metal-organic papers

# Di-μ-iodoacetato-bis[(2,2′-bipyridyl)(iodo-acetato)copper(II)] hemihydrate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.011 Å
Disorder in solvent or counterion
R factor = 0.047
wR factor = 0.131
Data-to-parameter ratio = 14.1

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

The title compound, $[Cu_2(C_2H_2IO_2)_4(C_{10}H_8N_2)_2]\cdot0.5H_2O$, is a copper(II) dimer, in which two Cu atoms are joined by two oxo bridges of iodoacetate groups. The distorted square-pyramidal environment of each Cu atom is completed by two N atoms of the 2,2′-bipyridine ligands (bpy), one iodoacetate O atom and two bridging iodoacetate O atoms. The dimer lies on an inversion center midway between the two Cu atoms.

Comment

The chemistry of copper complexes is of interest owing to their importance in biological and industrial processes. Mitchell and co-workers have reported that electronic effects such as favorable interactions between π-systems, between hydrophobic systems and between oppositely charged side groups contribute to the stability of metal complex structures (Mitchell & Sigel, 1978). The 2,2′-bipyridine ligand has been used in model complexes to mimic the non-covalent inter-actions in biological processes (Cravena *et al.*, 2003). Thus we designed and synthesized the title Cu complex, (I).

(I)
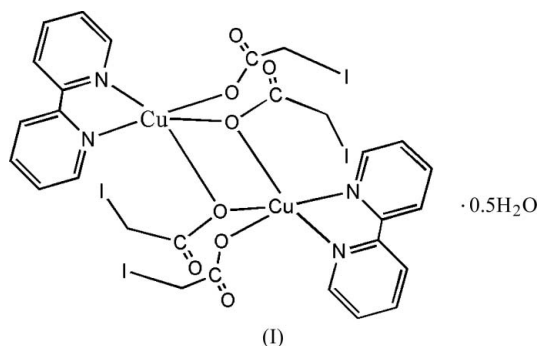
Each Cu^{II} ion of (I) exhibits a distorted square-based pyramidal geometry, CuN_2O_3, in identical environments, and the two Cu^{II} ions are bridged by two iodoacetate O atoms (Fig. 1). In each coordination environment, two N atoms of the 2,2′-bipyridine ligand, one iodoacetate O atom and one brid-ging iodoacetate O atom constitute the basal plane. The dimer lies on an inversion center located midway between the two Cu atoms, $[Cu\cdots Cu = 3.391\,(9)$ Å]. The Cu—O—Cu angle is 101.54 (18)°. The atom sequence $Cu1—O1—Cu1^i—O1^i$ [symmetry code: (i) $-x, -y, -z$] is a rather regular paralle-logram, with Cu1—O1 and $Cu1—O1^i$ distances of 1.976 (4) and 2.390 (5) Å, respectively. Water molecules are cocrys-tallized, forming O—H⋯O hydrogen bonds with $R_2^2(10)$ motifs (Etter *et al.*, 1990). Intermolecular C—H⋯O hydrogen bonds are also detected, and they play key roles in stabilizing the crystal packing. Details of the hydrogen-bond geometry is given in Table 2.
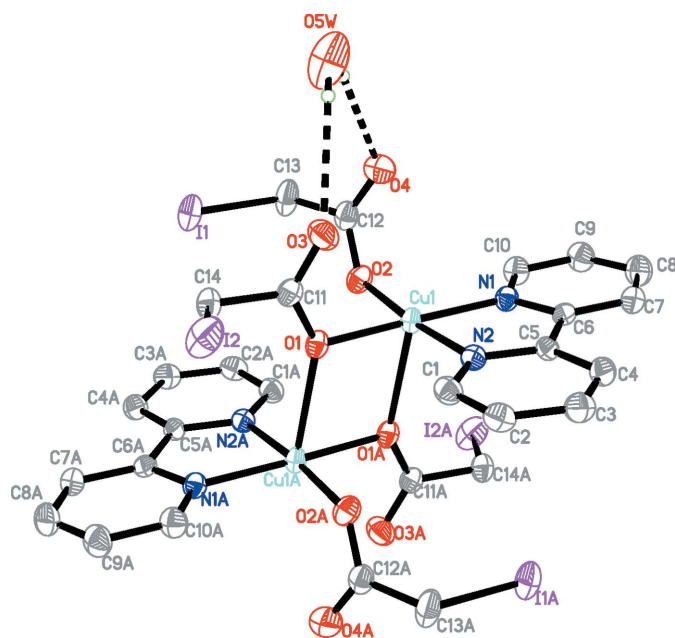
Figure 1
The structure of the title compound, with 30% probability displacement ellipsoids. H atoms have been omitted for clarity except for water H atoms. [Symmetry code: (A) −x, −y, −z.]

