

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

# Standard X-ray Diffraction Powder Patterns

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#### ERRATA

A book has been published containing card images of NBS Standard X-ray Diffraction Powder Patterns<sup>1</sup>. During preparation of the book, some errors were found and corrected on the card images. A list of them is available on request. The corrections below are in addition to those included on the card images.

Monograph 25

Sec. 14, p. 1, col. 1, footnote at asterisk: the zip code should be 94305. p. 12, at 20 = 45.75, d should be 1.981. p. 13, under Optical Data, delete the words "2V is large" and substitute the words "The optical sign is (+) and 2V = 88. p. 25, at d = 3.114, delete the hkl 301. p. 26, at d = 1.3085, hkl should be  $\overline{632}$ . Sec. 7, p. 60, in the paragraph "Structure," the space group should be P42/mbc.

Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA, 19081, \$150.00.)

#### STANDARD X-RAY DIFFRACTION POWDER PATTERNS

The following copies may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia, 22161. Where these publications are identified with a number, it must be used in ordering. They are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

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Volume 10.        .PB 178 911       Section 11.          Section 11.              Section 11.              Section 12.              Section 13.              Section 14. | Number         NBS Publication           Volume 1 | Number         NBS Publication           Volume 1 | Number         NBS Publication           Volume 1 | Number       Number       NBS Publication         Volume 1   < | Number       NBS Publication       Number       PB       178       903       Section 3       . |

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#### STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 15. --- Data for 112 Substances

by

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and

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Standard x-ray diffraction patterns are presented for 112 substances. Fiftyfour of these patterns represent experimental data and 58 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

#### INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the JCPDS - International Centre for Diffraction Data, the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the JCPDS, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 112 compounds (54 experimental and 58 calculated patterns), and is the twenty-fifth of the series of "Standard X-ray Diffraction Powder Patterns."2

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<sup>1</sup>JCPDS - International Centre for Diffraction Data 1601 Park Lane, Swarthmore, PA. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

#### EXPERIMENTAL POWDER PATTERNS

<u>Sample</u>. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the sample improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

OptiCal data. When reported, optiCal measurements were made by grain immersion methods, in white light, using oils standardized in sodium light, in the refractive index range 1.49 to 2.1 [Hartshorne and Stuart, 1970].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard. Choice of the standard was determined by the need for low angle and unobstructed reflections. The amount of standard was estimated so that the intensity of its strongest peak would be about equal to the intensity of the strongest peak of the sample.

To avoid errors associated with aberrations at the very top of the peaks, the readings of 20 were taken at positions about 20% of the way down from the top, and in the center of the peak width. The  $K\alpha_2$  peaks were occasionally read to assist in establishing a  $K\alpha_1$  peak position, but  $K\alpha_2$  peaks were not reported.

At low angles,  $K\alpha_1$  and  $K\alpha_2$  peaks were unresolved for both the sample and the internal standard. The internal standard corrections were established from the theoretical values for  $K\alpha_1$ and were applied to the unresolved, low angle peaks as well as to the resolved  $K\alpha_1$  peaks in the higher angle regions. If the internal standard correction varied along the length of the pattern, linear interpolations were used.

<sup>2</sup>See previous page for other published volumes.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in the table below; the  $2\theta$  angles were computed using cell dimensions uncorrected for index of refraction.

	Calculated 20	Angles, CuK $\alpha_1$	$\lambda = 1.540598 \mathring{A}$
hkℓ	W a=3.16524Å ±.00004	Ag a=4.08651Å ±.00002	Si a=5.43088Å ±.00004
110 111 200	40.262 58.251	38.112 44.295	28.443
211 220	73.184 86.996	64.437	47.303
310 311 222 321	100.632 114.923	77.390 81.533	56.123
400	153.535	97.875	69.131
331 420		110.499 114.914	76.377
422 511, 440	/333	134.871 156.737	88.032 94.954 106.710
531 620 533 444			114.094 127.547 136.897 158.638

The new internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Cell parameter data were also collected for a single crystal from the boules ground to prepare the powder. The lattice parameters from the two methods agreed within 3 parts in  $10^5$ [Hubbard et al. 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25  $\pm$  1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation:  $\lambda$  (CuK $\alpha_1$ , peak)= 1.540598Å [Deslattes and Henins, 1973].

Structure, lattice constants. The space groups were listed with short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography, Vol. I [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of *Crystal Data* [1973]. For primitive cells, the transformed cell axes are an alternate labelling of the reduced cell axes. For centered monoclinic cells, the transformed cell is the centered cell with the three shortest non-coplanar vectors.

A computer program [Evans et al., 1963] assigned hkl's and refined the lattice constants. Cell refinement was based only upon  $2\theta_{obs}$  values which could be indexed without ambiguity. The program minimized the value  $\Sigma (\Theta_{obs} - \Theta_{calc})^2$ . The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

In indexing cubic patterns, multiple hkl's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest <u>h</u> was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

<u>Densities</u>. These were calculated from the specified lattice constants, the Avogadro number  $6.0220943 \times 10^{23}$  [Deslattes et al., 1974] and atomic weights published by IUPAC [1972].

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10  $\mu$ m, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the





powdered sample was allowed to drift into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (as shown in Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. Any intensity larger than 20 was rounded to the nearer multiple of 5. At least 3 patterns for intensity measurements were prepared for each sample to check reproducibility.

Reference Intensity Ratio,  $I/I_{corundum}$ . The reference intensity ratio, I/I, has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the reflection 113(hexagonal) of corundum ( $\alpha$ -Al<sub>2</sub>O<sub>3</sub>) [Visser and de Wolff, 1964]. The ratio is tabulated for copper Ka radiation, for a 1:1 mixture by weight of the sample and corundum.

A new procedure has been adopted, to achieve greater statistical accuracy [Hubbard and Smith, 1977]. For any weight fractions of sample and corundum,  $x_s$  and  $x_c$  ( $x_s = 1-x_c$ ), intensities I(<u>h</u>) and I(<u>k</u>) are measured for several sets of reflections <u>h</u> and <u>k</u>, usually within the same region of 20, to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

I( <u>h</u> 0) =	<u>x</u>	$I_c^{rel}(\underline{k})$	I( <u>h</u> )
I_(113)	x	I <sup>rel</sup> (h)	I(k)

and  $(\underline{h_0})$  indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection  $(\underline{h_0})$  will be the one with I=100 since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio,  $I/I_c$ . These values yield the tabulated average  $\left< I/I_{C} \right>$  . From these data, the e.s.d.,  $\vartriangle$  , was obtained from

$$\Delta = \frac{\sum_{i=1}^{n} |(I/I_c)_i - \langle I/I_c \rangle|}{n}$$

where n is the number of measurements of the reference intensity ratio. The e.s.d. in the least significant figures is given in parentheses.

Format of tables. Part way through the preparation of this monograph, the printing of the data was computerized for the experimental patterns. In the new format, superimposed reflections were treated in one of two ways. If a dspacing had only two possible indices, an M was added to the d-spacing which was repeated on the next line, but with the second index. However, if there were more than two possible indices, a + sign was used in like manner. In both cases, the composite intensity was printed only once and aligned with the first reflection. The symbol "1L" in the intensity column was used to indicate "less than 1."

#### CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Clark, Smith and Johnson [1973] and modified at NBS.

Lattice parameters. Before the computations of the patterns, any necessary changes were made in the lattice constants in order to make them consistent with the revised value of  $\lambda$  (CuK $\alpha_1$ )= 1.540598Å [Deslattes and Henins, 1973]. Both the altered and the original published values are given. A lattice constant arrangement which follows the conventions of <u>Crystal Data</u> has been referred to as the "CD cell." In several of the calculated patterns, the literature lattice constants, the atom positions, and hence the final patterns were not given in the CD arrangement. For cross-reference purposes, the CD cell was calculated separately and included in the text.

<u>Scattering factors</u>. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, the factors were taken directly from the *International Tables for X-ray Crystallography*, *Vol. III*, [1962]. The factors were corrected for dispersion if the author had done so.

$$(-B \sin^2 \Theta)/\lambda^2$$

 $e^{-(h^2\beta_{11}+k^2\beta_{22}+\ell^2\beta_{33}+2hk\beta_{12}+2h\ell\beta_{13}+2k\ell\beta_{23})}.$ 

Other thermal parameters were converted to one of these two forms. The isotropic parameters were

used directly, if given by the structure reference. In a few of our patterns, anisotropic parameters were also used directly as given by the structure reference; in other work, instead of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined by:

$$B = 4 \begin{bmatrix} \frac{\beta_{11}\beta_{22}\beta_{33}}{a^{*2}b^{*2}c^{*2}} \end{bmatrix}^{\frac{1}{3}}$$

Structural information. The atom positions used in these calculated patterns varied somewhat in the degree of reliability. In our text, when the expression "the structure was determined by..." was used, the atomic parameters in the reference cited had been calculated from refinement of single crystal data. Otherwise, the atomic positions had been derived by analogy with similar compounds whose structure was known. In cases where isostructural relationships were used, the atoms were in fixed special positions or the ionic radii were closely related to the corresponding radii of the atoms in the known structure.

Integrated intensities. The theoretical integrated intensity of reflection i on the "absolute-relative" scale is  $I_{i}^{abs}/K$ , as defined by Hubbard, Evans, and Smith [1976] in the equation

$$\frac{I_{i}^{abs}}{K} = \frac{M_{i}Lp_{i}|F_{i}T_{i}|^{2}}{2\mu V^{2}}$$

where:

F is the structure factor T is the thermal correction

 $Lp = \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$  is the Lorentz-polarization term

M is the multiplicity for the reflection i  $\mu$  is the linear absorption coefficient V is the volume of the unit cell

When the largest integrated intensity was assigned a relative value of 100 and all other reflections were scaled relative to it, the intensities were placed on the relative intensity scale ( $I^{rel}$ ). Relative intensities were rounded to the nearest integer value before being listed, and reflections with  $I^{rel}$  less than 0.7 were omitted.

<u>Scale factor (integrated intensities)</u>. The scale factor,  $\gamma$ , was defined to convert the tabulated I<sup>rel</sup> to the "absolute-relative" scale [Hubbard, Evans, and Smith, 1976]. That is:

$$\gamma = \frac{M'Lp'|F'T'|^2}{200\mu V^2}$$

and

$$\frac{I^{abs}}{\kappa} = \gamma I^{rel}$$

The primes denoted the values for the largest integrated intensity. In earlier Monographs (1969–1975), a different scale factor,  $k_{\rm NBS}$ , was reported which is related to  $\gamma$ :

$$\frac{\gamma}{2\mu V^2} = \frac{1}{2\mu V^2}$$

From  $\gamma$ , the theoretical value of the Reference Intensity Ratio,  $I/I_{c}$ , was calculated:

$$I/I_{c} = \frac{\mu\gamma\rho_{c}}{\mu_{c}\gamma_{c}\rho}$$

where  $\rho$  is the density and the subscript c represents corundum ( $\alpha\text{-Al}_2\text{O}_3\text{)}$ .

For refined structures, the value of  $I/I_c$  was given. For those phases whose structures were postulated or were based only on analogy to other powder patterns,  $I/I_c$  was not included and any intensity above 20 was rounded further, to the nearer multiple of 5.

 $I/I_{\rm C}$  and  $\gamma$  are each based on the single strongest reflection, not on the overlapping sum of superimposed reflections.

Peak heights. The purpose of calculating peak height intensity was to provide a tabulated pattern similar to what might be obtained from experimental diffractometer measurements. For each predicted reflection, Cauchy profiles centered at both the  $\alpha_1$  and the  $\alpha_2$  peak positions were calculated and summed, forming a simulated powder pattern. The full width at half-maximum (FWHM) was allowed to vary to represent the changing FWHM as a function of  $2\theta$ . [The values of the FWHM vs 20 are given in the table below]. The resultant simulated powder pattern was then analyzed for peaks. In the regions of the predicted reflections several reflections could have identical or similar  $2\theta$  angles and produce only one composite peak in the simulated pattern. The 20 angle of the composite peak was assigned the hkl of the reflection having the greatest contribution to the peak height intensity. If any other peak contributed more than 10% of the intensity toward the composite peak height intensity, a plus sign(+) was appended to the hkl. Peaks due solely to  $\alpha_2$  lines were omitted. If an  $\alpha_1$  peak and an  $\alpha_2$  peak overlapped, the  $\alpha_1$  reflection was listed only when it contributed a significant intensity (>10%) at the peak 20.

The peak search routine located peaks only at 20 angles which were a multiple of  $0.02^{\circ}$ .

20		20	
CuKal	FWHM	CuKαl	FWHM
~ ~	0.100	140	0.000
0.0	0.120	140	0.230
20	.12	145	.255
40	.12	150	.285
60	.125	155	.315
80	.130	160	.360
100	.135	162.5	.410
120	.155	165	.500
130	.185		

#### UNITS

In this publication the Angström unit (10A=1nm) was selected for presentation of the d-spacings and lattice parameters to maintain consistence with (a) the earlier publications of Standard Xray Diffraction Powder Patterns (Circular 539 volumes 1-10 and Monograph 25 sections 1-15), (b) the publications of the International Union of Crystallography: Acta Crystallographica and the Journal of Applied Crystallography, and (c) the continuing publication of cards and search manuals of the Powder Diffraction File (now consisting of nearly 30,000 entires). The PDF search manuals are based on the d-spacing in  $\mathring{A}$  of the three strongest lines. Consistent with the choice of the A unit for length, the volume of the unit cell is expressed in  $A^3$  (=1 x 10<sup>-30</sup> m<sup>3</sup>). Other reported parameters and their units are density in g/cm<sup>3</sup>  $(1 \text{ gm/cm}^3 = 10^{-3} \text{ kg/m}^3)$  and the linear absorption coefficient in cm<sup>-1</sup>.

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Sample	d (Å)	I		hkl		20(°)
The sample was prepared by mixing solut Al $(NO_2)_2$ , Fe $(NO_2)_2$ , and $NH_2OH_2$ . Hydroxi	des of					
aluminum and iron precipitated and were	heated 2.394M		з	1	1	37.54
1/2 hr at 1350 °C	2.320	4	1	1	2	38.78
1/2 m. at 1550 C.	2.313	2	ō	Ā	ā	38-91
Color	2.237	11	2		1	40.29
Gray brown.	2.196	15	0	2	2	41.07
-						
Structure	2.185	30	3	2	1	41.29
Orthorhombic, $Pc2_1n(33)$ or $Pcmn(62)$ ,	$Z = 8, 2 \cdot 141$	4	4	0	С	42.18
isostructural with GaFeO <sub>3</sub> [Dayal et al., 1	.965].	14	1	2	2	42.47
	2.099	3	2	1	2	43.05
Lattice constants of this sample: a = 8.566(2) Å	2.033	2	2	4	0	44.52
b = 9.249(1)	1.969	6	4	0	1	46.07
c = 4.989(1)	1.940	15	0	з	2	45.80
	1.931	17	3	3	1	47.01
a/b = 0.9262	1.891	е	1	3	2	48.09
c/b = 0.5394	1.879	3	3	o	2	48.41
Volume	1.8085	6	1	5	0	50.42
395.2 A <sup>3</sup>	1.7676	4	2	З	2	51.67
	1.6959	12	0	4	2	54.03
Density	1,6915	16	З	4	1	54.18
(calculated) 4.397 g/cm <sup>3</sup>	1.6243	2	4	0	2	56.62
Peference intensity	1.5519	2	з	5	0	59.52
T/T = 1.04(9)	1.5390	8	1	2	3	60.07
corundum	1.5295M	4	5	2	ĩ	60.48
Ndditional matterna	1.5295M	~	2	1	-	60.49
Additional patterns	1.4974	14	5	-	0	61 00
<ol> <li>PDF card 11-562 [Atlas and Sumida, 195</li> <li>2. PDF card 18-633 [Dayal et al., 1965]</li> </ol>	8]		5	5	Ŭ	01.92
	1.4861	18	0	5	2	62.44
References	1.4825	40	З	5	1	62+61
Atlas, L. M. and Sumida, W. K. (1958), J	Amer. 1.4581	1	З	4	2	63.78
Ceram, Soc. 41, 150.	1.4370M	30	4	З	2	64.83
Dayal, R. R., Gard, J. A., and Glasser	, F. P. 1.4370M		З	0	3	64.83
(1965). Acta Crystallogr. <u>18</u> , 574.	1.4278	1.0	e	~	•	65 70
	1.7027	10	0	0	0	65.30
0	1.3923		2	6	1	67.18
$CuK\alpha_1 \lambda = 1.540598 \text{ A}; \text{ temp. } 25\pm1 \text{ °C}$	1.3047	11	2	3	3	67.60
0	1.3724M	3	6	0	1	68.29
Internal standard Si, a = 5.43088 A	1.3724M		3	2	3	68.29
d(A) I hkl 200	•) 1.3501	10	5	2	2	69.58
	1.3060	3	1	7	0	72.29
	1.2962	1	1	6	2	72.92
	1.2843	4	5	з	2	73.71
6.28 13 1 1 0 14.	09 1.2628	4	1	7	1	75.18
4.626 5 0 2 0 19.	17					
4.314 3 1 0 1 20.	57 1.2355	3	0	1	4	77.14
3.907 8 1 1 1 22.	74	-	•			
3.250 5 2 0 1 27.	42				-	
3.146 30 2 2 0 20	35					
3.066 6 2 1 1 20	10					
2.900 35 1 3 0 70	91					
1 3 0 30.	01					

