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An orthorhombic modification of lithium chloride monohydrate

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The structure of the title compound, $LiCl{\cdot}H_2O$, has already been determined three times. Interestingly, the different authors found different cell parameters and space groups. We present here an orthorhombic modification.

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(Li–O) = 0.0008 Å
R factor = 0.019
wR factor = 0.047
Data-to-parameter ratio = 14.0

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

Comment

The structure of the title compound, $LiCl{\cdot}H_2O$, has already been determined three times: Ott (1926) determined the structure by powder diffraction and reported a cubic cell with a = 3.830 Å and V = 56.2 $Å^3$ in $Pm\overline{3}m$; Datt *et al.* (1971) investigated $LiCl{\cdot}D_2O$ and found similar cell parameters ($a = b$ = 3.810 Å, c = 3.880 Å and V = 56.3 $Å^3$) but the tetragonal space group $P4/m$; Weiss *et al.* (1969) employed powder diffraction and obtained a bigger cell ($a = b$ = 7.669 Å, c = 7.742 Å and V = 455.3 $Å^3$) and a different tetragonal space group ($P4_2/nmc$). We report here an orthorhombic modification of $LiCl{\cdot}H_2O$ (Fig. 1) with the space group $Cmcm$.

The asymmetric unit comprises half a Cl anion on a mirror plane perpendicular to the c axis, half an O atom on a mirror plane perpendicular to the a axis, one H atom in a general position and two Li cations with one-quarter occupancy on $2/m..$ (Li1) and $m2m$ (Li2). The Cl anion is approximately octahedrally coordinated, with Li2 and its symmetry-equivalent in axial positions and Li1 and H1 and their symmetry-equivalents in the equatorial plane. The Li cations are also octahedrally coordinated, with Cl anions in the equatorial plane and two water molecules in axial positions. Apart from coordinating to Li the water molecules link two Cl anions by hydrogen bonds.

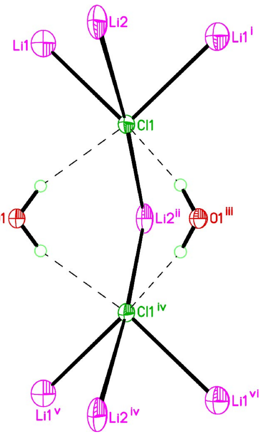

Figure 1
Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. [Symmetry codes: (i) $x, y, -z + \frac{1}{2}$; (ii) $x - \frac{1}{2}, y - \frac{1}{2}, z$; (iii) $x, y, -z + \frac{1}{2}$; (iv) $-x, y, z$; (v) $x - 1, y, z$; (vi) $x - 1, y, -z + \frac{1}{2}$.]

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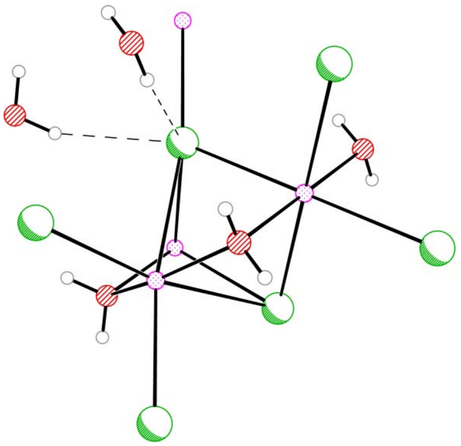

Figure 2
Perspective view of the title compound, showing the octahedral coordination of the Cl and Li ions. Colour scheme: Li pink, Cl green, O red, and H gray.

Unfortunately, Ott (1926) has not published the coordinates of the Li atom and Weiss *et al.* (1969) stated that the Li ion is disordered over three sites. Therefore, these two structures cannot be compared directly with the one we have determined. The fact that the cell parameters of Weiss *et al.* are so similar to those which we have determined leads us to assume that the structure of Weiss *et al.* is wrong. The cell parameter of Ott is approximately half as long as we determined for the three axes. Since the structure determination of Ott has also been performed by powder diffraction, we assume that this structure is also wrong. The third determination, by Datt *et al.* (1971), gives a dubious position for the D atom, leading to an Li$\cdots$D distance of just 1.570 Å. Whereas the coordination of their Li ion is similar to that which we found (the Li ion is hexacoordinated by four Cl ions and two water molecules), their Cl ion is coordinated by eight Li ions (Cl$\cdots$Li = 2.708 Å) and eight water molecules (Cl$\cdots$O = 3.317 Å). For the same reasons which we have stated for the structure of Ott, we propose that the structure of Datt *et al.* is also incorrect.

Experimental

X-ray quality crystals of the title compound were obtained after recrystallization from water at ambient temperature.

Crystal data

$LiCl\cdot H_2O$
$M_r = 60.41$
Orthorhombic, *Cmcm*
$a = 7.6259$ (13) Å
$b = 7.7107$ (16) Å
$c = 7.6592$ (13) Å
$V = 450.37$ (14) Å^3
$Z = 8$
$D_x = 1.782$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11303 reflections
$\theta = 3.1$–$29.4°$
$\mu = 1.27$ mm^{-1}
$T = 173$ (2) K
Block, colourless
0.25 × 0.23 × 0.21 mm

Data collection

Stoe IPDS–II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 1990; Blessing, 1995)
$T_{\min} = 0.742$, $T_{\max} = 0.777$
3852 measured reflections
349 independent reflections
325 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.049$
$\theta_{\max} = 29.2°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.047$
$S = 1.13$
349 reflections
25 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.43$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

$O1—Li2^{i}$	1.9943 (9)	$Cl1—Li1^{iv}$	2.6444 (4)
$O1—Li1^{ii}$	2.0405 (8)	$Cl1—Li1$	2.6444 (4)
$Cl1—Li2^{iii}$	2.572 (2)	$Cl1—Li2$	2.880 (2)
$Li2^{iii}—Cl1—Li2$	168.07 (9)		

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

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
$O1—H1\cdots Cl1$	0.829 (13)	2.396 (14)	3.1875 (7)	159.9 (12)

The H atom was located by difference Fourier synthesis and was refined isotropically.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991).

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