, B. J. & Nicholls, P. (1968). *J. Chem. Soc. A*, pp. 1678–1682.

Sheldrick, G. M. (1996). *SADABS.* University of Göttingen, Germany.

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

m592 Lin *et al.* • $[\mathrm{Cu(C_3H_{10}N_2)_2(H_2O)_2}](\mathrm{C_8H_4O_4})\cdot 2\mathrm{H_2O}$ *Acta Cryst.* (2005). E**61**, m590–m592