2.729

2.658

2.506

2.495

2.478

2.408

2.394M

5

100

20

17

9

13

25

3 1 0 2 2 1

0 0 2 3 0 1

0 1 2

1 0 2

1 3 1

32.79

33.69

35.81

35.96

36.22 37.32

37.54

Aluminum Sulfate,  $Al_2(SO_4)_3$ 

Sample A sample of Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> *18H <sub>2</sub> O was obtained from	CuK $\alpha_1 \lambda$ = 1.540598 Å; temp. 25±1 °C							
Fisher Scientific Co., New York. It was heated	Internal standard W, $a = 3.16524$ A							
at 600 °C for 6 hours to produce the anhydrous salt.	d(Å)	I	1	hkl		20(°)		
Color					····· ·			
Colorless	5.82	36	0	1	2	15.21		
	4.221	14	1	â	Δ	21.03		
Structure	4.024	11	1	1	0	22.07		
Hexagonal, $R3$ (148), $Z = 6$ , [Thiard, 1965].	3.502	100	1	1	3	25.41		
	3.317	1	2	ō	2	26.86		
Lattice constants of this sample:		-	_	-	_			
a = 8.055(1) Å	2.915	17	0	2	4	30.65		
c = 21.191(5)	2.654	16	1	1	6	33.74		
	2.618	10	2	1	1	34.22		
c/a = 2.6307	2.560	1	1	2	2	35.02		
	2.361	3	2	1	4	38.08		
Volume og								
1191.0 A <sup>3</sup>	2.327	20	3	0	0	38.66		
	2.285	1	0	2	7	39.40		
Density	2.209	5	З	0	З	40.82		
(calculated) 2.863 g/cm <sup>3</sup>	2.033	40	1	1	9	44.53		
	1.989	2	2	1	7	45.57		
Reference intensity								
1/1 = 6.0	1.942	3	З	0	6	46.75		
This makes is a should enclose a firm forward	1.903	1	З	1	2	47.76		
This material showed evidence of preferred	1.8693	2	1	2	8	48.67		
orientation for the nk% 119.	1.8169	2	1	З	4	50.17		
Additional mattern	1.7660	1	0	0	12	51.72		
Additional pattern								
1. PDF Card 22-21 [Ferret & ROSSO, 1900].	1.7494	3	2	2	6	52.25		
Deference	1.7209	1	0	4	2	53.18		
References	1.6522	3	2	1	10	55.58		
Chim France p 2700	1.6304	2	1	3	7	56.39		
Thiard R (1965) Thesis of 3rd Cycle in	1.6172	1L	1	1	12	56.89		
Physical Chemistry, Dijon, France,			-	_		c		
inysical chemistry, bijon, itance.	1.5957	14	3	2	1	57.73		
	1.5624	1	3	1	8	59.08		

Sample				d(Å)	I	hkl	20(°)
The sample	e was obtai	ined from The	City Chemical				
Corporatio	on of New Yo	ork.		2.243	3	315	40.18
<b>G</b> , <b>1</b> ,				2.227	2	413	40.47
Color				2.189	14	306	41.21
Colorless				2.170	14	324	41.58
Strugturo				2.158	/	502	41.82
Hovagonal	$P_{20}^{-}(167)$	7 - 6 isost	ructural with	2 000	2	0.43	42.07
K. CdClc	The struc	52 = 0, 15050	) CdPre was	2.099	3	241	43.07
determined	the Struc	cure or (NH4	14 CUBIG Was	2.072	16	226	43.64
determinet	I DY GIADOWS	SKI ANG SWALYCZ	SEMENT [1900].	2.031	10	217	44.57
Lattice cone	stants of th	vic camplo.		2.013	2	235	45.00
Lattice cons	stants of th	its sample:		1.996	11	511	45.40
a = 12.931	3(5) Å			1 00/	12	019	15 16
c = 16.206	5(1)			1.994	13	018	45.40
c/a = 1.25	532			1 952	12	152	40.29
-,				1.952	12	244	40.40
Volume .				1.866	14	600	40.40
2436.8 Å <sup>3</sup>				1.000	14	000	40.70
				1.856	10	137	49.03
Density				1 830	7	431	49.05
(calculate	d) 2.819 g/	′cm <sup>3</sup>		1 828	, 9	128	49.00
	,			1 8015	1	514	50.63
Reference in	tensity			1.7952		342	50.82
I/I	= 3.43(10)	))		1.7552	0	542	50.02
corundu	ım			1,7932	8	520	50.88
Additional p	attern			1.7724	4	425	51.52
1. PDF car	d 24-1455 [	Hardt & Pazen,	1971].	1.7343	< 1	119	52.74
				1.7197	2	327	53.22
References				1.7090	6	155	53.58
Grabowski,	M. and Sw	aryczewski, A.	(1966). Soc.				
Sci. Lod	lz. Acta Chi	.m. 11, 57.		1.7017	8	523	53.83
Hardt, H.	D. and Paz	en, F. (1971)	. Z. Anorg.	1.6843	1	336	54.43
Allgem.	Chem. 380,	16.		1.6767	1	434	54.70
		0		1.6710	2	612	54.90
CuKαl	$\lambda = 1.5405$	98 A; temp. 25	±1 °C	1.6413	3	048	55.98
			0				
Inter	nal standar	d Ag, a = 4.08	651 A	1.6038	6	1.0.10	57.41
0				1.5906	1	238	57.93
d (A)	I	hkl	20(°)	1.5733	4	164,229	58.63
6 55				1.5694	3	532	58.79
6.57	100	012	13.47	1.5569	< 1	0•2•10	59.31
6.47	60	110	13.67				
4.605	30	202	19.26	1.5483	2	443	59.67
4.145	20	113	21.42	1.5455	2	621	59.79
4.096	30	211	21.68	1.5350	1	606	60.24
2 010	10	104		1.5252	3	262	60.67
3.810	10	104	23.33	1.5179	2	517	60.99
3.751	3	122	23.70				
3.283	8	024	27.14	1.5135	2	2•1•10	61.19
3.235	4	220	27.55	1.5112	2	615	61.29
3.051	40	131	29.25	1.5024	1	508	61.69
2 0.20	0 E	214	20 51	1.4939	3	526	62.08
2.920	20	214	30.51	1.4874	6	354	62.38
2.901	30	312	30.80	1 4600		100	
2.774	10	223	32.24	1.4632	2	428	63.53
2.702	< 1	125	31 91	1.4496	2	624,419	64.20
2.575	× 1	125	54.04	1.4412	3	437	64.62
2,538	1	321	35 34	1.42/2	1 O	158	65.33
2.493	1	116	36.00	1.4115	2	452,630	66.15
2.465	- 11	134	36.00				
2 444	20	110	36.75				
2,303	6	404	39 09				
21000	0		59.00				

0			
d(A)	I	hkl	2⊖(°)
1.4027	1	4.0.10	66.62
1.3912	1	1.2.11	67.24
1.3869	2	446	67.48
1.3795	2	802	67.89
1.3652	< 1	633	68.70
1.3511	1	544,0.0.12	69.52
1.3217	1	1.1.12	71.30
1.3164	1	357	71.63
1.3129	2	0•5•10	71.85
1.3066	1	811	72.25
1.3058	1	618	72.30
1.3002	2	716	72.66
1.2964	2	274	72.91
1.2933	2	182,550	73.11
1.2867	1	2•4•10	73.55
1.2806	< 1	461	73.96
1.2780	1	2•3•11	74.13
1.2706	3	529	74.64
1.2621	3	5.1.10	75.23
1.2557	4	731,078	75.68
_			
1.2506	4	636	76.04
1.2471	4	814	76.29

Ammonium Cadmium Bromide,  $(NH_4)_4 CdBr_6$  (continued)

Sample	CuKa <sub>1</sub>
The sample was precipitated by adding a strong	Tation
following the method of Schwarz [1966].	Intern
forfowing the method of behaving (1900).	d (Å)
Color	7 21
Colorless	/.3L / 39
	3.66
Structure	3.613
Hexagonal, R3m (166), $Z = 3$ , isostructural with $Sr_3(PO_4)_2$ and many other double chromates and	3.237
sulfates [Schwarz, 1966]. The structure of	2.766
$(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].	2.623
Lattice constants of this sample.	2.587
a = 5.5321(3) A	2.439
c = 21.964(2)	2.382
	2.341
c/a = 3.9703	2.207
Valuma	2.196
582 14 Å <sup>3</sup>	2.103
J02.14 A	1.996
Density	1.904
(calculated) 2.703 g/cm <sup>3</sup>	1.830
	1.804
Reference intensity	1.786
corundum - 2.4(2)	1.674
Additional pattern	1.619
1. PDF card 19-71 [Schwarz, 1966]	1.597
	1.593
References Mallor C K (1954) Acta Chem Scand 8 8]	1.568
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344,	1.5604
41.	1 5065
	1.5119
	1.4643
	1.3973
	1.3831
	1 2500
	1 3415
	1.3366
	1.3192
	1.2942
	1,2720
	1.2355
	1.2238
	1.1553
	1.1370
	1,1165
	1.1035
	1.0978
	1.0942
	1.0792
	1.0704
	1.0662
	1.0455

СuКα	$\lambda = 1.5405$	\$98 Å; temp. 25±	:1 °C
Inter	nal standar	d Ag, a = 4.086	51 Å
d (Å)	I	hkl	20 (°)
7.31	95	003	12.09
4.39	60	012	20.22
3.66	2	006	24.33
3.613	2	104	24.62
3.237	100	015	27.53
2.766	50	110	32.34
2.623	10	107	34.15
2.587	30	113	34.64
2.439	3	009	36.82
2.382	3	018,021	37.74
2.341	1	202	38.43
2.207	18	116	40.86
2.196	15	024	41.06
2.103	15	205	42.97
1.996	17	1•0•10	45.40
1.904	2	027	47.74
1.830	7	0•0•12,119	49.78
1.804	9	208,211	50.54
1.786	6	122	51.09
1.674	6	125	54.80
1.619	2	0·2·10	56.82
1.597	5	300	57.69
1.593	4	1·0·13	57.82
1.568	3	217	58.85
1.5604	4	303	59.16
1.5265	2	1.1.12	60.61
1.5119	1	128	61.26
1.4643	3	0.0.15,306	63.48
1.3973	6	2.1.10	66.91
1.3831	6	220	67.69
1.3589	2	223	69.06
1.3415	1	1•2•11	70.09
1.3366	1	309	70.38
1.3192	< 1	1•0•16,312	71.45
1.2942	5	1•1•15,226	73.05
1.2720	3	315	74.54
1.2355	2	2·1·13	77.14
1.2238	1	137	78.02
1.1553	1	045	83.63
1.1370	2	2·0·17,1·3·10	85.29
1.1165 1.1035 1.0978 1.0942 1.0792	2 1 1 2	1.1.18 2.2.12 048,321 2.1.16,232 3.0.15	87.25 88.54 89.12 89.50 91.08
1.0704	1	0·1·20	92.05
1.0662	2	235	92.52
1.0455	2	410	94.92
1.0350	1	413	96.19

Ammonium Zinc Chloride, (NH<sub>4</sub>)<sub>3</sub>ZnCl<sub>5</sub>

Sample The sample was prepared by slow evaporation at room temperature of a 3:1 molar aqueous solution of NH4Cl and ZnCl2. Color Colorless Structure Orthorhombic, Pmcn (62), Z = 4. The structure was determined by Klug and Alexander [1944]. Lattice constants of this sample: a = 9.894(3) Åb = 12.638(4)c = 8.722(3)a/b = 0.7829c/b = 0.6901Volume 1090.6 Å<sup>3</sup> Density (calculated) 1.807 g/cm<sup>3</sup> Reference intensity I/I = 1.55(8) Additional pattern 1. PDF card 2-0548 [Canadian Industries Ltd.] Reference Klug, H. P., and Alexander, L. (1944). J. Amer. Chem. Soc. 66, 1056.

CuKa	$\lambda = 1.540$	598 A;	ten	np. 2	5±1 °C
Inte	rnal standa	rd Si,	a =	= 5.4	3088 Å
d (Å)	I	]	hkl		20(°)
7 70	4.5				
7 • 78	45	1	1	0	11.37
(+1)	13	0	1	1	12.33
6.32	8	0	S	0	14.00
5.805	75	1	1	1	15.25
D+110	05	0	2	1	17.32
4.946	50	2	0	0	17.92
4.549	11	1	2	1	19.50
4.363	18	0	0	2	20.34
4.122	17	0	1	2	21.54
4.074	20	2	1	1	21.80
3.992	12	1	0	2	22.25
3.875	50	1	3	0	22.93
3.803	12	1	1	2	23.37
3.552	12	2	2	1	25.05
3.165	100	2	1	2	28.17
		•	-		
3.030	25	0	3	2	29.46
3.011	25	2	3	1	29.65
2.969	55	0	4	1	30.07
2.993	50	2	2	2	30.77
2.847	12	1	4	1	31.40
2.772	14	3	2	1	32.27
2.725	17	1	1	3	32.84
2.663	8	2	4	0	33.63
2.643	15	0	2	З	33.89
2.632	15	З	0	2	34.04
2.557	9	0	4	2	35.07
2.487	25	3	3	1	36.08
2.474	40	4	0	ō	36.28
2.393	6	0	3	3	37.55
2.358	20	1	5	1	38.14
2. 730	6	6	1	•	39 45
2.273		4	*	•	30.43
2.228	6	<u>د</u>	2	2	3900Z
2.208	6	7	Δ	1	40.83
2.181M	6	0	0	4	40.00
202020	U	Ŭ	Ŭ		-1-01
2.181M		2	5	1	41.37
2 • 149M	10	3	1	3	42.00
2.149M		0	1	4	42.00
2.122	6	4	1	2	42.58
2.071	15	4	3	1	43.67
2.062M	15	З	2	з	43.88
2.062M		0	2	4	43.88
2.021	7	3	4	2	44.82
2.006M	6	3	5	0	45.17
2.006M		1	6	1	45.17
1.0702	۵	2	1	٨	46.03
1.90774	20	2	1	1	40.03
1.9077M	20	0	5	-	47.63
1.8027	15	2	6	1	47.03
10921	10	2	0	-	40.03

Sample	° d(A)	I	h	kl	2⊖(°)
The sample was from the K & K Laboratories,					
Jamaica, New York. The material was melted at					
about 90 °C before being run. The material was	3.204	18	2	3 0	27.82
somewhat hygroscopic.	3.098	35	0	4 0	28.79
	3.031	25	0	3 1	29.45
Color	2.970	70	3	20	30.05
Light gray	2.966	65	1	4 0	30.11
Structure	2.949	100	2	2 1	30.28
Orthorhombic, $P_{21}2_{12}(19)$ , $7 = 4$ . [Cushen and	2.904	€5	1	3 1	30.76
Hulme, 1964].	2.698	12	3	0 1	33.18
naime, 1904j.	2.646	9	2	4 0	33.85
Lattice constants of this sample.	2.603	30	2	3 1	34.43
a = 10.162(3) Å					
h = 12.388(2)	2.539	з	4	0 0	35.32
c = 4.459(1)	2.488	25	4	1 0	36.07
	2.468	25	1	4 1	36.37
a/b = 0.8203	2.409	14	1	5 0	37.30
a/b = 0.3599	2.287	6	3	4 0	39.37
C/D = 0.3333					
Volume .	2.258	6	3	31	39.89
561.3 A <sup>3</sup>	2.227	4	2	5 <b>0</b>	40.47
	2.165M	12	0	5 1	41.68
Density	2.165M		4	з О	41.68
(calculated) $4.277 \text{ g/cm}^3$	2.118	7	1	5 1	42.65
(					
Reference intensity	2.097	7	0	2 2	43.11
I/I = 1.13(8)	2.064	З	0	6 0	43.82
corundum	2.033	13	З	4 1	44.52
Polymorphism	1.999	15	3	5 0	45.32
Antimony bromide, in some cases, crystallizes in	1.993	13	2	5 1	45.48
a $\beta$ -form which is also orthorhombic, but in space					
group Phnm [Cushen and Hulme, 1962].	1.873	4	0	6 1	48.57
group that [busiless and harmon rough	1.842M	19	1	6 1	49.44
References	1.842M		3	1 2	49.44
Cushen, D. W. and Hulme, R. (1962) J. Chem. Soc.	1.824M	5	3	5 1	49.97
1962 2218	1.824M		5	з О	49.97
Cushen D W and Hulme R (1964) J Chem Soc					
1964 4162	1.808	20	0	4 2	50.42
1504, 4102.	1.782	2 <b>C</b>	1	4 2	51.23
	1.7622	20	3	6 0	51.84
(1) $(2)$	1.7575	19	2	6 1	51.99
Currando A = 1.540598 A; temp. 2511 °C	1.7432	5	1	7 0	52.45
Internal standard Si a = 5 42000 a					
Internal Standard SL, a = 5.43088 A	1.6967	9	з	3 2	54.00
	1.6755	10	4	0 2	54.74
	1.6239	7	1	7 1	56.67

