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Crystallographic data for sodium acetate trihydrate, sodium acetate tetrahydrate, and 2,5-bis(benzylidene)-cyclohexanone.

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Cell constants and space groups have been determined for single crystals of $CH_3COONa.3H_2O$, $CH_3COONa.4H_2O$, and $C_{20}H_{18}O$.

Table 1. *Crystal data*

	$CH_3COONa.3H_2O$*	$CH_3COONa.4H_2O$	$2,5\text{-}(C_6H_5CH{:})_2C_6H_6O$
a	12·475 (2)	11·788 (5)	10·40 (1)
b	10·407 (3)	8·671 (7)	18·24 (1)
c	10·449 (3)	7·754 (5)	9·50 (1)
β	112·65 (5)	116·44 (7)	121·7 (1)
D_o	1·45	1·44	1·185
D_c	1·45	1·44	1·19
Z	8	4	4
Space group	$C2/c$	$P2_1$ or $P2_1/m$	$P2_1/n$ $P2_1$

* Data for sodium acetate trihydrate has been reported by Padmanabhan (1952). He concluded that the space group was $C2/m$, but the $h0l$ reflexions are absent for $l=2n+1$ showing the presence of a c glide.

Sodium acetate crystallizes from water either as small hexagons or as large plates. All crystals are hygroscopic. The hexagons appear to be the trihydrate and the plates the tetrahydrate.

Cell constants were determined from rotation and zerolevel Weissenberg photographs calibrated with Al powder lines (λ Cu $K\alpha=1{\cdot}5418$ Å). Densities were found by flotation. The results are summarized in Table 1. No further work is planned on these compounds.

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Reference

PADMANABHAN, V. M. (1952). *Curr. Sci.* **21**, 97.

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The crystal structure of HgIn.

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The crystal structure of HgIn has been redetermined. HgIn is of the ordered CuPt–$L1_1$ type, space group $R\bar{3}m$, with $a=4{\cdot}84_6$ Å and $\alpha=43{\cdot}2_4°$.

In a recent paper, Mascarenhas (1970) describes the compound HgIn (see Elliott, 1965) as rhombohedral, α-Hg–$A10$ type, with 1 atom per cell and $a=3{\cdot}008$ Å, $\alpha=73°20'$. HgIn would then differ from α-Hg only by a small increase of the angle α [α(Hg) = 70°30'] and would constitute an almost unique case – a disordered intermetallic phase with a very narrow homogeneity range of simple stoichiometry.

A reinvestigation of the structure of HgIn in the course of a study of stable and metastable HgIn phases has now shown HgIn to be ordered. Liquid HgIn alloys were deposited on Cu substrates by the splat quenching technique (Duwez, 1966; Giessen & Willens, 1969) and were examined at −196°C on an X-ray diffractometer, as described in detail earlier (Giessen, Morris & Grant, 1967). No contamination from ice, frozen CO_2, or other Hg–In phases was present. The powder pattern (Table 1) was indexed as rhombohedral, CuPt–$L1_1$ type (Smithells, 1967), space group $R\bar{3}m$ with

$a=4{\cdot}84_6\pm0{\cdot}005$ Å and $\alpha=43{\cdot}2_4\pm0{\cdot}04°$, and
1 Hg in (a): 000; 1 In in (b): $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

This yields an average atomic volume of $48{\cdot}4_2$ Å^3 and a density of 10·81 g.cm^{-3}. The agreement of the intensities in Table 1 is satisfactory, with two exceptions:

(a): Of the six observed lines due to ordering (superstructure lines with $h+k+l=2n+1$ and $F=f_{Hg}-f_{In}$), at least four (111, 100, 210, and 320) are too weak. [The intensity of a further superstructure line (322) cannot be considered since it is enhanced by texture; see (b)]. The reduced intensities may be due to some residual disorder; for the first two lines (110 and 100), there is probably a low-angle absorption error due to finite sample size.