Experimental

All chemicals were of reagent grade and commercially available from the Beijing Chemical Reagents Company of China, and were used without further purification. At room temperature, an aqueous solution (5 ml) of $CuCl_2·2H_2O$ (0.1094 g, 0.64 mmol) was added dropwise to an aqueous solution (5 ml) of Na_2CO_3 (0.0848 g, 0.8 mmol), yielding a pale-blue deposit, which was separated by centrifugation and washed with distilled water four times. The precipitate was then dispersed in a water/methanol (1:1 v/v) solution, and bipyridine (0.0936 g, 0.6 mmol) was added and the mixture was stirred for 10 min. Subsequently, iodoacetic acid (0.2232 g, 1.2 mmol) was added and the precipitate dissolved slowly, forming a blue solution. Blue crystals were collected after the solution had been allowed to evaporate slowly for one week at room temperature.

Crystal data

$[Cu_2(C_2H_2IO_2)_4(C_{10}H_8N_2)_2]$·· $0.5H_2O$	$\gamma = 95.205\ (4)°$
$M_r = 1197.21$	$V = 894.5\ (6)\ \text{Å}^3$
Triclinic, $P\bar{1}$	$Z = 1$
$a = 9.447\ (3)$ Å	$D_x = 2.223\ \text{Mg m}^{-3}$
$b = 9.631\ (4)$ Å	Mo $K\alpha$ radiation
$c = 10.410\ (4)$ Å	$\mu = 4.69\ \text{mm}^{-1}$
$\alpha = 93.485\ (4)°$	$T = 298\ (2)$ K
$\beta = 107.740\ (5)°$	Block, blue
	$0.50 \times 0.40 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	3664 measured reflections
	3076 independent reflections
φ and ω scans	2745 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2000)	$R_{int} = 0.026$
$T_{min} = 0.119$, $T_{max} = 0.625$	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.047$	$+ 4.6211P]$
$wR(F^2) = 0.131$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3076 reflections	$\Delta\rho_{max} = 1.46\ \text{e Å}^{-3}$
218 parameters	$\Delta\rho_{min} = -0.99\ \text{e Å}^{-3}$
H-atom parameters constrained	Extinction correction: SHELXL97
	Extinction coefficient: 0.0058 (9)

Table 1
Selected geometric parameters (Å, °).

Cu1—O2	1.939 (5)	Cu1—N1	2.006 (5)
Cu1—O1	1.976 (4)	Cu1—O1^i	2.390 (5)
Cu1—N2	1.998 (5)		
O2—Cu1—O1	88.3 (2)	N2—Cu1—N1	80.8 (2)
O2—Cu1—N2	174.6 (2)	O2—Cu1—O1^i	90.21 (19)
O1—Cu1—N2	94.3 (2)	O1—Cu1—O1^i	78.46 (18)
O2—Cu1—N1	96.4 (2)	N2—Cu1—O1^i	94.95 (19)
O1—Cu1—N1	175.0 (2)	N1—Cu1—O1^i	102.97 (19)

Symmetry code: (i) −x, −y, −z.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C4—H4⋯O3^{ii}	0.93	2.52	3.387 (9)	155
C3—H3⋯O4^{ii}	0.93	2.41	3.139 (10)	135
C2—H2⋯O4^{iii}	0.93	2.51	3.430 (10)	172
O5W—H52⋯O3	0.76	2.69	3.252 (13)	132
O5W—H51⋯O4	0.82	2.30	2.874 (12)	127

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

Water H atoms were located in a difference Fourier map and their positions and isotropic displacement parameters were refined, with O—H restraints which led to O—H values in the range 0.82–0.83 Å. All other H atoms were positioned geometrically, treated as riding atoms and refined isotropically, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The highest residual electron-density peak is located near the I2 atom. The disorded water O atom was refined with a site-occupancy factor of 0.5.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXTL.

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