4

55

З

30

19

50

9

25

40

16

14

18

14

25

70

7.88 6.20

5.289

5.087

4.701

4.199

4.085

3.931

3.879

3.829

3.622

3.413

3.352

3.269

3.235

1 1 0

0 2 0

1 2 0

2 0 0

2 1 0

3 0

0 2 1

1 2 1

2 0 1

3 1 0

2 1 1

0 1 1

1

2

1

1

11.22

14.28

16.75

17.42

18.86

21.14

21.74

22.60

23.21

24.56

26.09

26.57

27.26

27.55

1.5866

1.5677M

1.5677M

1.5483

1.4476

13

5

7

4

5 4

3 7

8 0

8 1

6 3 0

0

1

1

0

58.09

58.86

58.86

59.67

64.30

Sample				
				d
The sampl	e was obta	ined from the	City Chemical	
COIP., Ne	W IOLK.			3.
Color				3.
Colorless	3			3.
				3.
Structure	mh a star	wature of Dog	101 . 411 0	3.
studied k	v Brassour	and de Rossen	$f_{0}$ $f_{0$	_
Perloff	19771 det	ermined the p	rimitive tri-	3.
clinic ce	ell by sin	gle crystal pre	cession tech-	3.
niques.				3.
				3.
Lattice cor $a = 87$	istants of 1	this sample:		
b = 9.0	00(2)			3.
c = 6.9	)10(1)			3.
$\alpha = 102.3$	38(2)°			3.
$\beta = 98.6$	58(2)			3.
γ = 98.9	)2(2)			
a/b = 0.9	727			2.
c/b = .7	7678			2.
				2.
/olume				2.
515.7 A <sup>3</sup>				
Density				2.
(calculat	ed) 2.986	g/cm <sup>3</sup> assuming	Z = 2	2.
				2.
References			- (1000) -	2.
Brasseur,	logr Kri	e Rosseniosse,	A. (1936). Z.	
		stallgeomtrie	Kristallnhvs	1 2
Kristal	lchem. A95	stallgeomtrie. . 474.	Kristallphys.	2.
Kristal Perloff,	lchem. <u>A95</u> A. (1977).	stallgeomtrie. , 474. Private Commu	Kristallphys. nication.	2.
Kristal Perloff,	lchem. <u>A95</u> A. (1977).	stallgeomtrie. , 474. Private Commu	Kristallphys. nication.	2 • 2 • 2 • 2 •
Kristal Perloff,	Lichem. A95 A. (1977).	stallgeomtrie. , 474. Private Commu	Kristallphys.	2 • 2 • 2 • 2 •
Kristal Perloff, CuKa	Llchem. <u>A95</u> A. (1977). $1 \lambda = 1.540$	stallgeomtrie. , 474. Private Commu 	Kristallphys. nication. 5±1 °C	2 • 2 • 2 • 2 • 2 •
Kristal Perloff, CuKa Inte	Llchem. A95 A. (1977). $\lambda = 1.540$ rnal standa	stallgeomtrie. , 474. Private Commu 	Kristallphys. nication. 5±1 °C 8651 Å	2 · 2 · 2 · 2 · 2 · 2 · 2 ·
Kristal Perloff, CuKa Inte	llchem. <u>A95</u> A. (1977). 1 $\lambda$ = 1.540 rnal standa	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0	Kristallphys. nication. 5±1 °C 3651 Å	2 · 2 · 2 · 2 · 2 · 2 · 2 · 2 ·
Kristal Perloff, CuKa Inte d(Å)	lichem. A95 A. (1977). 1 $\lambda$ = 1.540 rnal standa	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl	Kristallphys. nication. 5±1 °C 3651 Å 20(°)	2 2 2 2 2 2 2 2 2 2
Kristal Perloff, CuKa Inte	llchem. A95 A. (1977). 1 $\lambda$ = 1.540 rnal standa	stallgeomtrie. , 474. Private Commu 0598 A; temp. 2 ard Ag, a = 4.0 hkl	Kristallphys. nication. 5±1 °C 3651 Å 20(°)	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
Kristal Perloff, CuKa Inte d(Å)	llchem. A95 A. (1977). 1 $\lambda$ = 1.540 rnal standa I	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl	Kristallphys. nication. 5±1 °C 3651 Å 20(°)	2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -
Kristal Perloff, CuKa Inte d(Å) 8.61	llchem. <u>A95</u> A. (1977). 1 λ = 1.540 rnal standa I <b>95</b>	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 1C.26	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48	llchem. A95 A. (1977). 1 $\lambda$ = 1.540 rnal standa I 95 25	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 1C.26 10.42	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.67	lichem. A95 A. (1977). $1 \lambda = 1.540$ rnal standa I 95 25 8	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C -1 1 C	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 10.26 10.42 13.10	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.63 6.91	llchem. A95 A. (1977). $1 \lambda = 1.540$ rnal standa I 95 25 8 4 14	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 0 -1 1 0 0 0 1	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 1C.26 10.42 13.10 13.35 14 73	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.63 6.91	llchem. A95 A. (1977). $\lambda = 1.540$ rnal standa I 95 25 8 4 14	<pre>stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C -1 1 C 0 0 1 0 -1 1</pre>	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 1C.26 10.42 13.10 13.35 14.73	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.63 6.91 5.79	llchem. A95 A. (1977). 1 $\lambda = 1.540$ rnal standa I 95 25 8 4 14 9	<pre>stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 0 hkl 0 1 0 -1 1 0 0 0 1 0 -1 1 0 -1 1 -1 0 1</pre>	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 10.26 10.42 13.10 13.35 14.73 15.29	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.63 6.91 5.79 5.53	llchem. A95 A. (1977). A. (1977). I $\lambda = 1.540$ rnal standa I 95 25 8 4 14 9 100	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C -1 1 C 0 0 1 0 -1 1 0 -1 1 -1 3 1 1 0	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 10.26 10.42 13.10 13.35 14.73 15.29 16.01	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.63 6.01 5.79 5.53 4.996	llchem. A95 A. (1977). A. (1977). I $\lambda = 1.540$ rnal standa I 95 25 8 4 14 9 100 8	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C -1 1 C 0 0 1 0 -1 1 -1 0 1 1 1 0 -1 -1 1	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 1C.26 10.42 13.10 13.35 14.73 15.29 16.01 17.74	
Kristal Perloff, CuKa Inte d(A) 8.61 8.48 6.75 6.63 6.91 5.79 5.53 4.996 4.815 0.73	llchem. A95 A. (1977). A. (1977). A. $(1977)$ . I $\lambda = 1.540$ rnal standa I 95 25 8 4 14 9 100 8 35	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C -1 1 C 0 0 1 0 -1 1 -1 0 1 1 1 0 -1 -1 1 1 -1 1	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 1C.26 10.42 13.10 13.35 14.73 15.29 16.01 17.74 18.41	
Kristal Perloff, CuKa Inte d (Å) 8.61 8.48 6.75 6.63 6.91 5.79 5.53 4.996 4.815 4.731	llchem. A95 A. (1977). A. (1977). A = 1.540 rnal standa I 95 25 8 4 14 9 100 8 35 10	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C -1 1 C 0 0 1 0 -1 1 -1 0 1 1 1 0 -1 -1 1 1 -1 1 0 1 1	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 1C.26 10.42 13.10 13.35 14.73 15.29 16.01 17.74 18.41 18.74	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.63 6.01 5.79 5.53 4.996 4.815 4.731 4.631	llchem. A95 A. (1977). A. (1977). A. $(1977)$ . I $\lambda = 1.540$ rnal standa I 95 25 8 4 14 9 100 8 35 10 30	<pre>stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 0 -1 1 C 0 0 1 0 -1 1 0 -1 1 1 1 0 -1 -1 1 1 -1 1 0 1 1</pre>	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 1C.26 10.42 13.10 13.35 14.73 15.29 16.01 17.74 18.41 18.74	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.63 6.01 5.79 5.53 4.996 4.815 4.731 4.631 4.312	llchem. A95 A. (1977). A. (1977). A. $(1977)$ . I $\lambda = 1.540$ rnal standa I 95 25 8 4 14 9 100 8 35 10 30 3	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C -1 1 C 0 0 1 0 -1 1 -1 2 1 1 1 0 -1 -1 1 1 -1 1 0 2 0	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 10.26 10.42 13.10 13.35 14.73 15.29 16.01 17.74 18.41 18.74 19.15 20.58	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.63 6.01 5.79 5.53 4.996 4.815 4.731 4.631 4.312 4.134	llchem. A95 A. (1977). A. (1977). A. $(1977)$ . I $\lambda = 1.540$ rnal standa I 95 25 8 4 14 9 100 8 35 10 30 3 12	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C -1 1 C 0 0 1 0 -1 1 -1 1 1 1 -1 1 0 1 1 -1 1 1 0 2 0 -1 2 0	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 10.26 10.42 13.10 13.35 14.73 15.29 16.01 17.74 18.41 18.74 19.15 20.58 21.22	
Kristal Perloff, CuKa Inte d(Å) 8.61 8.48 6.75 6.63 6.91 5.79 5.53 4.996 4.815 4.731 4.631 4.312 4.134 4.141	llchem. A95 A. (1977). A. (1977). A. $(1977)$ . I $\lambda = 1.540$ rnal standa I 95 25 8 4 14 9 100 8 35 10 30 3 12 17	stallgeomtrie. , 474. Private Commu 0598 Å; temp. 2 ard Ag, a = 4.0 hkl 0 1 C 1 0 C -1 1 C 0 0 1 0 -1 1 -1 3 1 1 1 0 -1 -1 1 1 -1 1 0 1 1 -1 2 0 -2 1 0	Kristallphys. nication. 5±1 °C 3651 Å 20(°) 10.26 10.42 13.10 13.35 14.73 15.29 16.01 17.74 18.41 18.74 19.15 20.58 21.22 21.44	

d (A)	I	hkl	20(°)
3.929	40	-2 0 1	22.61
3.791	40	1 -2 1	23.45
3.626	30	-2 1 1	24.53
3.597	14	-1 -2 1	24.73
3.574	12	1 2 0	24.89
3.406	14	2 -1 1	26.14
3.381	10	0 -1 2	26.34
3.370	11	-2 2 0	26.43
3.331	40	-1 2 1	26.74
3.314	45	0 0 2	26.88
3.306	55	-1 0 2	26.95
3.272M	12	-1 -1 2	27.23
3.272M	~	0 2 1	27.23
3.051	6	2 - 2 1	29.25
3.020	4	1 -1 2	29.55
2.956	7	-2 2 1	30.21
2.90 5M	65	0 -3 1	30.75
2.905M		1 0 2	30.75
2.874	40	0 3 0	31.09
2.865M	50	0 1 2	31 • 19
			74.40
2.865M		-1 -2 2	31.19
2.851	40	1 - 3 1	31.35
2.830M	35		31.59
2.830M		300	31.07
2.191	40	1 -2 2	51.97
2.768	4	2 2 0	32.32
2.738	3	-3 1 1	32.68
2.680	8	-2 1 2	33.41
2.629	8	-2 3 0	34.07
2.609	25	-3 2 0	34.34
0.55.0	25	_ 7 _ 1 _ 1	74 40
2.598	25	-3 -1 1	75 01
2.547M	35	3 1 0	75 21
2.0347M	7	3 - 1 1	35.53
2.4954	12	-2 -2 2	35.96
2049311			
2.495M		-1 3 1	35.96
2.439	25	301	36.82
2.433	25	-1 2 2	36.92
2.408M	12	2 -2 2	37.31
2.408M		1 -3 2	37.31
2.388	0	-3 0 2	37.63
2.364	3	0 2 2	38.03
2.282M	5	-1 -1 3	39.46
2.282M	•	-2 -3 1	39.46
2.278	4	0 -1 3	39.53
2.260	6	-3 -2 1	39.86
2.246M	10	-3 3 0	40.11
2.246M		-1 0 3	40.11
2.215	19	0 -4 1	40.70
2.206+	20	0 0 3	40.87

Barium Cadmium Chloride Hydrate,  $BaCdCl_4 \cdot 4H_20$  - (continued)

d (Å)	I	hkl	20(°)
2.206+		311	40.87
2.193M	13	-1 4 0	41.13
2.193M		2 3 0	41.13
2.172M	10	-1 -2 3	41.55
2.172M		2 -3 2	41.55
2.157M	25	2 1 2	41.84
2.157M		0 4 0	41.84
2.152	20	3 - 7 1	41 04
2 1 7 2	10	-2 0 7	40 77
2.107	19	-2 0 3	42.037
20121	25	-2 -5 2	42047
2.121M	25	1 -1 3	42.59
2.121M		4 0 0	42.59
2.102	17	-331	42.99
2.096	14	-2 4 0	43.13
2.080M	40	1 -2 3	43.47
2000011			40041
2.080M		-3 2 2	43.47
2.075M	45	-1 -4 1	43.59
2.075M		-1 1 3	43.59
2.070	25	-4 2 0	43.69
2.051	з	0 -4 2	44.13
2.023M	8	1 -4 2	44.76
2.023M		3 - 2 2	44.76
2.017	10	-4 2 1	44.90
2.010	10	-1 3 2	45.06
2.007	14	-2 1 3	45.13
2.002	12	0 -3 3	45.25
1.976	6	4 - 1 1	45.88
1.973M	6	4 1 0	45.96
1.973M		3 0 2	45.96
1.963M	6	-1 -4 2	46.22
1.9634		-2 3 2	46.22
1.038	9	4 - 2 1	40.22
1 0704	14	4 - 2 1	40.04
1 0724	T.44		47.00
1.0184	15	-4 1 2	47.00
1.910+	15	4 0 1	47.35
1.918+		0 4 1	47.35
1.915	10	-3 -1 3	47.44
1.932M	6	-3 4 0	47.79
1.902M		-4 -1 2	47.79
1.894M	12	2 -1 3	48.00
1.894M		3-3 2	48.00
1.880M	4	2 - 2 3	48.37
1.880M		2 2 2	48.37
1.871	1	3 - 4 1	48.62
1.847+	10	-1 2 3	49.30
1.847+		-3 -3 2	49.30
1.975	5	-4 -3 1	49,64
1.035	5	-4 -2 1	49.04
1.822	3	-2 0 3	50.02
1.815+	2	-2 2 3	50.23
1.815+		4 -3 1	50.23

d (Å)	I	hkl	20(°)
1.7958M	4	0 2 3	5 <b>0.</b> 80
1.7860M	8	2 - 3 3	51 • 10 51 • 10
1.7821	6	4 1 1	51.22

Barium Chromium Oxide, Ba<sub>3</sub>(CrO<sub>4</sub>)<sub>2</sub>

Sample	CuK
The sample was prepared by heating a 2:1 molar mixture of $BaCrO_4$ and $Ba(OH)_2$ at 1000°C for 2 hours in a stream of Na	Int
nouis in a stream or N2.	d (Å)
Color Blackish green	7.12
	4.839
Structure	3.638
Hexagonal, $R3m$ (166), $Z = 3$ , isostructural with	3.242
Ba <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> [Wilhelmi and Jonsson, 1965]. The structure of Ba <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> was studied by Zachari-	2.872
asen [1948].	2.470
	2.420
Lattice constants of this sample:	2.376
a = 5.7406(5) A	2.353
c = 21.389(3)	2.254
c/a = 3.7259	2.235
	2.149
Volume.	1.965
610.44 A <sup>3</sup>	1.9283
	1.8722
Density	
(calculated) 5.256 g/cm <sup>3</sup>	1.8306
	1.7/31
Additional patterns	1.7203
1. PDF card 19-120 [Banks and Jaunarajs, 1965]	1 6214
2. PDF Card 21-64 [Gordeev and Serdyukov, 1967]	1.0214
References	1.5028
Banks, E. and Jaunarajs, K. L. (1965). Inorg.	1.4602
Chem. 4, 78.	1.4352
Gordeev, S. Ya. and Serdyukov, V. I. (1967).	1.4260
Inorg. Mater. USSR <u>3</u> , 1440.	1.4117
Wilhelmi, KA. and Jonsson, O. (1965). Acta	
Chem. Scand. <u>19</u> , 177.	1.3759
Zachariasen, W. H. (1948). Acta Crystallogr.	1.3593
<u>1</u> , 263.	1.3348
	1.3124
	1.3021

CuKo	$\alpha_1 \lambda = 1.5405$	598 Å; temp. 2	5±1 °C			
Inte	Internal standard Ag, $a = 4.08651 \text{ Å}$					
d (Å)	I	hkl	20 (°)			
7.12	l	003	12.43			
4.839	8	101	18.32			
3.638	8	104	24.45			
3.242	100	015	27.49			
2.872	85	110	31.12			
2.470	3	021	36.34			
2.420	6	202	37.12			
2.376	11	009	37.83			
2.353	1	018	38.22			
2.254	12	024	39.96			
2.235	3	116	40.32			
2.149	45	205	42.00			
1.965	30	1.0.10	46.15			
1.9283	1	027	47.09			
1.8722	1	211	48.59			
1.8306	11	119	49.77			
1.7731	2	214	51.50			
1.7203	25	125	53.20			
1.6568	11	300	55.41			
1.6214	11	0•2•10	56.73			
1.5028	<1	306	61.67			
1.4602	5	0•1•14	63.68			
1.4352	11	220	64.92			
1.4260	4	0.0.12	65.39			
1.4117	12	2•1•10	66.14			
1.3759	l	131	68.09			
1.3593	3	309	69.04			
1.3348	1	134	70.49			
1.3124	8	315	71.88			
1.3021	1	2•0•14	72.54			
1.2770	12	1•1•15	74.20			
1.2288	3	229	77.64			
1.2104	1	404	79.05			
1.1937	4	045	80.38			
1.1857	3	1•2•14	81.03			

