alloy specimen in either the 'as melted' or annealed condition. Filings were annealed in Vycor capillaries 'gettered' with zirconium wire.

The unit-cell dimensions for the intermetallic compounds are given in Tables 1 through 4. These dimensions were calculated on an IBM 1620 computer from back-reflection data using the analytical extrapolation method of Cohen (1935, 1936).

Table 1. CsCl *structure type**

| | $a$ | $\sigma(a)$ |
|---|---|---|
| HoTl | 3·720 Å | 0·002 Å |
| ErTl | 3·704 | 0·004 |
| HoIn | 3·774 | 0·003 |
| ErIn | 3·745 | 0·003 |

* *Strukturbericht*, 1, 74 (1931).

Table 2. $AuCu_3$ *structure type**

| | $a$ | $\sigma(a)$ |
|---|---|---|
| $HoTl_3$ | 4·667 Å | 0·002 Å |
| $ErTl_3$ | 4·659 | 0·005 |
| $HoIn_3$ | 4·570 | 0·004 |
| $ErIn_3$ | 4·563 | 0·004 |
| $HoPt_3$ | 4·058 | 0·002 |
| † | 4·064 | |
| $ErPt_3$ | 4·050 | 0·003 |
| $HoAl_3$‡ | 4·248 | 0·005 |
| $ErAl_3$ | 4·212 | 0·002 |
| § | 4·214 | |

* *Struckturbericht*, 1, 486 (1931).
† Dwight, Downey & Conner (1961).
‡ Not the major constituent of powder photograph and not all other lines of the pattern identified.
§ Krip'yakevich & Zalutskii (1963).

Table 3. $MoSi_2$ *structure type* (*tetragonal*)*

| | $a$ | $\sigma(a)$ | $c$ | $\sigma(c)$ |
|---|---|---|---|---|
| $HoAg_2$ | 3·682 Å | 0·001 Å | 9·172 Å | 0·004 Å |
| $ErAg_2$ | 3·668 | 0·001 | 9·135 | 0·002 |
| $HoAu_2$ | 3·676 | 0·001 | 8·934 | 0·001 |
| $ErAu_2$ | 3·665 | 0·002 | 8·932 | 0·003 |
| † | 3·66 | | 8·98 | |

* *Strukturbericht*, 1, 741 (1931).
† Dwight (1964).

Table 4. $Mn_5Si_3$ *structure type* (*hexagonal*)*

| | $a$ | $\sigma(a)$ | $c$ | $\sigma(c)$ |
|---|---|---|---|---|
| $Ho_5Ge_3$ | 8·410 Å | 0·003 Å | 6·300 Å | 0·005 Å |
| $Er_5Ge_3$ | 8·367 | 0·002 | 6·266 | 0·005 |

* *Strukturbericht*, 4, 24 (1936).

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# Optical and crystallographic data of uric acid and its dihydrate.

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The optical properties of uric acid crystals were first studied by Brun (1899) who found that the highest and the lowest principal refractive indices were 1·73 and 1·53 respectively. Winchell (1954) reported the corresponding values to be 1·830 and 1·573 and expressed the view that the substance examined by Brun was a dimorphous or hydrated form of uric acid. From the literature it is apparent that the optical properties of uric acid have not been studied in detail, nor are other single-crystal data available.

In the present study two optically different forms of uric acid are described. Slow cooling and evaporation of a solution of pure uric acid yielded monoclinic crystals. After more rapid cooling of the solution however, unstable orthorhombic crystals appeared.

Optical and X-ray crystallographic data were recorded from single crystals of both these modifications.

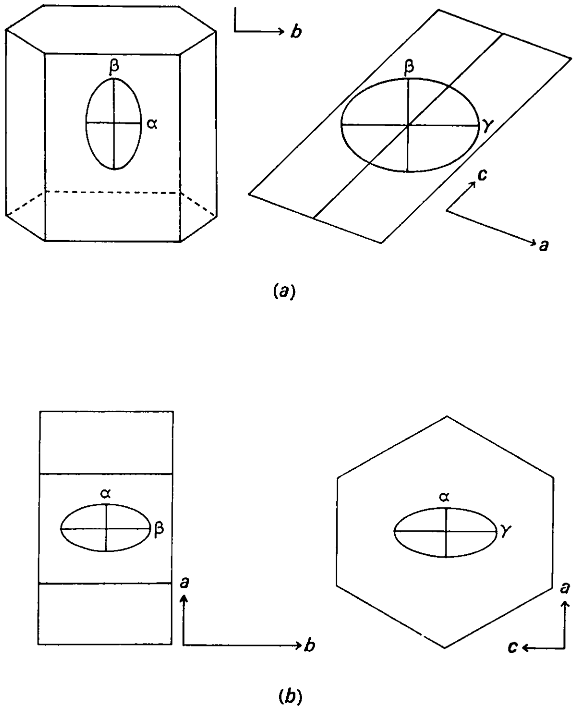
### *The monoclinic form*

Uric acid, $C_5H_4N_4O_3$, slowly crystallized from an aqueous solution, formed plates. The larger plates often showed multiple twinning parallel to the basal pinacoid. Some smaller crystals however, were not twinned and exhibited a monoclinic habit. Fig. 1(*a*) shows such a crystal in relation to the principal optic directions and the chosen crystallographic axes

