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The crystal structure of lithium acetate dihydrate $CH_3COOLi.2H_2O$.

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Lithium acetate dihydrate belongs to the orthorhombic class (Groth). Rotation and Weissenberg photographs taken around the three axes gave

$$a = 6{\cdot}86,\quad b = 11{\cdot}49 \quad\text{and}\quad c = 6{\cdot}59\ \text{Å}\,,$$

giving

$$a{:}b{:}c = 0{\cdot}60{:}1{:}0{\cdot}57\ .$$

Groth's value is 0·62 : 1 : –.

The density is found to be 1·30 g.cm.$^{-3}$ (flotation method) giving four molecules per unit cell.

The extinctions lead to the space groups *C*222, *Cmm*2 and *Cmmm*, but packing considerations of the four acetate ions uniquely fix the space group as *Cmm*2. The multiple-film technique was used to obtain intensity data with Cu $K\alpha$ radiation. The intensity values were corrected for all factors and were put to absolute scale by Wilson's method.

The four acetate ions were placed on the four-fold special positions $(0, y, z)$ as the other set $(x, 0, z)$ was found to be untenable. Similarly the four lithium atoms were found to occupy the positions $(x, 0, z)$. The eight water molecules occupy the general positions, the approximate positions being fixed by Patterson's method. The final structure was obtained after a series of trial and error and Fourier refinements. The mean reliability factor for $(h0l)$, $(0kl)$ and $(hk0)$ reflections is 0·18 (hydrogen contribution neglected). The atomic coordinates, bond lengths and angles are listed in Table 1.

As reported on zinc acetate (Niekerk, Schoening & Talbot, 1953), lithium acetate also exhibits a 'two-dimensional sheet' structure. The acetate ions are separated along *a* by *a*/2 and linked by weak hydrogen bonds of the water molecules (hydrogen-bond linkage 3·08 Å and 3·14 Å) and along *c* by the *c* spacing. Along *b* the nearest distance is 3·68 Å and along *c* 3·87 Å. Such weak forces account for the low melting point of the crystal. Lithium is surrounded by six oxygens, four of which belong to the acetate ions and the two other to the water molecules.

Table 1 *Atomic coordinates, bond lengths and angles*

Atomic parameters

	x	*y*	*z*
C_1	0	0·325	−0·248
C_2	0	0·272	−0·032
O_1	0	0·334	0·118
O_2	0	0·156	0·005
H_2O	0·156	0·140	0·452
Li	0·162	0	0·147

Bond distances and angles

C_1–C_2	1·55 Å	Li–O_2	2·27 Å
C_2–O_1	1·22	Li–H_2O	2·57
C_2–O_2	1·33	$\sphericalangle$ O_1–C_2–O_2	119° 24′

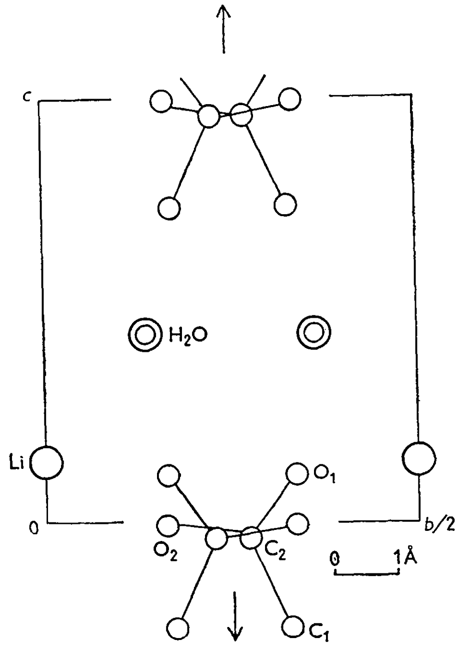

Fig. 1. The crystal structure of CH_3COOLi, 2 H_2O viewed down the *a*-axis.

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Redetermination of the oxygen parameters in zircon ($ZrSiO_4$).

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The crystal structure of zircon has been determined by Vegard (1926), Hassel (1926) and Wyckoff & Hendricks (1927), the results being in fairly good agreement. Since zircon is one of the first minerals on which the metamict state has been studied, and since the bond lengths in this structure have been used in the discussion of the nature of the metamict state, it appeared worth while to redetermine the oxygen parameters in this structure.