Barium Manganese Oxide,  $Ba(MnO_4)_2$ 

Sample The sample was obtained from K & K Laboratories, Jamaica, New York.				
Color	d (Å)	I	hkl	20(°)
Reddish purple				
	2.217	40	4 2 2	40.66
Structure	2.175	16	1 3 3	41.49
Orthorhombic, Fddd $(70)$ , Z = 8. The structure	2.0797	9	3 1 3	43.48
was determined by Hardy et al. [1971].	2.0527	10	0 6 2	44.08
	2.0015	5	1 7 1	45.27
Lattice constants of this sample:				
a = 11.915(1)A	1.9330	14	3 3 3	46.97
b = 14.778(1)	1.9183	7	620	47.35
c = 7.4278(7)	1.8751	4	153	48.51
	1.8572	8	0 0 4	49.01
a/b = 0.8063	1.8469	8	0 8 0	49.30
c/b = 0.5026				
	1.8078	11	371	50.44
Volume	1.7512	6	602	52.19
1307.9 A <sup>3</sup>	1.7236	2	2 2 4	53.09
	1.7126	7	3 5 3	53.46
Density	1.6901	6	4 6 2	54.23
(calculated) 3 811 g/cm <sup>3</sup>	1.0901	Ũ	4 0 2	04420
(carcarated) 5.011 g/cm	1 4501	7	0 0 0	66.33
Poforongo intensity	1.0591	, ,	7	55,55
T/T	1.6484	5	/ 1 1	55.72
1/1 corundum = 1.81(12)	1.5936	3	282	5/.81
	1.5891	4	1 9 1	57.99
Additional pattern 1. PDF card 14-697 [Hardy, 1962].	1.5824	10	642	58.26
	1.5755	9	4 0 4	58.54
References	1.5723	10	7 3 1	58.67
Hardy, A. (1962). Ann. Chim. Paris 7, 281.	1.5457M	5	6 6 C	59.78
Hardy, A., and Fourre, B. (1971), C. B. Acad.	1.5457M		5 7 1	59.78
Sci. Paris Ser. C. 273, 1508.	1.4893M	6	8 0 0	62.29
	1.4893M		373	62.29
	1.4868	8	3 9 1	62.41
	1.4670	2	1 1 5	63+35
	1.4408	6	<u> </u>	64.19
	1 4450	8	7 5 1	64.36
	1.440414	0	, U .	04000
0	1.4464		A 8 2	64.36
$CuK\alpha_1 \lambda = 1.540598 \text{ A}; \text{ temp. } 25\pm1 \text{ °C}$	1. 3062	3	7 1 3	66.97
	1.3902	5	315	67.57
Internal standard Si, a = 5.43088 A	1.3052	5		69.36
	1.3/29	5	0 10 2	60.07
$d(A)$ T $hk\ell$ 20(°)	1.3595M	2	1 9 3	69.03
	1 75054		8 2 2	69.03
	1.3595M	•	7 7 7	69.66
5.794 40 1 1 1 15.28	1.3487	4	7 3 3	70.25
3,882 13 1 3 1 22,80	1.3388	4		70.54
	1.3349	5	0 2 4	70+54
	1.3192	2	1 5 5	/1.45
				71 70
3.318 95 0 2 2 20.85	1.3140	2	1 11 1	11+18
	1.3099	З	084	72.04
2.981 14 4 0 0 29.95	1.3046	4	771	72.38
2.899 4 2 2 2 30.82	1.2939	4	393	73.07
2.855 45 3 3 1 31.31	1.2709	1	682	74.62
2.676 3 1 5 1 33.46				
2.399 12 2 4 2 37.46	1.2672	4	7 5 3	74.87
	1.2588	З	3 5 5	75.46
2.393 14 1 1 3 37.55	1.2544	3	3 11 1	75.77
2.320 4 4 4 0 38.78	1.2473	3	4 10 2	76.28
2.277 13 2 6 0 39.54	1.2312	2	0 12 0	77.46
2.258 45 3 5 1 39.90				
2.244 9 5 1 1 40.16				

Sample

The sample was obtained from K & K Laboratories, Inc., Plainview, N. Y.

Color

Colorless

Structure Hexagonal,  $P6_122$  (178) or  $P6_522$  (179), Z = 6. The structure was determined by Ferrari and Cavalca [1948].

Lattice constants of this sample: a = 7.0759 (3) A c = 17.897 (1)

c/a = 2.5293

Volume 776.0 Å<sup>3</sup>

Density

(calculated) 3.176 g/cm<sup>3</sup>

Reference intensity I/I = 1.36(12)

Additional pattern 1. PDF card 1-1112 [Hanawalt et al., 1938].

References

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Ferrari, A. and Cavalca, L. (1948). Period.
Mineral. <u>17</u>, 125.
Hanawalt, J. D., Rinn, H. W. and Frevel, L. K.
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(1938). Ing. Eng. Chem. Anal. Ed. <u>10</u>, 457.

CuKα	$\lambda = 1.540$	598 A; temp. 2	5±l °C
Inte	rnal standa	rd Ag, $a = 4.00$	8651 Å
d (Å)	I	hkl	20(°)
6.12	50	100	14.45
5.79	5	101	15.29
5.058	100	102	17.52
4.275	90	103	20.76
3.616	50	104	24.60
3.535	7	110	25.17
3.469	90	111	25.66
3.289	19	112	27.09
3.062	10	200	29.14
3.042	16	113	29.34
3.017	60	201	29.59
2.979	40	006	29.97
2.899	10	202	30.82
2.777	35	114	32.21
2.724	4	203	32.85
2.681	30	106	33.40
2.528	40	204	35.48
2.518	65	115	35.63
2.360	4	107	38.10
2.328	40	205	38.65

d (Å)	I	hkl	20(°)
2,316	14	210	38 85
2.310	45	210	20.00
2.200		116	39.20
2.280	, ,	110	39.49
2.241	22	212	40.20
2.159	25	213	41.80
2.137	7	206	42.25
2.101	11	108	43.01
2.073	14	117	43.63
2.057	16	214	43.98
2.043	6	300	44.30
2.030	4	301	44.61
1,992	6	302	45.50
1,963	14	207	46.20
1 944	15	215	46 69
1.932	20	303	46,99
1.891	16	109,118	48.09
1.858	2	304	48.99
1.830	2	216	49.79
1.807	2	208	50.45
1.769	2	220	51.64
1 760	2	221	51 01
1 726	9	221	52 69
1.730	15	1.0.10 217	52.09
1.700	15	1,0,217	53.31 E3.00
1.700	10	310	53.89
1.692	13	311	54.16
1.685	9	306	54.39
1.669	2	312,209	54.98
1.6454	9	224	55.83
1.6343	1	313	56.24
1.6089	8	218	57.21
1,5964	3	1•1•10.307	57.70
1.5859	2	225	58.12
1 5721	2	1•0•11	58 68
1 5450	2	2.0.10	59.81
1.5355	7	315	60.22
1 5316	-	460	60.20
1.5316	5	400	60.39
1.5220	3	226	60.81
1.5092	5	219,308	61.38
1.4915	2	0.0.12	62.19
1.4840	10	403	62.54
1.4770	20	316	62.87
1.4492	2	404,1.0.12	64.22
1.4374	4	2.0.11	64.81
1.4247	7	309	65.46
1.4158	11	2.1.10,317	65.92
1.4014	2	321	66.69
1.3889	13	322	67.37
1.3741	1	1.1.12	68.19
1.3685	1	323	68.51
1.3629	2	406	68,83
1.0025	2		

	d(A)	I	, hkl	20(°)
	1,3531	1	, 318	69.40
	1.3411	- 7	324.2.0.12	70.11
	1.3334	, 5	411	70.58
	1.3312	5	2•1•11	70.71
	1 3223	4	412 229	71 26
	1.3223	4	412,229	/1.20
	1.3086	2	325	72.12
	1.3047	5	413	72.37
	1.2834	3	1•1•13	73.77
	1.2812	6	414	73.92
	1.2717	3	326	74.56
	1.2582	3	2•2•10	75.50
	1.2558	3	2•0•13	75.67
ł	1.2516	б	1•0•14	75.97
	1.2320	2	3•1•10,327	77.40
	1.2228	3	501	78.09
ŀ	1.2138	4	502,409	78,78
	1.2045	2	3.0.12	79.51
	1,2021	2	1•1•14	79.70
	1,1906	5	328	80.63
	1,1838	4	2.1.13	81,19
1	1.1030	•	2 1 19	01.19
	1 <b>.1</b> 798	4	2•0•14,330	81.52
	1.1754	5	3•1•11	81.89
	1 <b>.17</b> 11	3	1.0.15	82.26
	1.1593	2	505	83.28
	1 <b>.1</b> 557	4	421	83.60
	1.1480	4	329	84,29
	1.1371	3	423	85,29
	1.1336	3	506	85,61
	1,1209	6	424.3.1.12	86,82
	1.1193	7	2•1•14	86.98
	1 1 1 7 7	0	2.0.15	07 70
	1.111/	2	2•0•15	87.72
	1.1097	3	419	87.92
	1.1054	5	3•2•10,507	88.35
	1.1019	4	425	88.70
	1.0986	6	511	89.04
	1.0922	2	512	89.70
	1.0795	1	426	91.05
	1.0708	4	4.1.10,337	92.00
	1.0697	4	3•1•13	92.13
	1.0687	5	514,4•0•12	92.24
	1.0665	3	1.1.16	92.49
	1.0605	2	2.1.15	93.16
	1.0549	2	427	93.81

Barium Nitrite Hydrate,  $Ba(NO_2)_2 \cdot H_2O$  (continued)

Beryllium Sulfate, BeSO<sub>4</sub>

			_				
Sample	CuK $\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å						
Beryllium nitrate was treated with H <sub>2</sub> SO <sub>4</sub> and evaporated. The process was repeated and the							
sample recrystallized from water. The tetra- hydrate so formed was dehydrated at 44 °C for over an hour.	d (Å)	I		hkl		20(°)	
Color	3.765	100	1	0	1	23.61	
Colorless	3.449	5	0	0	2	25.81	
001011035	3.177	З	1	1	0	28.06	
Structure	2.336	30	1	1	2	38.51	
Tetragonal. $T4(82)$ , $7 = 2$ . The structure was	2.0457	2	1	0	з	44.24	
studied by powder and single crystal methods							
[Grund, 1955; Kokkoros, 1956].	1.9287	10	2	1	1	47.08	
(orana, 1900, nonnorob, 1900).	1.8817	6	2	0	2	48.33	
Lattice constants of this sample:	1.7227	1L	0	0	4	53.12	
a = 4.4927(4) Å	1.5879	2	2	2	0	58.04	
b = 6.8937(8)	1.5126	10	2	1	з	61.23	
c/a = 1.6059	1.4639	1L	З	0	1	63.50	
	1.4432	2	2	2	2	64.52	
Volume	1.4203	2	З	1	0	65.69	
139.14 A <sup>3</sup>	1.3675	4	2	0	4	68.57	
	1.3134	2	З	1	2	71.82	
Density							
(calculated) 2.507 g/cm <sup>3</sup>	1.2544	2	3	0	З	75.77	
	1.2261	4	3	2	1	77.84	
Reference intensity	1.1680	1L	2	2	4	82.52	
$I/I_{1} = 1.9(2)$	1.1369	2	2	1	5	85.30	
Corundum	1.0956	2	3	2	з	89.35	
Additional patterns	1 000/				,		
1. PDF card 15-612 [Petersen, D. R., Rinn,	1.0804	1	1	1	6	90.95	
H. W. and Sutton (1963. Dow Chemical Co.,	1.0/04	2	4	1	1	91.39	
Midland, Michigan 48640].	1.0500	1	4	5	2	92.31	
2. Grund, A. [1955].	1.0390	1.	3	3	4	93.34	
	1.0229	1	٢	U	0	91.11	
References	1.0142	2	7	0	5	68.84	
Grund, A. (1955). Tschermak's Mineral.	1.0123	1	3	3	2	99.10	
Petrogr. Mitt. <u>5</u> , 227.	1.0044	1	4	2	0	100.16	
Kokkoros, P. (1956). Tschermak's Mineral.	.9845	11	4	1	3	102.96	
Petrogr. Mitt. <u>6</u> , 116.				•	-		

Sample	o d (A)	I		hkl	20(°)	
The sample was prepared by heating a 1:1 mixture						
or Tiu <sub>2</sub> , anatase, and Cou in a torch, then heat-	1.9206	8	1	0 7	47.29	
ing in a furnace at 700 °C for approximately 65	1.7985	25	1	1 6	50.72	
nours.	1.7171	14	0	1 8	53.31	
On loss	1.7040	5	2	1 1	53.75	
Colorless	1.6707	2	1	2 2	54.91	
	1.5569	30	2	1 4	59.31	
Structure	1.5490	4	ō	2 7	59.64	
Hexagonal, $R3(148)$ , $Z = 6$ , isostructural with	1.5130	20	З	0 0	61.21	
ilmenite, FeTiO <sub>3</sub> . The structure of FeTiO <sub>3</sub> was	1.4851	3	1	2 5	62.49	
determined by Barth and Posnjak [1934].	1.4466	2	3	0 3	64.35	
Lattice constants of this sample:	1 4760	•	~		64 69	
a = 5.2403(1) Å	1.4300	4	2	0 0	66 22	
c = 14.8380(6)	1.7051	0	1	1 0	67 07	
	1.3335	4	1	1 7	20.57	
c/a = 2.8315	1.3100	e	2	2 0	72.03	
17- June		-	-	-		
	1 • 29 30	3	0	1 11	73.13	•
552.07 A	1.2901	4	3	0 E	73.32	
Dongity	1.2664	2	2	2 3	74.93	
(a)(a)(a)(a)(a) = 0	1.2593	é	1	28	75.42	
(calculated) 5.001 g/cm	1.2540	2	1	3 1	75.80	
Reference intensity	1.2419	5	0	2 10	76.67	
$I/I_{corundum} = 5.0(3)$	1.1918	10	1	3 4	80.53	
COT MINUM	1.1591M	5	2	0 11	83.30	
Polymorphism	1.1591M	•	3	1 5	83.30	
According to Posnjak and Barth [1934], a high	1.1576	5	2	2 6	83.43	
temperature perovskite modification found by						
Zachariasen [1928] exists when CdTiO <sub>3</sub> is pre-	1.1312	1L	4	0 1	85.84	
pared at temperatures above 1050 °C.	1.1220	5	2	1 10	86.71	
Additional anthrony	1.1181	4	1	1 12	87.09	
Additional patterns	1.0849	5	4	04	90.47	
Ltd.].	1.0823	6	1	37	\$0.75	
2. Posnjak and Barth [1934].	1 06 04					
	1.0604	4	1	2 11	93.18	
References	1.0705	5	3	1 8	95.40	
Barth, T. F. W. and Posnjak, E. (1934). Z.	1.0321	3	3	2 1	95.70	
Kristallogr. Kristallgeometrie Kristallphys.	1.0257	11	2	2 9	90.55	
Kristallchem. 88A, 265.			-		57000	
Posnjak, E. and Barth, T. F. W. (1934). Ibid.	1.0024	9	З	2 4	100.43	
271.	.9903	11	4	1 0	102.13	
Zachariasen, W. H. (1928). Skr. Nor. Vidensk.	.9824	1	2	3 5	103.27	
Akad. Oslo, No. 4.	.9711	3	4	1 3	104.97	
	.9680	З	0	4 8	105.46	
$CuK\alpha_1 \lambda = 1.540598 \text{ Å: temp. } 25\pm1 \text{ °C}$	.9602	٩	2	0.14	106 69	
	.9345	1	7	2 7	111.03	
Internal standard Ag, $a = 4.08651$ A	.9256	4	1	1 15	112.66	
	.91 94	8	4	1 6	113.83	
$d(A)$ I $hk\ell$ 2 $\Theta(^{\circ})$	.9079	4	2	3 8	116.09	
4.946 7 0 0 3 17.92	•9016	7	1	2 14	117.38	
4.344 18 1 0 1 20.43		5	U	3 4	127 76	
3.870 14 0 1 2 22.96	•0734	5	3	3 0	123.70	
2.873 100 1 0 4 31.11	L					
2.620 70 1 1 0 34.20						
2.4834 7 0 1 5 36.14						
2.3150 25 1 1 3 38.87						
2.2431 10 0 2 1 40.17						
2.1692 1 2 0 2 41.60						
1.9357 35 0 2 4 46.90						

