

(Zachariassen, 1965), and in LiAlO_2 (Marezio, 1965*b*). In both cases the $\text{Cu } K\alpha$ wavelength is less than one fourth that of the nearest critical absorption edge.

During the determination of the structure of LiGaO_2 , the intensities of all $0kl$, $1kl$, $h0l$, $h1l$, $hk0$ and $hk1$ reflections were measured with $\text{Cu } K\alpha$ radiation and a General Electric XRD-3 spectrometer rebuilt for single-crystal work and equipped with a proportional counter. The dispersion effect was observed for the $0kl$, $1kl$, $h0l$ and $h1l$ reflections. It was not observed for the $hk0$ and $hk1$ reflections, in the first case because $X_H=0$ by symmetry, and in the second case because the intensities corresponding to \bar{H} were not measured. The half width of the distribution function for the $|X_H|$ values is 2.9%, which is not much greater than the accuracy of the intensity measurements. It was estimated that the standard deviation for each measurement varied from 1% for strong reflections to 3% for the weakest reflections.

A comparison between observed and calculated X_H is given in Table 1 for those reflections which have $|X_H|$ greater than the accuracy of the intensity measurements. The X 's were obtained using $\Delta f''_{\text{Ga}}=0.903$ and $\Delta f''_{\text{O}}=0.035$, which are the values calculated from the atomic absorption coefficients given in *International Tables for X-ray Crystallography* (1962). As was pointed out by Zachariassen (1965) fairly good values for $\Delta f''$ can be calculated from the atomic absorption coefficients, $\mu_a=(2e^2\lambda/mc^2)\Delta f''$, on the assumption that true absorption is the predominant process. During the refinement of the structure of LiGaO_2 the real part of the anomalous dispersion correction was applied to the scattering factor of gallium. The value used ($\Delta f'_{\text{Ga}}=-1.5$) was taken from *International Tables for X-Ray Crystallography* (1962).

As can be seen, the dispersion effect is small as expected, but distinctly noticeable, even though the nearest critical absorption edge of the long wave side of $\text{Cu } K\alpha$ wave length is the L absorption edge of gallium (11.149 Å). Although the agreement obtained between $|X_c|$ and $|X_o|$ is satisfactory, it is not good enough for a calculation of $\Delta f''_{\text{Ga}}$ and $\Delta f''_{\text{O}}$ independently. In the fourth column of Table 1 the calculated $\Delta f''_{\text{Ga}}$ values are shown for those reflections for which $|X| \geq 0.05$ when $\Delta f''_{\text{O}}$ is assumed to be 0.028, which was

Table 1. *Anomalous dispersion data for LiGaO_2*

hkl	$X_o \cdot 10^2$	$X_c \cdot 10^2$	$\Delta f''_{\text{Ga}}$
002	-3.5	-4.2	
121	7.6	6.4	0.98
201	7.1	6.4	0.95
212	3.0	1.5	
203	5.1	2.5	
401	6.5	5.3	1.01
114	3.3	2.4	
214	2.5	2.3	
134	4.9	2.3	
403	4.5	2.6	
511	3.7	5.6	
413	-4.6	-4.9	
161	5.0	5.0	0.90
512	3.3	1.4	
414	3.6	2.7	
513	3.4	2.6	
071	6.3	5.5	0.96
601	6.6	9.1	0.73
163	4.1	3.0	
154	3.6	2.9	
602	-3.9	-5.6	
172	5.4	5.0	0.93
006	5.9	6.3	0.81
116	3.0	2.2	
064	-9.9	-10.0	0.85
073	4.8	2.9	
126	5.1	6.8	0.69
206	7.2	6.5	0.93

obtained experimentally in LiAlO_2 (Marezio, 1965*b*). The average of the $\Delta f''_{\text{Ga}}$ - values shown in Table 1 is 0.89 ± 0.03 , which is in fairly good agreement with the value calculated from the atomic absorption coefficient (0.90) and with the value (0.9) given in the *International Tables for X-Ray Crystallography* (1962).

References

- International Tables for X-Ray Crystallography* (1962). Vol. III. Birmingham: Kynoch Press.
 MAREZIO, M. (1965*a*). *Acta Cryst.* **18**, 481.
 MAREZIO, M. (1965*b*). *Acta Cryst.* In the press.
 ZACHARIASSEN, W. H. (1965). *Acta Cryst.* **18**, 714.

