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Determination of the amplitudes of thermal vibration in MnHg at 298 °K.*

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The r.m.s. amplitudes of vibration in MnHg (*B*2 structure type) at 298 °K are Hg: 0·117 Å, with e.s.d. 0·003 Å; Mn: 0·145 Å with e.s.d. 0·014 Å. These values are not significantly different, in agreement with the results of recent experimental and theoretical studies on some alkali halides.

Theoretical studies show that, at temperatures well above the Debye temperature, the amplitudes of thermal vibration of individual atoms or ions in ordered cubic crystals should be equal even though their masses may be very different (Waller, 1925; quoted by Blackman, 1956). These general conclusions have been illustrated for some alkali halides by calculations based on the shell model (Pryor, 1966) and the available experimental results [for summaries see Pryor (1966) and Lonsdale (1962)] are in reasonable agreement with theory. The recent experimental results of Barnea & Post (1966) for CsCl also show equal vibration amplitudes for the two ions. These results are all for ionic crystals; we have therefore thought it of interest to report the vibration amplitudes determined for the intermetallic compound MnHg (Royce & Kahlenberg, 1931) which has been shown (Lihl, 1955; de Wet, 1955) to have the *B*2 (CsCl) structure with $a = 3·316 \pm 0·002$ Å. Magnetic measurements (Nagakawa & Hori, 1961; Plessis & Alberts, 1964) and neutron diffraction studies (Nagakawa, Watanabe & Hori, 1964; Oles, 1965) have shown MnHg to be antiferromagnetic with a Néel temperature of 460 °K; below 198 °K there is a slight distortion to tetragonal symmetry (Nagakawa & Hori, 1962).

The sample used was prepared by vacuum-evaporation of mercury from mercury-rich mixtures at temperatures above the decomposition temperature of Mn_2Hg_5 (de Wet, 1959). The material is a soft grey powder which can be ground to an impalpable fineness between the fingers. Diffracted intensities were measured (at 298 °K) with Mo $K\alpha$ (Zr filter) radiation by using a Philips PW1010 stabilized generator, a PW1050 diffractometer, a PW1064 specimen spinner and associated counting equipment. Integrated intensities were obtained by planimetry of peak profiles determined, for strong reflexions from chart records and for weak reflexions by point-by-point counting using an automatic device developed by Mr. W. W. Schroeder of this Laboratory. Structure factors, on a relative scale, were derived from measured intensities by application of appropriate Lorentz-polarization factors. No corrections were made for temperature-diffuse scattering peaked at the Bragg reflexions.

The individual isotropic temperature factors of Mn and Hg were obtained from a least-squares refinement on the Elliott 503 computer at the Technion, using the Daly, Stephens & Wheatley (1965) programming system. The function minimized was $R' = \Sigma\, w(|F_{\rm obs}| - k|F_{\rm calc}|)^2$, the weights w being assigned following Cruickshank & Pilling (1961). Dirac–Slater atomic scattering factors were used (Cromer & Waber, 1965), with similarly calculated corrections for anomalous dispersion (Cromer, 1965). The final R value was 5·3 % and $R_1 = 1.9\,\%$ ($R_1 = \{R'/\,\Sigma\, w|F_{\rm obs}|^2\}^{\frac{1}{2}}$). The final values of observed and calculated structure factors are given in Table 1.

Table 1. *Results of least-squares refinements of Debye–Waller factors of* Mn *and* Hg *in* MnHg

hkl	$\lvert F_{\rm obs}\rvert$	$F_{\rm calc}$
110	78·1	79·87
111	43·4	41·21
200	63·9	66·94
210	36·2	36·48
211	58·6	57·74
220	53·9	50·62
300	31·3	29·81
310	43·0	44·95
311	26·4	27·26
222	44·1	40·22
320	25·4	25·03
321	39·7	36·26
400	34·8	32·88
410	21·1	21·24
411	26·8	29·90
331	24·6	19·63
420	26·8	27·31
421	16·9	18·12
332	27·9	25·03
422	22·3	22·99
510	22·2	21·14
521	16·1	18·00

The individual isotropic r.m.s. vibration amplitudes obtained for Hg and Mn were ($\langle u^2\rangle_j = B_j/8\pi^2$)

$$\text{Hg}: \langle u^2\rangle^{\frac{1}{2}} = 0·117\ \text{Å e.s.d.} = 0·003\ \text{Å}$$
$$\text{Mn}: \langle u^2\rangle^{\frac{1}{2}} = 0·145\ \text{Å e.s.d.} = 0·014\ \text{Å}$$

The weighted mean atomic vibration amplitude is 0·118 Å with an e.s.d. of 0·005 Å. Neither of the individual values differs significantly from the weighted mean (for Mn Student's $t = 1·85$). These results show that only the vibration amplitude of Hg has been determined with satisfactory precision; this is a consequence of the different atomic numbers of the two components and the inaccuracies in the measured structure factors. As the neutron scattering lengths ($b_{\rm Hg} = 1·3$, $b_{\rm Mn} = -0·36 \times 10^{-12}$ cm) are in much the same ratio as the atomic numbers, only more accurate intensity measurements will yield better results for the vibration amplitudes of *both* atoms. An average Debye temperature was calculated for MnHg using the method proposed by Lonsdale (1948); the value obtained was 150 °K.