Sample	CuKαl	$\lambda = 1.5405$	98 A;	temp.	25±1	L °C
The sample was prepared by heating a 3:1 molar mixture of CaCO <sub>3</sub> and $Cr_2O_3$ at 950 °C for 6 days, with intermittent grindings	Intern	al standar	d Ag,	a = 4	1.0865	51 Å
with internitient grindings.	d(A)	I	h	kl		20(°)
Color						
Black	8.39	ç	0	1	2	10.54
Chanadana	6.66	9	1	0	4	13.29
Structure Howagonal $B_{2n}$ (167) 7 - 21 The structure has	5.391	25	1	1	0	16.43
heen studied by Sinha and Srivastava [1973]	4.962	2	1	1	з	17.86
Earlier the formula was given as $Ca_9Cr_6O_{24}$ (or	4.535	14	2	0	2	19.56
was present in two valences Glasser and Osborn	4.237	8	0	1	8	20.95
[1958] suggested the probability that all Cr	4 • 193	20	0	2	4	21.17
ions were in a valence of 5 and that the struc-	4.115	4	1	1	6	21.58
ture is closely related to $Ca_3(PO_L)_2$ (whitlockite).	3.524	40	1	0 1	10	25.25
	3.469	З	1	2	2	25.66
Lattice constants of this sample:	3.308	50	2	1	Δ	26.93
a = 10.779(1) Å	3.176	4	ō	0 1	12	28.07
c = 38.099(8)	3.109	10	3	0	0	28.69
/ 2.5246	2.951	100	0	2 1	10	30.26
c/a = 3.5346	2.834	25	1	2	8	31.54
Volume 。				_		
3833.6 A <sup>3</sup>	2.795	6	3	0	6	32.00
	2.00	10	1	1 1	.2	32071
Density	2.636	6	2	2	3	33.09
(calculated) 3.204 g/cm <sup>3</sup>	2.612	4	ō	1	14	34.30
Reference intensity	_					
I/I = 1.00(7)	2.588	16	2	1 1	10	34.63
-/ corundum	2.480	10	2	2	6	36.19
Additional patterns	2.453	5	3	1	5	36.60
1. PDF card 11-415 [Glasser & Osborn, 1958]	2.351	2	2	01	.4	38.26
2. PDF card 25-130 [British Steel Corp.,	2.315	o	U	4	۷	38.87
Rotherham, England	2.308	10	1	0 1	16	38.99
3. Ford & Rees [1949]	2.273M	4	З	1	8	39.61
4. Sinna and Srivastava [1975]	2.273M		2	2	9	39.61
References	2.269	5	4	0	4	39.70
Ford, W. F. and Rees, W. J., (1949). Trans. Brit.	2.222	5	З	0 1	12	40.57
Classer E P and Osborn E E (1958) J Am	2.139	4	3	2	1	42.22
Ceram Soc 41 358	2.129	5	2	3	2	42.43
Sinha, D. P. and Srivastava, B. C. (1973). Indian	2.122	З	0	2 1	16	42.57
J. Phys. 47 746.	2.096	8	0	4	8	43.12
·	2.091	7	3	2	4	40024
	2.054	2	2	2 1	12	44.06
	2.011	З	4	1	3	45.05
	1.990	30	4	0 1	10	45.54
	1.953	6	2	3	8	46.45
	1.940M	14	1	31	13	46.80
	1.940M		4	1	6	46.80
	1.876	4	З	1 1	14	48.48
	1.868M	12	3	2 1	0	48.72
	1.868M		0	1 2	20	48.72
	1.8323	11	0	5	4	49.72
	1.7972	2	з	з	0	50.76
	1.7785	2	З	3	З	51.33
	1.7638	35	2	0 2	20	51.79
	1.7509	7	3	0 1	8	52.20
	1.7382	7	5	0	8	52.61

d (Å)	I	hkl	20(°)
1.7352	8	2 4	4 52.71
1.7150	4	4 1 3	12 53.38
1.6821	4	2 3	14 54.51
1.6767M	7	0 5	10 54.70
1.6767M		1 2	20 54.70
1.6663	5	4 0 3	16 55.07
1.6525M	6	51	4 55.57
1.6525M		33	9 55.57
1.6007	12	24	10 57.53
1.5924	10	3 2	16 57.86
1.5819	5	1 5	8 58.28
1 • 56 29	З	33	12 59.06
1.5557	8	60	0 59.36
1•5339M	З	3 1	20 60.29
1.5339M		4 3	1 60.29
1.5150	5	4 3	4 61.12
1.4943	2	52	0 62.06
1.4755	7	0 4 3	20 62.94
1.4672M	5	4 1	18 63.34
1.4672M		33	15 63.34
1.4604	4	34	8 63.67
1.4550M	8	5 1	13 63.93
1.4550M		52	6 63.93
1.4231+	6	4 3	10 65.54
1.4231+		23	20 65.54

Calcium Chromium Oxide,  $Ca_3(CrO_4)_2$ 

å (Å)

Sample The sample of sodium fluoride phosphate hydrate obtained from Alfa Inorganics, Inc., Beverly, Mass. was dissolved and filtered. Calcium chloride was then added and the solution was filtered. The solution was placed at 0 °C over- night. The crystallites were dried in a dessi- cator.
*Insufficient sample was available to complete the intensity measurements. The powder data peak height intensities given in the table were calculated from the structure data [Perloff, 1972].
Major impurities 0.001-0.01% Na
Color Colorless
<pre>Structure Triclinic, Pl(2), Z = 2. The structure was determined by Perloff [1972].</pre>
Optical data Biaxial (+), $\mathrm{N}_{\alpha}$ = 1.485, $\mathrm{N}_{\beta}$ = 1.495, $\mathrm{N}_{\gamma}$ = 1.512. 2V is large.
Lattice constants of this sample: a = 6.225(2) A b = 8.378(2) c = 5.738(1) $\alpha = 93.31(2)^{\circ}$ $\beta = 114.75(2)$ $\gamma = 109.07(2)$
a/b = 0.7430 c/b = 0.6849
Volume °3 250.17 Å <sup>3</sup>
Density (calculated) 2.311 g/cm <sup>3</sup>
Reference Perloff, A.(1972). Acta Crystallogr. <u>B28</u> , 2183.

CuK $\alpha_1 \lambda = 1.540598 \text{ Å}$ ; temp. 25±1 °C Internal standard W, a = 3.16524 Å

I\*

hkl

20(°)

7.60	100	0 1	0	11.50
7.09	100		~	11.00
5.211	2	1 0	0	17.00
4.971		-1 0	1	17.83
4.759	2	0 -1	1	18.63
4.485	44	-1 1	1	19.78
3.924	59	-1 -1	1	22.64
3.857M	9	0 1	1	23.04
3.857M		0 2	•	23.04
3.0074		1 1	~	23.04
3.705	1	1 1	0	24.00
3.472	1	0 -2	1	25.64
3.287	47	-1 2	1	27.11
3.072	3	-2 1	1	29.04
3.006	21	1 0	1	29.70
2.932	30	1 -2	1	30.46
2 949	30	_1 _2		21.37
2.049	30	-1 -2	1	31.37
2.820	4	-2 1	0	31.70
2.7824	7	0 2	1	32.15
2.782M		-2 2	1	32.15
2.697	13	-2 2	0	33.19
2.605	30	2 0	Ň	34.30
2.000	30	2 0	0	34.37
	0.4		~	24 60
2.590	24	0 -1	2	34.60
2.569	11	03	0	34.89
2.538M	3	0 0	2	35.34
2.538M		0 -3	1	35.34
2.512	6	1 1	1	35.72
2000-		• •	•	300.2
2 472	6	-2 1	2	26.32
2.472	0	-2 1	2	30.32
2.431	6	1 -3	1	36.95
2.382	2	0 -2	2	37.73
2.349	4	-1 -2	2	38.29
2.339	4	-2 3	0	38.45
2-315	10	-2 3	1	38.87
2 264	7	0 1	2	70.70
2.204			2	39079
2.157	IL	-1 -3	1	41.85
2.110	6	0 3	1	42.83
2.053M	13	-2 -2	1	44.08
2.053M		0 -3	2	44.08
2.053M	3	0 -3	2	44.08 44.91
2.053M 2.017	3	0 -3	2	44.08 44.91
2.053M 2.017 1.952M	3 10	0 -3 1 3 -2 4	200	44.08 44.91 46.48
2.053M 2.017 1.952M 1.952M	3 10	0 -3 1 3 -2 4 1 0	2 0 0 2	44.08 44.91 46.48 46.48
2.053M 2.017 1.952M 1.952M 1.927	3 10 7	0 -3 1 3 -2 4 1 0 0 4	2 0 2 0	44.08 44.91 46.48 46.48 47.13
2.053M 2.017 1.952M 1.952M 1.927	3 10 7	0 -3 1 3 -2 4 1 0 0 4	20020	44.08 44.91 46.48 46.48 47.13
2.053M 2.017 1.952M 1.952M 1.927 1.898	3 10 7 8	0 -3 1 3 -2 4 1 0 0 4 -3 3	2 0 2 0	44.08 44.91 46.48 46.48 47.13 47.90
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526	3 10 7 8 6	0 -3 1 3 -2 4 1 0 0 4 -3 3 2 2	2 0 2 0 1 0	44.08 44.91 46.48 46.48 47.13 47.90 49.14
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282	3 10 7 8 6 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2 0 2 0 1 0 3	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282	3 10 7 8 6 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2 0 2 0 1 0 3 3	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84 51.09
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282 1.7863	3 10 7 8 6 2 5	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2 0 2 0 1 0 3 3	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84 51.09
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282 1.7863 1.7750	3 10 7 8 6 2 5 4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2 0 2 0 1 0 3 3 3	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84 51.09 51.44
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282 1.7863 1.7750	3 10 7 8 6 2 5 4	$\begin{array}{c} 0 & -3 \\ 1 & 3 \\ -2 & 4 \\ 1 & 0 \\ 0 & 4 \\ \end{array}$ $\begin{array}{c} -3 & 3 \\ 2 & 2 \\ -2 & 1 \\ -1 & 1 \\ -1 & -2 \end{array}$	2 0 2 0 1 0 3 3 3	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84 51.09 51.44
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282 1.7863 1.7750 1.7463M	3 10 7 8 6 2 5 4 5	$\begin{array}{c} 0 & -3 \\ 1 & 3 \\ -2 & 4 \\ 1 & 0 \\ 0 & 4 \\ \hline \\ -3 & 3 \\ 2 & 2 \\ -2 & 1 \\ -1 & 1 \\ -1 & -2 \\ \hline \\ -3 & -1 \end{array}$	2 0 2 0 1 0 3 3 3 2	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84 51.09 51.44
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282 1.7863 1.7750 1.7463M 1.7463M	3 10 7 8 6 2 5 4 5	$\begin{array}{c} 0 & -3 \\ 1 & 3 \\ -2 & 4 \\ 1 & 0 \\ 0 & 4 \\ \\ -3 & 3 \\ 2 & 2 \\ -2 & 1 \\ -1 & 1 \\ -1 & -2 \\ \\ -3 & -1 \\ -3 & -1 \end{array}$	2 0 2 0 1 0 3 3 3 2 1	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84 51.09 51.44 52.35 52.35
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282 1.7863 1.7750 1.7463M 1.7463M 1.7355	3 10 7 8 6 2 5 4 5 4 5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 0 2 0 1 0 3 3 3 2 1 2	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84 51.09 51.44 52.35 52.35 52.70
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282 1.7863 1.7750 1.7463M 1.7463M 1.7355 1.7141	3 10 7 8 6 2 5 4 5 4 5 4	$\begin{array}{c} 0 & -3 \\ 1 & 3 \\ -2 & 4 \\ 1 & 0 \\ 0 & 4 \\ -3 & 3 \\ 2 & 2 \\ -2 & 1 \\ -1 & 1 \\ -1 & -2 \\ -3 & -1 \\ -3 & -1 \\ 0 & -4 \\ -1 & -4 \end{array}$	2 0 2 0 1 0 3 3 3 2 1 2 1	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84 51.09 51.44 52.35 52.35 52.70 53.41
2.053M 2.017 1.952M 1.952M 1.927 1.898 1.8526 1.8282 1.7863 1.7750 1.7463M 1.7463M 1.7355 1.7141	3 10 7 8 6 2 5 4 5 4 5 4 1	$\begin{array}{c} 0 & -3 \\ 1 & 3 \\ -2 & 4 \\ 1 & 0 \\ 0 & 4 \\ \end{array}$ $\begin{array}{c} -3 & 3 \\ 2 & 2 \\ -2 & 1 \\ -1 & 1 \\ -1 & -2 \\ \end{array}$ $\begin{array}{c} -3 & -1 \\ -3 & -1 \\ 0 & -4 \\ -1 & -4 \\ \end{array}$	20020 10333 2121	44.08 44.91 46.48 46.48 47.13 47.90 49.14 49.84 51.09 51.44 52.35 52.35 52.35 52.70 53.41 54.18

d (A)	I *	hkl	20(°)
1.691.5M		C O 3	54.18
1.6801M	2	0 4 1	54.58
1.68014	-	1 2 1	54-58
1.6652M	٨	-1 5 0	55.11
1.0052M	-+	-1 -2 -2 -7	55+11
I.CCD2M		-2 -2 3	22011
1.6440	3	-2 4 2	55.88
1.6296M	5	1 -5 1	56.42
1.6296M		0 3 2	56.42
1.6162	1	1 4 0	56.93
1.6079M	2	-3 2 3	57.25
1.6079M		2 -2 2	57.25
1.5538M	2	2 3 0	59.44
1.5538M		1 2 2	59.44
1.5385M	5	-1 5 1	60.09
1.5385M		3 -1 1	60.09
1.5313+	4	-2 3 3	60.40
1.5313+		-4 1 2	60.40
1.4954	2	-3 3 3	62.01
1.4703	1	-3 5 0	63.19
1.4508	2	301	64.14
1.4443	2	0 -4 3	64-46
1.43214	2	-4 0 1	65-08
1.43214	2	-2 0 1	65.08
1.43217	2	-2 0 4	65.42
1.42557	2	-4 1 3	65 40
1.4255+		-2 -4 2	00+42
1.4153	1	-1 -5 1	65.95
1.4109	2	-4 2 0	66.18
1.3905+	1	0 5 1	67.28
1.3905+		-4 4 2	67.28
1.3854M	2	2 1 2	67.56
- 1.3854M		-2 6 0	67.56
1.3722+	3	1 -6 1	68.30
1.3722+		-3 -3 2	68.30
1.3443	2	1 5 0	69.92

Sample	C
The compound was made by reacting $HIO_3$ with $Cs_2CO_3$ , filtering and drying.	I
Color Colorless	d (Å)
Structure	4.66
type structure [Zachariasen, 1928].	2.69
Lattice constant of this sample: a = 4.6736(2)  Å	2.09
Volume	1.90
102.08 A <sup>3</sup>	1.47
(calculated) 5.007 g/cm <sup>3</sup>	1.34
Reference intensity I/I = 7.7(4)	1 • 29 1 • 24 1 • 16
Additional pattern 1. PDF card 20-279 [Bousquet et al., 1967].	1.13
References Bousquet, J., Rivière, R. and Remy, JC. (1967). C. R. Acad. Sci. Ser. C <u>265</u> , 712. Zachariasen, F. W. H. (1928). Skr. Nor. Vidensk. Akad. Oslo <u>1</u> , #4.	1.07 1.04 1.01 .99 .95 .93

$CuK\alpha_1 \lambda = 1.540598 A$ ; temp. 25±1 °C								
Internal standard W, a = $3.16524 \text{ \AA}$								
d (Å)	I	h	ıkl		20(°)			
4.665	2	1	0	0	19.01			
3.303	100	1	1	õ	26.97			
2.697	3	-	1	1	33.19			
2.336	30	2	ō	0	38.50			
2.090	1L	2	1	0	43.25			
1.9077	35	2	1	1	47.63			
1.6525	13	2	2	0	55.57			
1.5585	1L	з	0	0	59.24			
1.4783	16	З	1	0	62.81			
1.4092	1	З	1	1	66.27			
1.3494	4	2	2	2	69.62			
1.2967	1L	з	2	0	72.89			
1.2491	15	З	2	1	76.15			
1.1684	1	4	0	0	82.49			
1.1336	1L	4	1	0	85.61			
1.1013	5	з	з	0	88.76			
1.0719	1	з	з	1	91.88			
1.0449	3	4	2	0	94.99			
1.0197	1L	4	2	1	98.12			
.9965	3	3	3	2	101.25			
•9540	2	4	2	2	107.69			
.9347	1	4	З	0	111.00			
. 91 66	6	5	1	0	114.37			
. 8994	1L	5	1	1	117.85			
.8679	1L	5	2	0	125.12			
.8533	3	5	2	1	129.04			