Acta Cryst. (1965). **19**, 285

Some new intermetallic compounds of holmium and erbium with Ag, Au, Pt, Al, In, Tl, and Ge. By J. L.

MORIARTY, R. O. GORDON*, and J. E. HUMPHREYS, *Lunex Company, Pleasant Valley, Iowa, U.S.A.*

(Received 4 January 1965)

During an extensive investigation of the binary alloy systems of holmium and erbium in combination with twenty-one metallic elements a number of new intermediate phases were identified. The general approach and pattern of this study was suggested by results of earlier work described by Moriarty (1960). Structural data for compounds formed in similar systems with gadolinium and dysprosium can be found in reports by Baenziger & Moriarty (1961), also by McMasters & Gschneidner (1964).

* Present address: Harvard University, Cambridge, Massachusetts.

Alloys were prepared by arc-melting stoichiometric proportions of the components on a water cooled copper hearth under an argon gas atmosphere. Each specimen was remelted repeatedly to improve homogeneity. Final weights differed from initial weights by less than 1.0%. Purities of the metals used were: holmium and erbium, 99.8%; all others were greater than 98.5%.

In all cases the phases were identified by indexing the X-ray diffraction powder photographs. Diffraction equipment included a basic Norelco X-ray unit, using filtered copper radiation, 114.6 mm Debye-Scherrer cameras and Ansco Superay C film. The photographs were made of the

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*

	<i>a</i>	$\sigma(a)$
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. AuCu₃ structure type*

	<i>a</i>	$\sigma(a)$
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	

* *Strukturbericht*, 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. MoSi₂ structure type (tetragonal)*

	<i>a</i>	$\sigma(a)$	<i>c</i>	$\sigma(c)$
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. Mn₅Si₃ structure type (hexagonal)*

	<i>a</i>	$\sigma(a)$	<i>c</i>	$\sigma(c)$
Ho ₅ Ge ₃	8.410 Å	0.003 Å	6.300 Å	0.005 Å
Er ₅ Ge ₃	8.367	0.002	6.266	0.005

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

The authors thank Professor N. C. Baenziger for helpful discussions during the course of this work. The cooperation of Harvard University Department of Chemistry in providing computer time is gratefully acknowledged.

References

- BAENZIGER, N. C. & MORIARTY, J. L. (1961). *Acta Cryst.* **14**, 948.
 COHEN, M. U. (1935). *Rev. Sci. Instrum.* **6**, 68.
 COHEN, M. U. (1936). *Rev. Sci. Instrum.* **7**, 155.
 DWIGHT, A. E. (1964). Argonne Natl. Lab. Rept. ANL 6868.
 DWIGHT, A. E., DOWNEY, J. W. & CONNER, R. A., JR. (1961). *Acta Cryst.* **14**, 75.
 KRIP'YAKEVICH, P. & ZALUTSKII, I. (1963). *Dopovidi Akad. Nauk Ukr. RSR*, No. 1, 61.
 MCMASTERS, O. D. & GSCHNEIDNER, K. A., JR. (1964). *Nuclear Metallurgy Series*, X, 93-158.
 MORIARTY, J. L. (1960). Ph. D. Thesis, Diss. Abstr. **21**, 1391-2.

Acta Cryst. (1965). **19**, 286

Optical and crystallographic data of uric acid and its dihydrate. By HANS RINGERTZ, Department of Medical Physics, Karolinska institutet, Stockholm, Sweden

(Received 22 January 1965 and in revised form 15 February 1965)

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, C₅H₄N₄O₃, 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

$$\gamma = 1.898 \pm 0.003$$

$$\beta = 1.739 \pm 0.003$$

$$\alpha = 1.588 \pm 0.003$$

$$2V_{calc} = 83.8^\circ \pm 0.6^\circ$$

$$B = 0.31$$

Weissenberg and rotation photographs taken with Cu K α radiation revealed that the unit cell was monoclinic, belonging to space group *P*2₁/*a*. The morphological parameters were

$$a = 14.464 \pm 0.003 \text{ \AA}$$

$$b = 7.403 \pm 0.002$$

$$c = 6.208 \pm 0.001$$

$$\beta = 65.10^\circ$$

$$V = 602.9 \text{ \AA}^3$$