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Crystal Structure
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Cadmium copper tetrachloride tetrahydrate

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The double salt $[CuCl_2(H_2O)_2\{CdCl_2\}]\cdot 2H_2O$ crystallizes in the triclinic rather than the monoclinic system as reported previously. The structure consists of sheets in the *ac* plane with slightly distorted octahedral $CdCl_6$ [Cd—Cl 2.5813 (8)–2.6943 (8) Å] connected by Cd—Cl—Cd bridges in the Cd equatorial plane along **a**, and by Cd—Cl—Cu bridges to layers of square-planar $CuCl_2(H_2O)_2$ along **c**. There are long axial Cu—Cl interactions of 2.8623 (7) Å and additional water of hydration is hydrogen bonded to coordinated water and chloride ligands. The additional water connects the *ac* sheets into a three-dimensional network. Both Cd and Cu occupy different $P\overline{1}$ sites. The Cu···Cu and Cd···Cd distances are 3.8274 (6) Å.

Comment

The structural analysis of the title salt was performed in support of an examination of its magnetic behavior. A previous Weissenberg camera diffraction study using Cu radiation (Thrierr-Sorel *et al.*, 1969) indicated a C-centered monoclinic cell. In contrast, we find the structure to be triclinic with a cell one-quarter the volume of that reported earlier. The green columnar crystals tend to twin and only parallelepiped-shaped crystals were indexed successfully.

The title structure (Fig. 1) consists of approximately octahedral $CdCl_6$ linked into a linear polymer by double Cl bridges running along **a**. The Cl—Cd—Cl angles are within 8° of 90 or 180°. The axial Cl ligand bridges to Cu, which forms square-planar $CuCl_2(H_2O)_2$, and these Cl bridges connect the Cd and Cu atoms into sheets in the *ac* plane (Fig. 2). Cl1 also forms a long interaction with a neighboring Cu atom with an axial Cu—Cl distance of 2.8623 (7) Å. Angles around copper are within 6° of 90 or 180°. The water coordinated to Cu is hydrogen bonded to non-coordinated lattice water, which is in turn hydrogen bonded to Cl2. These hydrogen bonds connect the sheets along the *b* direction to form a three-dimensional network. The Cu and Cd atoms occupy different $P\overline{1}$ sites such that the closest Cd···Cd and Cu···Cu distances are both one-unit translations along the *a* axis, *i.e.* 3.8274 (6) Å.

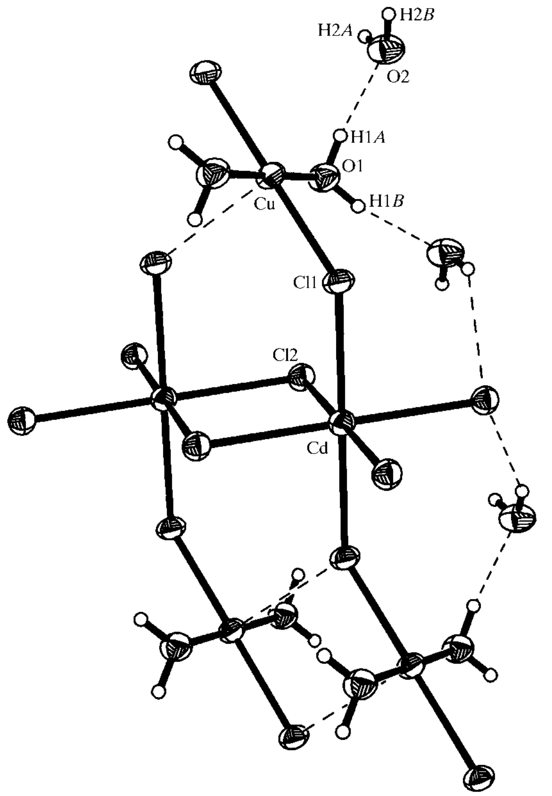

Figure 1
View of the title compound showing the numbering scheme and 50% probability ellipsoids.