Sample	CuK $\alpha_1 \lambda$ = 1.540598 Å; temp. 25±1 °C						
The sample was prepared at the National Institutes of Health using a modified method of Joseph and	Inte	ernal standa	ard Si	, a	= 5.4	13088 Å	
Rae (1917) as described by Ness, Smith, and Evans (1952). Chemical analysis at NIH showed that the material conformed to the above formula. At NBS.	d (Å)	I		hkl		20(°)	
the material was recrystallized out of solution with $(NH_{4})_2HPO_4$ .	5.783	7	4	с	0	15.31	
	5.622	25	0	1	1	15.75	
Color	5.349	11	1	1	1	16.56	
Purplish gray	5.257	25	-2	1	1	16.85	
	4.876M	40	2	1	1	18.18	
Optical data					, in the second s		
Biaxial(-). $N_{g} = 1.568$ , $N_{g} = 1.592$ , $N_{g} = 1.599$ ,	4.876M		С	0	2	18.18	
2V≃15°.	4.779	18	-2	0	2	18.55	
	4.356	11	З	1	1	20.37	
Structure	4.237	100	-4	1	1	20.95	
Monoclinic, $A2/a(15)$ , $Z = 8$ . This appears to be isostructural with MqSO4•6H <sub>2</sub> O. The initial lattice	4.066	25	-4	0	2	21.84	
constants were obtained by using a syntex P21	3-855M	45	6	0	C	23-05	
diffractometer.	3-855M		4	1	1	23.05	
	3.756	7	-5	1	1	23-67	
Lattice constants of this sample:	3-460	30	4	<sup>1</sup>	2	25.07	
a = 23.473(5) Å	3.446	25	ō	2	2	25.83	
b = 6.890(1)	5.440	25	v	2	v	20.00	
c = 9.882(2)	3.408	-	1	2	0	26.13	
$R = 99.42(2)^{\circ}$	3.400	6	-6	1	1	20.13	
p = 55.22(2)	3.334	6	-0	2	1	20.12	
a/b = 3.4069	3.300	o	-6	2	9	27.00	
c/b = 1.4343	3.050	6	6	1	2	29.26	
	5.000	, in the second s	Ũ	•	•	27020	
Volume	2.970	6	1	1	З	30.06	
1576.76 A <sup>3</sup>	2.956	8	-2	1	3	30-21	
	2.939	6	0	1	3	30.39	
Density	2-893M	7	3	1	3	30.88	
(calculated) 2.149 g/cm <sup>3</sup>	2.893M		8	0	õ	30.88	
Deference intensity	0.000	2.0		0	-		
T/T = 1.21(R)	2.826	20	-1	2	2	31.04	
corundum - 1.21(0)	2.812M	25	0	2	2	31.80	
Additional nattorn	2.812M	7.0		0	2	31.80	
Additional pattern	2.795M	30	-2	2	2	32.00	
[Sullivan and McMurdie, 1952]	2.795M		-4	1	з	32.00	
	2.762M	3	5	2	0	32.39	
References	2.762M		1	2	2	32.39	
Joseph, A. F. and Rae, W. N. (1917). J. Chem. Soc.	2.728	5	-3	2	2	32.80	
<u>III, 196.</u>	2.689	13	9-	0	2	33.29	
Ness, A.T., Smith, R. E., and Evans, R. L. (1992). J. Am. Chem. Soc. <u>74</u> , 4685.	2.677M	11	-8	1	1	33.45	
Swanson, H. E. and Fuyat, R. K., (1951). Joint	2.677M		2	2	2	33.45	
Committee Fellowship Report, Nat'l. Bur. Stand.,	2.569M	10	6	2	0	34.90	
U.S., October.	2.569	10	3	2	2	34.90	
Sullivan, B.M. and McMurdie, H. F. (1952). J. Res.	2.525	2	-6	1	3	35.63	
Nat. Bur. Stand. <u>48No.2</u> , 159.	2.512	2	- 5	2	2	35.72	
	2.479M	9	8	1	1	36.20	
	2.479M		4	1	3	36.20	
	2.469	9	-2	0	4	36.36	
	2.442	3	4	2	2	36.78	
	2.428	3	-9	1	1	37.00	
	2.390	4	- 4	0	4	37.60	
	2.383	4	-6	2	2	37.72	
	2.379	4	-7	1	3	37.78	
	2.328	2	8	0	2	38.65	
	2.312M	2	2	0	4	38.92	

d (Å)	I	hkl			20(°)
2.312M		5	2	2	38.92
2.262	1	9	1	1	39.82
2.250	3	-7	2	2	40.04
2.233+	9	-8	1	З	40.35
2.233+		-1	З	1	40.35
2.216+	6	-10	1	1	40.69
2.216+		8	2	0	40.69
2.187	7	6	1	3	41.24
2.178M 2.178M	7	2	3	1 2	41.42
2,169	6	-3	7	1	41.61
2.121	5	-8	2	2	42.60
2.113	<u>م</u>	· = 4	7	1	42.76
2.007	1	· _ q	1	-	47.11
2.060	2	4	3	1	43.92
2.035M	4	-8	0	4	44.49
2.035M		-11	1	1	44.49
2.00EM	2	-2	2	4	45.17
2.006M		1	2	4	45.17
1.994	3	-9	2	2	45.44
1.992	З	-3	2	4	45.49
1.964	3	-4	2	4	46.18
1.924M	14	-5	2	4	47.21
1.924M		6	0	4	47.21
1.9032M	3	e	3	1	47.75
1.9032M		-12	0	2	47.75
1.8998	3	-2	1	5	47.84
1.8755M	4	0	1	5	48.50
1.8755M	_	0	3	3	48.50
1.8730M	5	-4	1	5	48.57
1.8730M		- <del>6</del>	2	4	48.57
1.8554	2	1	3	3	49.06
1.8431	16	° <b>⇔</b> 5	1	5	49.41
1.8357M	1L	-10	0	4	49.62
1.8357M		-4	3	3	49.62
1.8088M	8	4	2	4	50.41
1.8088M		9	1	3	50.41
1.8035M	7	-6	1	5	50.57
1.8035M		-8	3	1	50.57
1.7985	6	-5	3	3	50.72
1.7743	5	12	1	1	51.46
1.7686	4	-11	2	2	51.64
1.7528M	2	-6	3	3	52.14
1.7528M	_	-8	2	4	52.14
1.7376M	3	8	3	1	52.63
1.7376M		4	3	3	52.63
1.7174	4	1	4	0	53.30
1.7017+	11	12	C	2	53.83
1.7017+		-8	1	5	53.83
1.6832M	2	12	2	0	54.47
1.6832M		5	З	3	54.47
1.6668	2	-12	2	5	55.05

Chromium Phosphate Hydrate,  $CrP0_4 \cdot 6H_20$  - (continued)
Cobalt Hydroxide,  $\beta$ -Co(OH),

```
CuKa<sub>1</sub> \lambda = 1.540598 A; temp. 25±1 °C
Sample
   The sample was precipitated by adding a solution
  of NaOH to a hot solution of Co(NO_3)_2. It was
  filtered, washed with H20 and dried at 150 °C.
Color
  Reddish gray
Structure
  Hexagonal, P3ml (164), Z = 1, isostructural with
  Zn(OH)_2 and Ni(OH)_2
                          [Lotmar and Feilknecht,
  1936].
Lattice constants of this sample:
  a = 3.1830(4) Å
  c = 4.6520(9)
  c/a = 1.4615
Volume
  40.817 Å<sup>3</sup>
Density
  (calculated) 3.781 g/cm<sup>3</sup>
Reference intensity
  I/I 1.5(3)
Polymorphism
  There is a less stable, blue-green form, called \alpha
  [Weiser and Milligan, 1932].
Additional patterns
  1. PDF card 3-913 [Lotmar and Feilknecht, 1936]
  2. PDF card 2-925 [Weiser and Milligan, 1932]
References
 Lotmar, W., and Feilknecht, W. (1936). Z. Kris-
    tallogr. Kristallgeometrie Kristallphys.
    Kristallchem. 93, 368.
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Weiser, H. B., and Milligan, W. O. (1932). J.

Phys. Chem. 36, 729.

	-				
Inte	rnal standa	rd Si,	a =	= 5.43	8088 Å
d (Å)	I		hkl		20(°)
4.653	6C 45	0	0	1	19.06
2.371	100	1	0	1	37.92
1.7776	45	1	0	2	51.36
1.5911	35	1	1	0	57.91
1.5507 1.5059	4 25	0 1	0 1	3 1	59.57 61.53
1.3786 1.3512	5 13	2 1	0 0	0 3	67.94 69.51
1.3213	13	2	0	1	71.32
1.3138	6	1	1	2	71.79

1 . B

Sample	CuKa <sub>1</sub> $\lambda$ = 1.540598 Å; temp. 25±1 °C						
the metals with $HNO_3$ and heating the resultant	Inter	nal standar	d Si,	a =	5.43	088 Å	
lines of $SnO_2$ and $Co_3O_4$ present.	d (Å)	I	ł	nkl		20(°)	
Color							
Black ,	4.987	25	1	1	1	17.77	
	3.056	15	2	2	0	29.20	
Structure	2.605	100	3	1	1	34.40	
Cubic, Fd3m (227), Z = 8, spinel structure [Natta	2.493	20	2	2	2	35.99	
and Passerini, 1929].	2.1593	30	4	0	0	41.80	
Lattice constants of this sample:	1.9820	4	з	з	1	45.74	
a = 8.6376(3) A	1.7632	7	4	2	2	51.81	
	1.6621	30	5	1	1	55.22	
Volume	1.5268	45	4	4	0	60.60	
644.43 Å <sup>3</sup>	1.4599	5	5	З	1	63.69	
Density	1.3655	1	6	2	0	68.68	
(calculated) 6.196 g/cm <sup>33</sup>	1.3172	9	5	З	з	71.58	
	1.3021	8	6	2	2	72.54	
Reference intensity	1.2466	5	4	4	4	76.33	
$I/I_{corundum} = 3.5(2)$	1.2097	2	7	1	1	79.10	
Additional patterns	1.1542	1	6	4	2	83.73	
1. PDF card 1-1137 [Hanawalt et al., 1938]	1.1243	15	7	З	1	86.49	
2. PDF card 2-1391 [Natta and Passerini, 1929]	1.0796	4	8	0	0	91.04	
	1.0178	1	8	2	2	98.37	
References	.9975	9	7	5	1	101+11	
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K.							
(1938). Ind. Eng. Chem. Anal. Ed. 10, 457.	.9909	4	6	6	2	102.04	
Natta, G. and Passerini, L. (1929). Gazz, Chim. Ital. <u>59</u> 640.	• 96 58	6	8	4	0	105.80	

Creatinine,  $C_4 H_7 N_3 0$ 

	·····				
Synonym 2-amino-1,5-dihydro-1-methyl-4H-imidazol-4-one	<b>CuK</b> α <sub>1</sub> λ	= 1.54059	8 A; tem	p. 25±1	°C
	Internal	. standard	W, a =	3.1652	4 A
Sample NBS standard reference material #914. The mate-	d (A)	I	hkl	-	2⊖(°)
sure to x-rays, i.e. peak heights would decrease	6.90	36	_1 (		12.84
if the same sample were re-run.	6.21	25	-1	) I ) I	14.24
II the band bangit word to take	5.690	1	2		15.56
Color	5.257	30	1		16.85
Colorless	4.754	1	0	1 1	18.65
Structure	4.496	40	-1	1 1	19.73
Monoclinic, $P2_1/n$ (14), $Z = 4$ . The structure was	4.103	5	2	L 0	21.64
determined by du Pré & Mendel [1955].	3.775	12	-2	1 1	23.55
	3.537	2	2	1 1	25.16
Lattice Constants of this sample: a = 11.432(2) Å	3.445	100	-2	0 2	25.84
b = 5.931(2)	3, 708	e	0	1 2	26.93
c = 8.019(2)	3.257	75	-1		20.93
$\beta = 96.29(2)^{\circ}$	3,101	1	-		27.94
	3.108	1	2		28.70
a/b = 1.9275	3-061		-3	1 1	29-15
c/b = 1.3520	JUCI	0	5		29010
	2.980	20	-2	1 2	29.96
Volume	2.868	2	1	2 0	31.16
540.4 A <sup>3</sup>	2.842	1	4	0 0	31.45
	2.779	2	0	2 1	32.18
Density	2.723	3	-1	2 1	32.86
(calculated) 1.390 g/cm <sup>3</sup>		-			
	2.676	2	1	2 1	33.46
Reference intensity	2.630	2	2	2 0	34.06
I/I = 1.46(10)	2.562	2	4	1 0	34.99
corundum	2.512	4	-4	1 1	35.71
Additional pattern	2.442	1	-4	02	36.78
i. Di culu / /24 [du lic and hendely 1955]	2.423M	2	0	1 3	37 07
Reference	2.423M	2	-1	1 3	37.07
du Pré. S. and Mendel, J. (1955). Acta Crystal-	2.385	2	1	1 2	37.68
logr. 8. 311.	2.332	1	3	2 0	38.57
	2.317	1	-2	1 3	38.84
	2.297M	1	-3	0 З	39.19
	2.297M		1	2 2	39.19
	2.247	з	-2	2 2	40.09
	2.202M	1	З	2 1	40.96
	2.202M		4	0 2	40.96
	2.122	1	5	1 0	42.56
	2.071	1	З	03	43.68
	2.051	1L	4	2 0	44.13
	2.000	2	5	1 1	45.30
	1.979	1	0	23	45.82
	1.957M	2	З.	2 2	46.36
	1.957M		-5	1 7	46.36
	1.944	1	-4	1 J	40.69
	1.9179M 1.9179M	2	-2	2 3 3 1	47.36
	1,8857	1	- 4	2 2	48.22
	1.8278	2	-5	0 3	45-85
	1.8156	2	-3	2 3	50.21
	1.8008	1	-6	1 1	50.65
	1.7644	4	-3	1 4	51.77
		•	-		

Sample The sample was a natural mineral from Ivigtut, Greenland, U. S. Nat. Museum #132849. X-ray	CuK $\alpha_1 \lambda = 1.540598 \text{ Å}; \text{ temp. } 25\pm1 \text{ °C}$ Internal standard Si, a = 5.43088 Å					
tained from 1 to 2% of Mn.	d (Å)	I	h	kl	20(°)	
Color Light yellowish brown	3.593	25	0	1 2	24.76	
Structure Hexagonal, $R_{3c}(167)$ , $Z = 6$ , isostructural with calcite (CaCO <sub>3</sub> ) and other bivalent carbonates. The structure was determined by Erenburg and Samilov [1963]	2.564 2.346 2.134	1L 20 20 20	0 1 1 2	0 6 1 0 1 3 0 2	34.97 38.34 42.32 46.16	
Lattice constants of this sample: a = 4.6935(2)  Å c = 15.3860(8)	1.7968 1.7382 1.7315 1.5291	12 30 35 3	0 0 1 2	2 4 1 8 1 6 1 1	50•77 52•61 52•83 60•50	
c/a = 3.2782	1.5063 1.4390	14 3	1 1 2	2 2 0 10	61.51 64.73 65.36	
293.53 Å <sup>3</sup>	1.3969	6 3	2	0 8 1 9	66•93 67•76	
Density (calculated) 3.932 g/cm <sup>3</sup>	1.3548	11 5	3 0	0 0 0 12	69.30 73.84	
Additional pattern 1. PDF card 8-133 [Andrews, United Steel Co., Ltd.]	1.2269	3 5	0	2 10 2 8	77.78 79.85	
Reference Erenburg, B. G. and Samilov, O. Ya. (1963). Zh. Strukt. Khim. <u>4</u> , 868.	1.1977 1.1737 1.1254 1.1154 1.0872	4 2 4 1 3	3 2 1 3 2	0 6 2 0 1 12 1 2 1 10	80.05 82.04 86.39 87.36 90.23	
	1.0820 1.0671 .9825 .9724 .9666	5 4 5 5 2	1 2 4 3 2	3 4 2 6 0 4 1 8 0 14	90.78 92.42 103.26 104.78 105.68	
	•9358 •9309 •9256	2 6 3	1 3 2	0 16 2 1 3 2	110.80 111.68 112.66	

•

Sample It was prepared by treating Na <sub>2</sub> HPO <sub>4</sub> with FeCl <sub>3</sub> ,	СиКа1	λ = 1.5405	98 Å;	tem	ıp. 25	5±1 °C °
in solution. The resulting precipitate was dried	Interr	nal standar	d Si,	a =	= 5.43	3088 A
	d (Å)	I		hkl		20(°)
Color Vellowish white						
	4.360	19	1	0	0	20.35
Structure	4.966	2	1	0	1	21.84
Hexagonal, $P3_12_1$ (152), $Z = 3$ , analogous to the	3.750	2	0	0	з	23.71
structure of low quartz [Cagliotti, 1935].	3.445	100	1	Э	2	25.84
Because of the ordering of the cations, the lat- tice parameter "c" is double the size of the "c"	2.843	1L	1	0	З	31.44
of the analogous quartz phase.	2.518	7	1	1	0	35.63
	2.458	1	1	1	1	36.53
Lattice constants of this sample:	2.362	14	1	0	4	38.07
a = 5.0347(4)Å	2.298	7	1	1	2	39.17
c = 11.245(1)	2.180	10	2	0	0	41.38
c/a = 2.2335	2.142	1L	2	0	1	42.16
	2.090	1L	1	1	з	43.25
Volume	2.0335	З	2	0	2	44.52
246.86 Å <sup>3</sup>	1.9986	2	1	0	5	45.34
	1.8846	12	2	0	З	48.25
Density				_		
(calculated) 3.044 g/cm <sup>3</sup>	1.7221M	6	2	0	4	53.14
	1.7221M	_	1	0	6	53.14
Polymorphism	1.6772	1	1	1	5	54.68
PDF card 3-379 is labelled FePO4 [Hanawalt et	1.6304	1	2	1	1	56.39
al., 1938]. It appears to be a mixture, or an entirely different phase.	1.5814	8	2	1	2	58.30
	1.5081M	З	2	1	з	61.43
An inversion from low to high temperature phase	1.5081M		1	0	7	61.43
takes place at 707+5°C, analogous to the simi-	1.5035	2	1	1	6	61.64
lar inversion from $\alpha$ - to $\beta$ -quartz. No inversions	1.4214M	10	2	1	4	65.63
to other forms were found.	1.4214M		2	0	6	65.63
Additional patterns	1.4063	4	З	0	2	66.40
1. PDF card 17-837 [Schafer et al., 1956]	1.3376	3	1	0	8	70.32
2. PDF card 18-649 [Kleber et al., 1965]	1.2912	2	з	0	4	73.25
(composition uncertain)	1.2588	1L	2	2	0	75.46
	1.2375	2	2	1	6	76.99
References		_			_	
Cagliotti, V. (1935). Atti Accad. Naz. Lincei	1.2273	2	1	1	8	77.75
C1. Sci. Fis. Mat. Natur. Rend. 22, 146.	1.2093	2	3	1	0	79.13
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K.	1.0889	1	1	0	10	90.05
(1938). Ind. Eng. Chem. Anal. Ed. 10, 457.	1.0059	2	4	0	2	92.11
Chem. Erde 24, 77.	1.0449	1	2	2	C	94.99
Schafer, E. C., Schafer, M. W., and Roy, R.	1.0268	1L	1	1	10	97.21
(1956). Z. Kristallogr. Kristallgeometrie,	1.0160M	2	4	0	4	98.60
Kristallphys. Kristallchem. 108, 263.	1.0160M		З	1	6	98.60

#### Sample

```
The sample was prepared at NBS by W. S. Brower.
High purity \alpha-Fe<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> were ground in
acetone, pressed into pellets, and heated to
800 °C in air. The sample was again ground in
acetone, pressed, and heated in air at 1000 °C.
Three of the pellets were stacked and heated
in an iron crucible for 1.5 hrs. at 1100 °C in
an atmosphere of 95% N<sub>2</sub> and 5% H<sub>2</sub>. The middle
pellet was ground and leached in dilute HCl to
remove faint trace of Fe.
```

#### Color

Gray, metallic

#### Structure

Hexagonal,  $R\overline{3}$ (148), Z = 6; ilmenite is used as a structure type. The structure was determined by Barth and Posnjak [1934].

