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Crystal data for $Zn(NO_3)_2 . 4H_2O$ and $Zn(NO_3)_2 . 2H_2O$.

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Unit-cell dimensions and space groups for $Zn(NO_3)_2.2H_2O$ and $Zn(NO_3)_2.4H_2O$ have been determined on the basis of rotation and Weissenberg photographs. Crystals of $Zn(NO_3)_2.4H_2O$ are isostructural with $Ni(NO_3)_2.4H_2O$.

As a part of our interest in nitrate hydrates of bivalent metals, we have examined crystals of zinc nitrate tetrahydrate and zinc nitrate dihydrate. Both compounds were prepared by methods already described (Mellor, 1952). The crystallization was performed in a dessicator over calcium-chloride or phosphorus pentoxide. The crystals obtained were colorless and quite hygroscopic monoclinic prisms. For further examination the crystals were sealed in capillary tubes. Crystal data, as determined from the analysis of rotation and Weissenberg photographs, are listed in Table 1 along with the data for $Ni(NO_3)_2 . 4H_2O$ (Gallezot, Weigel & Prettre, 1967) for comparison. The densities were determined by flotation in bromoform–ethyl iodide.

Similar values of lattice constants and the same space-group extinctions for zinc nitrate tetrahydrate and nickel nitrate tetrahydrate, whose crystal structure was solved recently (Gallezot *et al.*, 1967) suggest either isomorphism or close relationship of their structures. The determination of the crystal structure of $Zn(NO_3)_2 . 2H_2O$ is in progress.

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Table 1. *Crystal data*

	a (Å)	*b* (Å)	*c* (Å)	*β*	*V* (Å³)	*Z*	Space group	D_m (g.cm⁻³)	D_x (g.cm⁻³)	Reference
$Zn(NO_3)_2.2H_2O$	5·754 ±0·006	5·978 ±0·005	8·557 ±0·005	91°2′ ±20′	294·34	2	$P2_1/c$	2·50	2·54	This work
$Zn(NO_3)_2.4H_2O$	5·321 ±0·003	27·36 ±0·02	5·730 ±0·003	113°40′ ±20′	764·03	4	$P2_1/n$	2·22	2·27	This work
$Ni(NO_3)_2.4H_2O$	5·305 ±0·01	27·24 ±0·03	5·705 ±0·01	114° ±20′	753	4	$P2_1/n$	2·21	2·24	Gallezot *et al.* (1967)

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An I.C.T. Fortran program for least-squares refinement of crystal-structure cell dimensions.

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A computer program is described for the accurate calculation of unit-cell dimensions when the 'd_{hkl}' values (or simply line positions) and *hkl* indices are known. A weighted least-squares extrapolation method is used with provision for an eccentricity correction. The cubic, tetragonal, hexagonal, rhombohedral and orthorhombic crystal systems are included, and both single-crystal and powder data are acceptable. Various forms of data input and output are available.

The program was designed to be as general as possible whilst remaining simple to use. The crystal systems included are cubic, tetragonal, hexagonal, rhombohedral and orthorhombic. The rhombohedral indices must be referred to hexagonal axes. The input data required are the *hkl* indices and either 'd_{hkl}' values or 'line positions'. This latter can be in the form of 2θ values, or distances measured on the film from some arbitrary origin. Although the program was designed primarily for measurements made on films mounted in the Straumanis setting, it may be used without change with other film arrangements.

The calculation is made with each reflexion weighted according to the scheme suggested by Hess (1951)

$$w=1/[\sin^2(\pi-2\theta)]\,.$$

Using the Nelson & Riley (1945) function to allow for the effect of absorption and beam divergence on the measurements, it can be shown that