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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-$(C_6H_5CH:)_2C_6H_6O$
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 $K\alpha=1·5418$ 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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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 $R\overline{3}m$, with $a=4·84_6$ Å and $\alpha=43·2_4$°.

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 $a=3·008$ 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 $R\overline{3}m$ with

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

This yields an average atomic volume of $48·4_2$ 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 $F=f_{\rm Hg}-f_{\rm In}$), 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.

Table 1. *X-ray Diffraction pattern of* HgIn (– 196°C)

		d (Å)		*I*	
*hkl**	*hkl*†	Obs.	Calc.	Obs.	Calc.
111	—	4·375	4·386	3·4	6·4
100	—	3·090	3·011	2·4	7·8
110	100	2·804	2·799	298‡	100·0
211	110	2·243	2·253	54·2	54·2
222	111	2·176	2·193	14·0	16·8
221	—	2·006	2·004	3·0	3·0
$1\bar{1}0$	$\bar{1}10$	1·786	1·786	25·6	26·7
210	—	1·656	1·654	2·4	3·0
322	—	1·599	1·606	3·3‡	1·4
$11\bar{1}$	—		1·536	–	1·2
200	$11\bar{1}$	1·505	1·505	17·0	15·4
333	—		1·462	1·2	1·0
332	211	1·448	1·452	11·4	13·7
220	200	1·400	1·399	20·0‡	12·1
321	210	1·384	1·385	20·0	23·4
311	—		1·333	–	0·8
433	221	1·201	1·211	5·7	7·7
331	—		1·194	–	0·6
$\bar{2}10$	—		1·164	–	1·0
$21\bar{1}$	$2\bar{1}0$	1·150	1·151	14·0	13·4
432	—		1·131	–	1·0
422	220	1·124	1·127	5·7	6·3
443	—		1·116	–	0·5
310	$2\bar{1}1$	1·099	1·101	14·2	12·0
444	222	1·098	1·096	5·1	6·0
320	—	1·070	1·068	6·0	8·8
$2\bar{1}\bar{1}$	$\bar{2}11$	1·031	1·031	4·0	5·3

* Rhombohedral, 2 atoms/cell (this work). Lines with $h+k+l$ odd are superstructure lines and cannot be indexed in terms of the rhombohedral cell with 1 atom/cell.

† Rhombohedral, 1 atom/cell (Mascarenhas, 1970).

‡ Intensity enhanced by texture.

(*b*) Texture effects common in quenched foils (Giessen, Morris & Grant, 1967) occur. After quenching, there was a strong (110) texture (closepacked planes); on annealing the foil at ~ –40°C, there was a change to a pronounced (222) texture. Since unfortunately the textured (110) is also the plane of highest reflected intensity, the comparison of intensities for a quenched foil was carried out by matching $I(211)_{\text{obs}}$ and $I(211)_{\text{calc}}$.

As seen in Table 1, the superstructure lines cannot be indexed in terms of a smaller rhombohedral cell with 1 atom per cell and $a = 3{\cdot}01_2$ Å, $\alpha = 72{\cdot}7_8^{\circ}$. This cell corresponds to that of Mascarenhas (1970) who failed to observe these relatively weak lines. The correct rhombohedral cell is equivalent to a hexagonal cell with 6 atoms per cell and $a = 3{\cdot}57_2$, $c = 13{\cdot}16_8$. The intensities of the order lines did not change appreciably over the temperature range – 196°C to > – 56°C, which includes the temperature of – 75°C (Mascarenhas, 1970). HgIn melts at – 18°C.

The observed unit cell could alternately be of lower symmetry: *R*3*m*, with Hg in (*a*) $(x_1x_1x_1)$ with $x_1 \simeq 0$ and In in 1(*a*): $(x_2x_2x_2)$ with $x_2 \simeq 0{\cdot}5$. Calculations with $x_2 < 0{\cdot}5$ lead to progressively poorer intensity agreement for the weak lines; this confirms the high-symmetry structure assumed above.

The closest interatomic distances are:

$$d(\text{Hg–Hg}) = d(\text{In–In}) = 3{\cdot}57_2 \text{ Å},$$
$$d(\text{Hg–In}) = 3{\cdot}01_2 \text{ Å}.$$

Thus, unlike (first nearest) neighbors in alternating layers are considerably closer than like (second-nearest) neighbors within each layer.

The structure of HgIn is a superstructure based on the *A*10–Hg type in the same way in which the structure of CuPt is a superstructure based on the A1–Cu type; both structures differ from the parent types by small changes of the rhombohedral angle occurring upon ordering on alternate close-packed planes. Crystal-chemically, phases of the *A*1, *A*6, or *A*10 types and their superstructures would be expected for Hg–In phases; the prevalence of the *A*1 type and its distortion variants in stable or metastable *B* metal alloys with ~2·3 to >3 valence electrons per atom has been demonstrated (Giessen, 1969). Indeed, metastable Hg–In phases show further, complex distortions of the α-Hg type.

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Lattice parameters and space groups of the acetates of IVb group elements.

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Lattice parameters and space groups of the acetates of IVb group elements are recorded. Crystals of tin(IV) acetate are isostructural with lead(IV) acetate.

The crystals of silicon(IV) acetate, germanium(IV) acetate, tin(IV) acetate and lead(IV) acetate were prepared by the methods described in the literature of Brauer (1960). Since these acetates are very sensitive to moisture, the crystals were sealed in capillary tubes in a dry-box under nitrogen. Crystal data as determined from oscillation and Weissenberg photographs are listed in Table 1. The densities were determined pycnometrically. The systematic absences of the