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Redetermination of the crystal structure of uracil.

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The crystal structure of uracil, originally reported by Parry in 1954, has been redetermined. The unit-cell parameters are $a=11\cdot938\pm0\cdot001$, $b=12\cdot376\pm0\cdot0009$, $c=3\cdot6552\pm0\cdot0003$ Å; $\beta=120°54'\pm0\cdot4'$. The space group is $P2_1/a$. Three dimensional X-ray diffraction data were measured by diffractometry with Mo $K\alpha$ radiation. The final R was 0·045. The redetermined structure is essentially a confirmation of Parry's structure. The C(5)–C(6) bond length (1·340 Å, e.s.d. 0·002 Å) in this work, however, is 0·07 Å shorter than the value (1·41 Å, e.s.d. 0·011 Å) reported by Parry.

The crystal structure of uracil was first reported by Parry (1954). One interesting feature of the structure is the close approach of an oxygen atom to carbon atoms in different molecules. The reported distances are 3·19 and 3·28 Å. Another interesting result is the C(5)–C(6) bond length of 1·41 ± 0·01 Å, a value considerably greater (0·07 Å) than for a similar bond found in 1-methylthymine (Hoogsteen, 1963*a*, *b*), thymine monohydrate (Gerdil, 1961) and 1-methyluracil (Green, Mathews & Rich, 1962). The accuracy of the results, unfortunately, was limited by the quality of the uracil crystal. We report here the structural results of an X-ray diffraction investigation of a uracil crystal.

High quality single crystals of uracil were grown by heating the powder to its decomposition point in a Pyrex test tube with a sharp temperature gradient. Single crystals of stubby habit with prominent forms {001} and {110} grew on the walls of the tube at a temperature somewhat below the decomposition point. One precession and several Weissenberg photographs confirmed the space group $P2_1/a$ as reported by Parry (1954). Accurate cell parameters were determined on a Picker X-ray diffractometer with a General Electric quarter circle goniostat. The parameters for the monoclinic cell are:

$$a=11\cdot938\pm0\cdot001\ \text{Å}$$
$$b=12\cdot376\pm0\cdot0009$$
$$c=3\cdot6552\pm0\cdot0003$$
$$\beta=120°54'\pm0\cdot4'$$
$$\lambda(\text{Mo}\ K\alpha)=0\cdot71069\ \text{Å}.$$

Table 1. *Final atomic parameters*

The temperature factors are of the form

$$T_i=\exp\left[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)\right] \text{ and } T_{\text{H}}=\exp\left[-B(\sin\theta/\lambda)^2\right].$$

Estimated standard deviations, in parenthesis, are right adjusted:
e.g. For O(7), $\sigma(x)=11\cdot10^{-5}$ and for H(9), $\sigma(x)=16\cdot10^{-4}$.

	x	y	z	$10^4\beta_{11}$	$10_4\beta_{22}$	$10^4\beta_{33}$	$10^4\beta_{12}$	$10^4\beta_{13}$	$10^4\beta_{23}$
O(7)	0·08497 (11)	0·28677 (9)	−0·02173 (43)	80 (1)	41 (0·8)	1670 (22)	11 (0·8)	252 (4)	30 (3)
O(8)	0·12987 (10)	−0·07706 (8)	0·01962 (44)	66 (1)	35 (0·7)	1537 (19)	−6 (0·8)	228 (4)	−17 (3)
N(1)	0·27283 (12)	0·21750 (11)	0·05336 (50)	58 (1)	36 (0·9)	1157 (22)	−7 (0·9)	176 (4)	5 (4)
N(3)	0·11208 (12)	0·10468 (10)	0·00406 (48)	43 (1)	37 (0·8)	1040 (19)	−2 (0·8)	143 (4)	0 (3)
C(2)	0·15191 (14)	0·20933 (12)	0·00913 (56)	58 (1)	41 (1)	924 (22)	−3 (1)	143 (5)	10 (4)
C(4)	0·17988 (14)	0·01237 (12)	0·03494 (54)	52 (1)	40 (1)	829 (21)	−2 (1)	129 (5)	−10 (4)
C(5)	0·30519 (14)	0·02857 (13)	0·08193 (58)	51 (1)	44 (1)	1026 (25)	2 (1)	158 (5)	−9 (4)
C(6)	0·34620 (15)	0·12977 (12)	0·08905 (59)	49 (1)	51 (1)	940 (22)	−6 (1)	145 (5)	−14 (4)
H(9)	0·3536 (16)	−0·0322 (14)	0·0986 (56)	3·41 (39): B_{H}					
H(10)	0·4279 (16)	0·1464 (13)	0·1120 (50)	3·04 (35)					
H(11)	0·2964 (15)	0·2804 (14)	0·0416 (52)	3·15 (39)					
H(12)	0·0343 (16)	0·0947 (13)	−0·0320 (52)	3·33 (39)					