*Optical* Biaxial positive
$\gamma = 1{\cdot}898 \pm 0{\cdot}003$
$\beta = 1{\cdot}739 \pm 0{\cdot}003$
$\alpha = 1{\cdot}588 \pm 0{\cdot}003$
$2V_{calc} = 83{\cdot}8^\circ \pm 0{\cdot}6^\circ$
$B = 0{\cdot}31$

Weissenberg and rotation photographs taken with Cu $K\alpha$ radiation revealed that the unit cell was monoclinic, belonging to space group $P2_1/a$. The morphological parameters were

$a = 14{\cdot}464 \pm 0{\cdot}003$ Å
$b = 7{\cdot}403 \pm 0{\cdot}002$
$c = 6{\cdot}208 \pm 0{\cdot}001$
$\beta = 65{\cdot}10^\circ$
$V = 602{\cdot}9$ Å$^3$



(a)

(b)

Fig. 1. Common habit, the indicatrix and chosen crystallographic axis of (*a*) uric acid (*b*) uric acid dihydrate. The differences between the principal optic axes are exaggerated five times.

The observed density 1·844 g.cm$^{-3}$ gives $Z = 3{\cdot}985$ molecules of $C_5H_4N_4O_3$, molecular weight 168·11, per unit cell. $D_{calc} =$ 1·851 g.cm$^{-3}$. The monoclinic crystals thus consist of pure anhydrous uric acid.

*The orthorhombic form*

Under conditions mentioned above, uric acid can crystallize in an orthorhombic form which disintegrates when allowed to dry in air and is converted into a polycrystalline aggregate of the monoclinic form. This conversion has been followed by powder diffraction and no detectable intermediate crystalline form has been observed. However, stable crystals of the orthorhombic form were found in some rare human bladder stones and on the inside of hatched eggshells of hens.

The most common crystal habit in relation to principal optical directions and corresponding crystallographic axes is shown in Fig. 1(*b*).

*Optical* Biaxial negative

$\gamma = 1{\cdot}728 \pm 0{\cdot}003$
$\beta = 1{\cdot}691 \pm 0{\cdot}003$
$\alpha = 1{\cdot}508 \pm 0{\cdot}003$
$2V_{obs} = 40{\cdot}4° \pm 0{\cdot}6°$
$2V_{calc} = 44° \pm 4°$
$B = 0{\cdot}22$

Weissenberg and rotation photographs taken with Cu $K\alpha$ radiation showed that the unit cell was orthorhombic. The systematic absences varied between different, optically untwinned crystals, without any change of the unit-cell dimensions. Consistent absences for all crystals were $hk0$ when $k$ was odd. In addition $h00$ and $00l$ were absent when $h$ and $l$ were odd, but because of the small number of reflexions these absences could not be regarded as trustworthy. The $h0l$ reflexions when $h$ was odd were very few and varied moreover in intensity. So did, to even greater extent, the $0kl$ reflexions when $k+l$ was odd. These variations can probably be assigned to changes in the water content. Hence the space group could not be determined with certainty.

The lattice parameters were

$a = 7{\cdot}40 \pm 0{\cdot}01$ Å
$b = 17{\cdot}55 \pm 0{\cdot}01$
$c = 6{\cdot}35 \pm 0{\cdot}005$
$V = 825{\cdot}7$ Å$^3$

The observed density 1·650 g.cm$^{-3}$ gives four formula units with a molecular weight of 204·96. As this crystal form (1) was formed in water solution,(2) disintegrated upon drying and (3) converted into anhydrous uric acid, it is probable that it contains water. The calculated molecular weight for uric acid with two $H_2O$ (204·15) is in good agreement with the observed value. The calculated density $= 1{\cdot}643$ g.cm$^{-3}$. Thus it seems likely that the orthorhombic unit cell contains four formula units of $C_5H_4N_4O_3 \cdot 2H_2O$. Further support for this concept was gained in measuring the weight loss after heating a sample of this compound to 105 °C for five hours.

The crystal structure of uric acid is now under investigation.

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## A three-dimensional refinement of the structure of crocoite, PbCrO₄.

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### Introduction

A complete determination of the crocoite structure and two-dimensional refinement have already been carried out (Quareni & De Pieri, 1964). By means of this early study it was possible to refine the lead and chromium parameters and to determine the positions of the oxygen atoms. The