```
Lattice constants of this sample:

a = 5.0884(2) A

c = 14.0932(6)
```

c/a = 2.7697

#### Volume

316.01 A<sup>3</sup>

#### Density

(calculated) 4.784 g/cm<sup>3</sup>

Reference intensity I/I\_\_\_\_\_\_ = 1.77(11)

#### Additional patterns

- PDF card 3-0781 [United Steel Companies, Sheffield, Eng.]
- 2. Barth and Posnjak [1934].
- 3. Michel and Pouillard [1948].

#### References

- Barth, T.F.W. and Posnjak, E. (1934). Z. Kristallogr. Kristallgeometrie Kristallphys.
  Kristallchem. <u>88A</u>, 265.
  Michel, A. and Pouillard, E. (1948). Bull. Soc.
- Chim. Fr. <u>15</u>, 962.

CuKαl	$\lambda = 1.5405$	98 Å;	temp. 25	5±1 °C						
Inter	Internal standard Si, a = $5.43088 \text{ Å}$									
d (Å)	I	h	kl	20(°)						
3.737 2.754 2.544 2.349 2.237	30 100 70 2 30	0 1 1 0	1 2 0 4 1 0 0 6	23.79 32.49 35.25 38.29						
2.1772	2	0	2 1	41.44						
2.1032	2	2	0 2	42.97						
1.8683	40	0	2 4	48.70						
1.8309	1	1	0 7	49.76						
1.7261	55	1	1 6	53.01						
1.6535	2	2	1 1	55.53						
1.6354	9	0	1 8	56.20						
1.6206	3	1	2 2	56.76						
1.5057	30	2	1 4	61.54						
1.4686	35	3	0 0	63.27						
1.4342	1	1	2 5	64.97						
1.3757	3	2	0 8	68.10						
1.3421	13	1	0 10	70.05						
1.3337	5	1	1 9	70.56						
1.2834	1	2	1 7	73.77						
1.2719	8	2	2 0	74.55						
1.2453	3	3	0 6	76.42						
1.2279	2	2	2 3	77.71						
1.2101	4	1	2 8	79.07						
1.2040	3	3	1 2	79.55						
1.1871	6	0	2 10	80.92						
1.1744	1	0	0 12	81.98						
1.1547	9	1	3 4	83.69						
1.1185	8	2	2 6	87.05						
1.0884	1	0	4 2	90.10						
1.0758	8	2	1 10	91.45						
1.0663	1	1	1 12	92.51						
1.0516	3	4	0 4	94.19						
1.0156	1L	1	2 11	98.66						
1.0042	3	3	1 8	100.18						
.9872	1L	2	2 9	102.58						
.9813	3	0	1 14	103.44						
.9719	7	3	2 4	104.86						
.9617	6	4	1 0	106.45						
.9421	1	4	1 3	109.70						
.9341	2	0	4 8	111.10						
.9233	6	1	3 10	113.09						
.9156	5	2	0 14	114.55						
.8899	8	4	1 6	119.90						
.8814	1	1	1 15	121.84						
.8769	2	2	3 8	122.90						
.8680	4	4	0 10	125.11						
.8638	2	1	0 16	126.19						
.8615	6	1	2 14	126.80						
.8550	5	0	5 4	128.57						

#### Sample

The sample was prepared by heating stoichiometric amounts of  $La(C_2H_3O_2)_3 \cdot 1.5H_2O$  and  $TiO_2$  at 1400° for one hour. The product was then ground and reheated at 1500 °C for 5 hours.

Color

Colorless

Structure

Monoclinic, P2<sub>1</sub>(4) or P2<sub>1</sub>/m(11), Z = 4. The structure was determined by Gasperin [1975] and the compound was shown to be isostructural with monoclinic Ca<sub>2</sub>Nb<sub>2</sub>O<sub>7</sub>. La<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> could be indexed on a pseudo-orthorhombic cell a<sub>0</sub>=4a<sub>m</sub>sin $\beta$ , b<sub>0</sub>=b<sub>m</sub>, c<sub>0</sub>=c<sub>m</sub> like the Ca<sub>2</sub>Nb<sub>2</sub>O<sub>7</sub> reported by Rowland et al., [1958]. Brandon and Megaw [1970] attributed the Rowland et al. pseudocell to twinning. Brandon and Megaw [1970] reported another pseudo-orthorhombic cell for monoclinic Ca<sub>2</sub>Nb<sub>2</sub>O<sub>7</sub>: a<sub>0</sub>%2a<sub>m</sub>sin $\beta$ , b<sub>0</sub>=b<sub>m</sub>, c<sub>0</sub>=c<sub>m</sub>/2,  $\beta$ %90°8' which would index the data when weak l=2n + 1 reflections are ignored.

Lattice constants of this sample: a = 13.015(2) Å b = 5.5456(7) c = 7.817(1) β = 98.64(2)° a/b = 2.3468 c/b = 1.4096