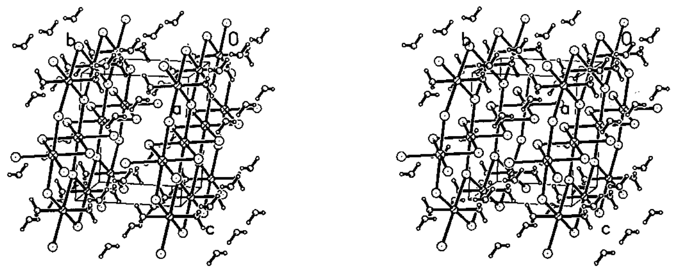

Figure 2
Stereopacking diagram viewed along the *a* axis with *c* down and *b* to the left.

Experimental

The $CdCl_2$–$CuCl_2$–H_2O system has been explored previously (Bassett & Strain, 1952). Crystals were obtained after about four weeks by evaporation from a solution containing $CuCl_2\cdot 2H_2O$ (18.75 g, 0.11 mol) and $CdCl_2$ (9.17 g, 0.05 mol) dissolved in H_2O (20 ml).

Crystal data

$[CuCl_2(H_2O)_2\{CdCl_2\}]\cdot 2H_2O$
$M_r = 389.80$
Triclinic, $P\overline{1}$
$a = 3.8274$ (6) Å
$b = 7.1591$ (11) Å
$c = 8.7756$ (13) Å
$\alpha = 87.595$ (2)°
$\beta = 82.735$ (2)°
$\gamma = 75.639$ (2)°
$V = 231.06$ (6) Å^3

$Z = 1$
$D_x = 2.801$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2232 reflections
$\theta = 5.88$–56.58°
$\mu = 5.716$ mm^{-1}
$T = 299$ (2) K
Column, green
0.38 × 0.10 × 0.05 mm

Data collection

CCD area-detector diffractometer	1033 reflections with $I > 2\sigma(I)$
ω scans	$R_{\rm int} = 0.028$
Absorption correction: multi-scan (Blessing, 1995)	$\theta_{\max} = 28.29°$
$T_{\min} = 0.475$, $T_{\max} = 0.810$	$h = -5 \rightarrow 5$
2771 measured reflections	$k = -9 \rightarrow 9$
1094 independent reflections	$l = -11 \rightarrow 11$
	Intensity decay: see below

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.0268P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.027$	$(\Delta/\sigma)_{\max} < 0.001$
$wR(F^2) = 0.071$	$\Delta\rho_{\max} = 0.646$ e Å^{-3}
$S = 1.074$	$\Delta\rho_{\min} = -0.837$ e Å^{-3}
1094 reflections	Extinction correction: *SHELXL*97
66 parameters	Extinction coefficient: 0.417 (14)
All H-atom parameters refined	

Crystal decay was monitored by recollection of the first 50 frames periodically throughout the data collection. No decay was observed. H atoms were refined isotropically from observed positions.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SHELXTL* (Sheldrick, 1997*a*); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BR1267). Services for accessing these data are described at the back of the journal.

Table 1
Selected geometric parameters (Å, °).

Cd—Cl2	2.5813 (8)	Cl1—Cu	2.3139 (7)
Cd—Cl2$^{\rm i}$	2.6303 (7)	Cu—O1	1.935 (2)
Cd—Cl1	2.6943 (8)	Cu—Cl1$^{\rm ii}$	2.8623 (7)
Cu—Cl1—Cd	130.99 (3)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2	0.85 (5)	1.87 (5)	2.718 (4)	174 (4)
O1—H1B···O2$^{\rm i}$	0.82 (5)	1.95 (5)	2.752 (4)	165 (5)
O2—H2A···O1$^{\rm ii}$	0.76 (7)	2.57 (6)	3.050 (4)	124 (6)
O2—H2A···Cl2$^{\rm ii}$	0.76 (7)	2.66 (7)	3.259 (3)	138 (6)
O2—H2B···Cl2$^{\rm iii}$	0.85 (8)	2.46 (8)	3.269 (3)	158 (6)

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

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