```
Density
(calculated) 5.782 g/cm<sup>3</sup>
```

```
Reference intensity
I/I = 1.7(1)
```

Additional patterns

3. Roth [1956]

- PDF card 27-1182 [Nanot et al., 1974]
   MacChesney and Sauer [1962]
- References Brandon, J. K. and Megaw, A. D. (1970). Phil. Mag. <u>21</u>, 189.
  - Gasperin, M. (1975). Acta Crystallogr. <u>B31</u>, 2129. MacChesney, J. B. and Sauer, H. A. (1962). J. Amer. Ceram. Soc. <u>45, No. 9</u>, 416.
  - Nanot, M., Queyroux, F., Gilles, J., Carpy, A., and Galy, J. (1974). J. Solid State Chem. <u>11</u>, 272.
  - Roth, R. S. (1956). J. Res. Nat. Bur. Stand. <u>56</u>, 17.
  - Rowland, J.F., Bright, N. F. H., and Jongejan, A. (1958). Advan. X-ray Anal. 2, 97.

	СиКа <sub>1</sub> λ	= 1.540598	3 Å;	temp	p. 25±1	°C
	Internal	standard	Aq,	a =	4.08651	° A
0				1.0		00 ( 0 )
d (A)			1	nkl	· · · · · · · · · · · · · · · · · · ·	20(0)
12.84	4	7	1	0	0	6.88
6.42	26	10	2	ō	0	13.77
5.09	95	8	1	1	0	17.39
4.20	01	40	2	1	0	21.13
4.0	14	4	-3	0	1	22.13
3.80	54M	11	0	0	2	23.00
3.80	54M		-1	0	2	23.00
3.54	46	2	2	1	1	25.09
3.39	92	11	З	1	0	26.25
3.2	51	S	-3	1	1	27.41
3.2	17	50	4	0	0	27.71
3.17	72M	30	0	1	2	28.11
3.1	72M		-1	1	2	28.11
3.1	12M	13	2	0	2	28.66
3.1	12M		-3	0	2	28 <b>.66</b>
2.99	9 5 M	100	1	1	2	29.81
2.9	95M		-2	1	2	29.81
2.7	82	50	4	1	0	32.15
2.7	74	50	0	2	0	32.25
2.7	1 3M	55	2	1	2	32.99
2.7	1 3M		=3	1	2	32.99
2.6	77M	25	3	0	2	33.44
2.6	77M		-4	0	2	33.44
2.5	73M	З	C	0	3	34.84
2.5	7 3M		5	0	0	34.84
2 5	60	2	- 5	0	1	35.03
2.5	16	2		1	1	35.66
2.00	11M	2		1	2	37.27
2 4	1 1 14	3	- 0	1	2	37.27
2.4	76	2	- 4	2	1	37.84
2.3	10	2	2	۲		57804
2.3	55	4	-1	1	з	38.18
2.3	36M	5	0	1	3	38.51
2.3	36M	•	5	1	0	38.51
2.3	29	6	3	2	0	38.62
2.3	07M	5	4	0	2	39.01

-5 0 2

-3 2 1

2 0 3

0 2 2

1 2

-2 2

32

-3 1

6 0

4 1 2

=5 1 2

4 2 0

2 2 2

-3 2 2

2

2

2

1

З

0

-1 2

з

Δ.

20

6

5

11

17

25

17

39.01

39.46

39.54

39.99

39.99

41.24

41.24

41.36

41.36

42.11

42.39

42.39

43.02

43.67

43.67

2.307M

2.282

2.277

2.253M

2.253M

2.187M

2.187M

2.181M

2.181M

2.144

2.131M

2.131M

2.1008

2.0711M

2.0711M

Lanthanum Titanium Oxide,  $La_2Ti_2O_7$  - (continued)

d (Å)	I	hJ	cl		20(°)
2.0261	2	-4	1	3	44.69
2.0078M	0	6	0	2	45.12
2.0007	8	-0	1	0	45.29
1.9783	2	4	2	1	45.83
1.0540	7.0	· _ •	•		46 47
1.02644	30	-1	2	4	40.43
1 02644	20	- 0	2	2	47 14
1.9204M	70		2	2	47 14
1.8865+	50	0	2	3	48.20
1 07054			~	_	40 54
1.8385M	2	1	2	3	49.54
1.0300	2		-	0	49.34
1 83404	2	1	5	0	49.70
1.8240M	2	-2	1	4	49.90
1002400		- 2	•	-	49.90
1.8018	2	= 3	2	З	50.62
1.7873	З	5	2	1	51.06
1.7772	8	2	З	0	51.37
1.7718M	15	1	1	4	51.54
1.7718M		-3	1	4	51.54
1.7664M	11	6	0	2	51.71
1.7664M		-7	0	2	51 • 71
1.7572	5	-7	1	1	52.00
1.7447	4	7	1	0	52.40
1.7309	1	7	0	1	52.85
1.7156	2	2	з	1	53.36
1.6967+	8	з	З	0	54.00
1.6967+		6	2	0	54.00
1.6933M	7	2	1	4	54.12
1.6933M		-4	1	4	54.12
1.6821M	7	٤	1	2	54.51
1.6821M		-7	1	2	54.51
1.6691+	20	З	0	4	54.97
1.6691+		-5	0	4	54.97
1.6522	3	7	1	1	55.58
1.6402M	11	1	з	2	56.02
1.6402M		-2	з	2	56.02
1.6256M	З	5	2	2	56.57
1.6256M		-6	2	2	56.57
1.6025	13	4	З	0	57.46
1 • 59 77	25	-1	2	4	57.65
1.5889M	16	2	з	2	58.00
1.5889M		-3	з	2	58.00
1.5851M	9	0	2	4	58.15
1.5851M		=2	2	4	58.15
1.5708M	4	7	0	2	58.73
1.5708M		-8	0	2	58.73
1.5554	з	4	2	З	59.37
1.5446	6	8	1	0	59.83
1.5211M	З	3	з	2	60.85

d (Å)	I	hl	cl		20(°)
			_		
1+5211M		-4	3	2	60.85
1.5110M	8	7	1	2	61.30
1.5110M		-8	1	2	61.30
1.4984M	з	4	1	4	61.87
1.4984M		-6	1	4	61.87
1.4893+	6	6	2	2	62.29
1.4893+		-7	2	2	62.29

Lead Hydrogen Phosphate,  $PbHPO_4$ 

The samp	e was pre	pared by addi	ng acidified Pb
acotato	colution t	a a cold solu	tion of NaHPO.
The preci	pitate wa	s then washed	with distilled
water and	dried in	the air.	
7-1-0-			
Colorless			
001011000			
structure			
Monoclini	.c, P2/a (1	3), $Z = 2.$ T	he structure of
PDHPO4 Wa	s stualea.	by Bengtsson	[1941].
Lattice con	stants of	this sample:	
a = 5.78	22(5)Å		
b = 6.64	54(5)		
$\beta = 97.14$	(1)°		
P 3701-	(1)		
a/b = 0.8	701		
c/b = 0.7	049		
olume			
178.6 A <sup>3</sup>			
ensity		- (3	
(Calculat	eu) 5.636 g	g/ cm	
Reference i	ntensity		
I/I corund	um = 5.2(2)	)	
dditional	nattorn		
dditional l. PDF c	pattern ard 6-274	[X-ray Diffr	action Patterns
dditional l. PDF c <u>of Le</u>	pattern ard 6-274 ad Compound	[ <u>X-ray Diffr</u> ds,1954].	action Patterns
dditional 1. PDF c <u>of Le</u>	pattern ard 6-274 ad Compound	[ <u>X-ray Diffr</u> ds,1954].	action Patterns
dditional 1. PDF c <u>of Le</u> References Bengtsson	pattern ard 6-274 ad Compound , E. (1941)	[X-ray Diffr ds,1954]. ). Ark. Kemi	action Patterns Mineral. Geol.
dditional 1. PDF c of Le References Bengtsson <u>15B</u> , No	pattern ard 6-274 ad Compound , E. (1941) . 7.	[ <u>X-ray Diffr</u> ds,1954]. ). Ark. Kemi	action Patterns Mineral. Geol.
dditional 1. PDF c of Le References Bengtsson <u>15B</u> , No <u>X-ray Di</u>	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction	[ <u>X-ray Diffr</u> ds,1954]. ). Ark. Kemi Patterns of	Action Patterns Mineral. Geol. Lead Compounds
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dditional 1. PDF c of Le eferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto	[ <u>X-ray Diffr</u> ds,1954]. ). Ark. Kemi <u>Patterns of</u> n Research Ce d.) p. 54.	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell
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dditional 1. PDF c of Le References Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKa <sub>1</sub>	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$	[X-ray Diffr ds, 1954]. ). Ark. Kemi Patterns of n Research Ce d.) p. 54. 598 Å; temp. 2	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C
dditional 1. PDF c of Le seferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKa <sub>1</sub> Intern	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar	[X-ray Diffr ds, 1954]. ). Ark. Kemi Patterns of n Research Ce d.) p. 54. $\hat{o}$ 598 Å; temp. 2 cd W, a = 3.2	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å
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dditional 1. PDF c of Le seferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKa <sub>1</sub> Intern d(Å)	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I	[X-ray Diffr ds,1954]. ). Ark. Kemi Patterns of n Research Cen d.) p. 54. 598 Å; temp. 2 cd W, a = 3. hkl	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å 20(°)
dditional 1. PDF c of Le Seferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKα <sub>1</sub> Intern d(Å)	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I	[X-ray Diffrds, 1954].). Ark. KemiPatterns ofn Research Centd.) p. 54.598 Å; temp. 2cd W, a = 3.2hkl0 1 0	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å 20(°) 13.33
dditional 1. PDF c <u>of Le</u> eferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKa <sub>1</sub> Intern d(Å) 6.64 4.650 4.301	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30	[ <u>X-ray Diffr</u> ds, 1954]. ). Ark. Kemi <u>Patterns of</u> n Research Cen d.) p. 54. 598 Å; temp. 2 cd W, a = 3.2 hkl 0 1 0 0 0 1	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å 20(°) 13.33 19.07 20.11
dditional 1. PDF c <u>of Le</u> eferences Bengtsson <u>15B</u> , No X-ray Di (1954). Petrole CuKa <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11	<pre>[X-ray Diffr ds, 1954]. ). Ark. Kemi Patterns of n Research Cen d.) p. 54. 598 Å; temp. 2 cd W, a = 3.2 hkl 0 1 0 0 0 1 1 1 0 0 1 1</pre>	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å 20(°) 13.33 19.07 20.44 23.34
dditional 1. PDF c of Le eferences Bengtsson <u>15B</u> , No X-ray Di (1954). Petrole CuKa <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.332	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90	[ <u>X-ray Diffr</u> ds,1954]. ). Ark. Kemi <u>Patterns of</u> n Research Ce d.) p. 54. 598 Å; temp. 2 cd W, a = 3.2 hkl 0 1 0 0 0 1 1 1 0 0 1 1 -1 1 1	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å 20(°) 13.33 19.07 20.44 23.34 26.73
ditional 1. PDF c of Le eferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKα <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.332	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90	[X-ray Diffr ds, 1954]. ). Ark. Kemi Patterns of n Research Cen d.) p. 54. 598 Å; temp. 2 cd W, a = 3. hkl 0 1 0 0 0 1 1 1 0 0 1 1 -1 1 1	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å 20(°) 13.23 19.07 20.44 23.34 26.73
dditional 1. PDF c of Le eferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKα <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.332 3.325	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90 1C0	[ <u>X-ray Diffr</u> ds, 1954]. ). Ark. Kemi <u>Patterns of</u> n Research Ce d.) p. 54. 598 Å; temp. 2 cd W, a = 3.2 hkl 0 1 0 0 0 1 1 1 0 0 1 1 -1 1 1 c 2 0	Action Patterns Mineral. Geol. Lead Compounds Inter, The Shell 25±1 °C 16524 Å 20(°) 13.33 19.07 20.44 23.34 26.79
dditional 1. PDF c of Le eferences Bengtsson <u>15B</u> , No X-ray Di (1954). Petrole CuKa <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.332 3.325 3.032 2.876	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90 100 80 70	[X-ray Diffrds, 1954].). Ark. KemiPatterns ofn Research Centricd.) p. 54.598 Å; temp. 2cd W, a = 3.2hkl0 1 00 1 11 1 00 1 1-1 1 10 2 01 1 1	Action Patterns Mineral. Geol. Lead Compounds Inter, The Shell 25±1 °C 16524 Å 20(°) 13.33 19.07 20.44 23.34 26.73 26.79 29.44
dditional 1. PDF c of Le eferences Bengtsson 15B, No <u>X-ray Di</u> (1954). Petrole CuKα <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.332 3.325 3.032 2.876 2.868	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90 10 80 30 35	[X-ray Diffrds, 1954].). Ark. KemiPatterns ofn Research Cend.) p. 54.598 Å; temp. 2cd W, a = 3.2hkl0 1 00 1 11 1 00 1 1-1 1 10 2 01 1 11 2 02 0 0	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å 20(°) 13.33 19.07 20.44 23.34 26.73 26.79 29.44 31.07 31.16
dditional 1. PDF c of Le eferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKα <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.325 3.325 3.325 3.032 2.876 2.868 2.702	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90 1C0 80 30 35 15	[X-ray Diffrds, 1954].). Ark. KemiPatterns ofn Research Cend.) p. 54.598 Å; temp. 2cd W, a = 3.hkl0 1 00 1 11 1 00 1 1-1 1 10 2 01 1 11 2 02 0 00 2 1	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å 20(°) 13.23 19.07 20.44 23.34 26.79 29.44 31.07 31.16 33.13
dditional 1. PDF c of Le Seferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKα <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.332 3.325 3.032 2.876 2.868 2.702	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90 1C0 80 30 35 15	[X-ray Diffrds, 1954].). Ark. KemiPatterns ofn Research Centricd.) p. 54.598 Å; temp. 2cd W, a = 3.2hkl0 1 00 1 11 1 00 1 1-1 1 12 02 0 00 2 1	Action Patterns Mineral. Geol. Lead Compounds Inter, The Shell 25±1 °C 16524 Å 20(°) 13.33 19.07 20.44 23.34 26.79 29.44 31.07 31.16 33.13
dditional 1. PDF c of Le References Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKa <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.332 3.325 3.032 2.876 2.868 2.702 2.632 2.580	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90 100 80 30 35 15 7	[X-ray Diffrds, 1954].). Ark. KemiPatterns ofn Research Cenderd.) p. 54.598 Å; temp. 2598 Å; temp. 25	Action Patterns Mineral. Geol. Lead Compounds Inter, The Shell 25±1 °C 16524 Å 20(°) 13.33 19.07 20.44 23.34 26.79 29.44 31.07 31.16 33.13 34.03
dditional 1. PDF c of Le eferences Bengtsson 15B, No X-ray Di (1954). Petrole CuKα <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.332 3.325 3.032 2.876 2.868 2.702 2.632 2.589 2.516	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90 1C0 80 30 35 15 7 13 20	[X-ray Diffrds, 1954].). Ark. KemiPatterns ofn Research Cend.) p. 54.598 Å; temp. 2cd W, a = 3.2hkl0 1 00 1 1-1 1 11 2 02 0 10 2 11 2 02 0 1-2 0 1-1 2 1	Action Patterns Mineral. Geol. Lead Compounds Inter, The Shell 25±1 °C 16524 Å 20(°) 13.33 19.07 20.44 23.34 26.73 26.79 29.44 31.07 31.16 33.13 34.03 34.62 35.65
dditional 1. PDF c of Le eferences Bengtsson <u>15B</u> , No <u>X-ray Di</u> (1954). Petrole CuKα <sub>1</sub> Intern d(Å) 6.64 4.650 4.341 3.808 3.332 3.325 3.032 2.876 2.868 2.702 2.632 2.589 2.516 2.380	pattern ard 6-274 ad Compound , E. (1941) . 7. ffraction (Thornton um Co., Lto $\lambda = 1.5405$ hal standar I 25 30 50 11 90 1C0 80 30 35 15 7 13 20 5	[X-ray Diffrds, 1954].). Ark. KemiPatterns ofn Research Cendd.) p. 54.598 Å; temp. 2cd W, a = 3.hkl0 1 00 1 1-1 1 10 2 01 1 11 2 02 0 00 2 12 1 0-2 0 1-1 2 11 2 1	Action Patterns Mineral. Geol. Lead Compounds nter, The Shell 25±1 °C 16524 Å 20(°) 13.23 19.07 20.44 23.34 26.79 29.44 31.07 21.16 33.13 34.03 34.62 35.65 37.77

d (A)	I	hkl	20 (°)
2.316	20	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	38.86
2.216	7		40.69
2.186	6		41.26
2.171	18		41.57
2.133	17		42.34
2.066	7	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	43.79
2.042	12		44.32
1.9994	10		45.32
1.9726	9		45.97
1.9271	10		47.12
1.9206	10	-1 3 1	47.29
1.9047	15	0 2 2	47.71
1.9002	17	2 2 1	47.83
1.8650	4	-1 2 2	48.79
1.8572	9	1 3 1	49.01
1.8511	8	-2 1 2	49.18
1.8375	11	3 1 0	49.57
1.7834	13	-3 1 1	51.18
1.7531	16	2 3 0	52.13
1.7046	7	2 0 2	53.73
1.6832	3	-2 3 1	54.47
1.6665	7	-2 2 2	55.06
1.6618	4	0 4 0	55.23
1.6577	3	3 2 0	55.38
1.6429	7	3 1 1	55.92
1.6175	5	-3 2 1	56.88
1.6030	9	0 3 2	57.44
1.6005	10	2 3 1	57.54
1.5957	11	1 4 0	57.73
1.5797	1	-1 3 2	58.37
1.5638 1.5495 1.5339 1.5252 1.5170	1 3 7 7	$\begin{array}{ccccccc} 0 & 4 & 1 \\ 0 & 0 & 3 \\ -3 & 1 & 2 \\ -1 & 4 & 1 \\ 2 & 2 & 2 \end{array}$	59.02 59.62 60.29 60.67 61.03
1.5106M 1.5106M 1.5044 1.4932 1.4536	7 7 7 5	1 3 2 3 2 1 -1 1 3 1 4 1 -2 3 2	61.32 61.32 61.60 62.11 64.00
1.4474	2	3 3 0	64.31
1.4402	3	-2 0 3	64.67
1.4374	4	2 4 0	64.81
1.4344	4	4 0 0	64.96
1.4235	4	-3 2 2	65.52
1.4204M 1.4204M 1.4174 1.4045 1.4010	6 8 3 5	-4 0 1 -3 3 1 1 1 3 0 2 3 -1 2 3	65.68 65.68 65.84 66.52 66.71
1.3645 1.3509M 1.3509M 1.3467 1.3371	2 3 4 2	3 1 2 0 4 2 2 3 2 3 3 1 -1 4 2	68.74 69.53 69.53 69.78 70.35

1

1			•		• •	
	CuKa <sub>1</sub>	$\lambda = 1.54059$	8 A;	temp	25	±l °C
	Tuto	1 040-11	1.7		2 1 4	504 P
	Intern	al standard	Ψ,	a =	3.16	524 A
	Å) b	Т		hk l		20(°)
		-		1156~		20( )
	1.3291M	4	1	2	З	70.84
I	1.3291M		0	5	0	70.84
	1.3215	3	-2	2	3	71.31
	1.3167	4	4	2	0	71.61
J	1.3071	1	-4	2	1	72.22
	1.2947+	F		•	2	77 02
	1.2947+	5	- 4	0	2	73.02
	1.2947+		1	5	0	73.02
	1.2841	1	-3	3	2	73.72
	1.2780	3	ō	5	1	74.13
1					-	
	1.2697	з	0	З	з	74.70
	1.2672	3	- 1	З	З	74.87
I	1.2611	4	-3	1	З	75.30
ł	1.2582	3	-2	4	2	75.50
I	1.2541	2	3	4	0	75.79
ł		_	_		_	
L	1.2367	3	-3	4	1	77.05
ł	1.2305	2	4	2	1 7	79.79
ł	1.20.62M	1	2	5	0	70.38
	1.2062M	,	-4	2	2	79.38
l	100000		•	-	-	
	1.2043	6	4	з	0	79.53
I	1.1965	2	-4	З	1	80.15
	1.1900	1	2	4	2	80.68
	1.1869	4	З	4	1	80.93
	1.1826	3	-2	5	1	81.29
	1 1600		•	~		07 04
	1.1520	1	0	0	4	83.04
	1.1571	2	4	5	2	83.83
	1.1435	2	-3	4	2	84.70
	1.1408	2	4	1	2	84.94
		-	-	•	-	0.001
	1.1373	1	4	з	1	85.27
	1.1312+	6	-5	1	1	85.84
	1.1312+		-1	4	з	85.84
	1.1312+		5	1	0	85.84

## Lead Hydrogen Phosphate, $PbHPO_4$ - (continued)

Magnesium Chromium Oxide Hydrate,  $MgCrO_4 \cdot 5H_2O$ 

Sample The sample was prepared at NBS from an aqueous solution of MgCrO4 by slow evaporation at room temperature. Color Vivid orange yellow Structure Triclinic, PI(2), Z = 2. The structure was determined by Bertrand et al. [1971], and the compound was shown to be isostructural with  $CuSO_4 \cdot 5H_2O$ . Lattice constants of this sample: a = 6.4186(9) Åb = 10.787 (2) с = 6.1592(9)  $\alpha = 98.60 (1)^{\circ}$  $\beta = 108.80 (1)$  $\gamma = 75.58 (2)$ a/b = 0.5950c/b = 0.5710Volume 389.87 A<sup>3</sup> Density (calculated) 1.962 g/cm<sup>3</sup> Reference intensity  $I/I_{corundum} = 0.58(3)$ Additional pattern 1. PDF card 23-1223 [Thrierr-Sorel and Lallemant, 1969]. The cell and indexing on it are incompatible. PDF card 1-0243 labelled 7H2O appears to be a mixture with the  $5H_2O$ . References Bertrand, G., Dusausoy, Y., Protas, J. and Watelle-Marion, G. (1971). C. R. Acad. Sci. Ser. C 272, 530. Thrierr-Sorel, A. and Lallemant, M. (1969). C. R. Acad. Sci. Ser. C 268, 1748.

СиКа	$\lambda = 1.54059$	8 Å;	tem	p. 25	±1 °C
Inte	rnal standard	Ag,	a =	4.08	651 A
d (Å)	I	h	kl		20(°)
10.43	10	0	1	0	8.47
5.94	45	1	0	0	14.90
5.70	15	1	1	0	15.52
5.248	45	0 -	-1	1	16.88
4.971	100	-1 -	-1	1	17.83
4.414	30	1	2	0	20.10
4.128	8	-1 -	-2	1	21.51
4.035	30	0 -	-2	1	22.01
3.740	60	0	2	-	23.11
3.647	9	1	0	1	24.39
3.553	30	-1	2	0	25.04
3.473	17	0	3	0	25.63
3.353	50	1 -	-1	1	26.56
3.323	20	1	3	0	26.81
3.237	35	-1 -	-3	1	27.53
3.220	30	-1	2	1	27.68
3.138	14	-2 -	-1	1	28.42
3.114	45	1	2	1	28.64
3.087	25	0 -	-3	1	28.90
3.032M	35	-2	0	1	29.44
3.032M		2	1	0	29.44
2.987	55	-1	0	2	29.89
2.979	60	-2 -	-2	1	29.97
2.906	9	0	0	2	30.74
2.873	14	1 -	-2	1	31.11
2.855M	50	2	2	0	31.30
2.855M		0 -	-1	2	31.30
2.826	35	-1 -	-2	2	31.64
2.749M	70 /	-1	З	0	32.54
2.749M		0	1	2	32.54
2.741		- 1	1	2	32.64
2.651	4	-2 -	-3	1	33.79
2.605	20	0	4	0	34.40
2.598	20	1	4	0	34.50
2.578	8	-1 -	-4	1	34.77
2.541	12	2	з	0	35.30
2.484	11	-2 -	-2	2	36.13
2.475	12	-2	0	2	36.26
2.462	16	0	2	2	36.47
2.415	13	1 -	•3	1	37.20
2.404	15	-1	2	2	37.38
2.387	10	2	1	1	37.66
2.373	13	2	0	1	37.88
2.349	З	1	0	2	38.29
2.312	8	0	4	1	38.93
2.302	19	1	1	2	39.10
2.300	20	-2 -	- 3	2	39.14
2.280	3	1 -	-1	2	39.50
2.246	14	2 -	-1	1	40.11
2.216	8	- 1	4	0	40 60

Magnesium Chromium Oxide Hydrate,  $MgCr0_4 \cdot 5H_20$  - (continued)

d (Å)	I	hkl	20(°)	d (A)	I	hkl	20(°)
2.207	18	2 4 0	40.86	1.6566+		-3 -3 3	55.42
2.122	12	1 -2 2	42.57	1.6454	18	-1 3 3	55.83
2.113+	16	-1 -5 1	42.76	1.6196M	12	-2 -6 2	56.80
2.113+		1 5 0	42.76	1.6196M		350	56.80
2.084	9	0 5 0	43.39	1.6092M	8	-2 4 2	57.20
				1 (000)		- 7 7 1	E7 20
2.062	18	-2 -4 2	43.87	1.6092M	-	-3 3 1	57.50
2.052+	30	-2 2 2	44.10	1.5992		-4 -2 1	57.59
2.052+		2 - 2 1	44.10	1.5821	10	-2 -5 3	58.27
2.024	7	3 1 0	44.75	1.5792+	15	-3 3 0	58+39
2.015M	5	0 -4 2	44.94	1.5792+		-1 -5 3	58.39
2.015M		-3-31	44.94	1.5770+	12	152	58.48
1.997M	20	320	45.38	1.5770+		-1 5 2	58+48
1.997M		-1 -2 3	45.38	1.5672	3	-4 -3 1	58.88
1.978M	6	300	45.84	1.5597M	7	3 4 1	59.19
1.978M		-3 -2 2	45.84	1.5597M		-4 -1 2	59.19
1 073		-2 -5 -	45 07	1.5559M	7	2 4 2	59.35
4.973	0	-2 -5 1	42.97	1.5559M	•	-2 5 0	59.35
1.945	13	-2 -1 3	40.00	1.5443	6	-4 -3 2	59.84
1.930M	18	0 0 3	40.05	1.5420M	6	0 = 6 2	59.94
1.938M		-1 1 3	40.85	1.5420M	Ŭ	-2 5 1	59.94
1.923+	10	-3 0 2	41.22	103420		2 3 1	
1.923+		-2 -2 3	47.22	1.5334M	5	-1 -1 4	60.31
1.917	16	0 5 1	47.38	1.5334M		-3 -6 1	60.31
1.904+	30	-3 -3 2	47.74	1.5222	6	1 7 0	60.80
1.904+		3 3 0	47.74	1.5182M	8	1 -6 1	60.98
1.881+	12	-1 -3 3	48.35	1.5182M		-2 -1 4	60.98
1.8814		-1 -5 2	48.35	1.5164M	6	-4 0 2	61.06
1 0714	15	-7 -5 2	40.52	1.5164M	-	4 2 0	61.06
1.0714	15	-3 1 0	40.02	1.5061M	5	2 6 1	61.52
1 945		-7 -4 1	49.79	1.5061M	-	-4 -4 1	61.52
1 9414	11	-3 -4 1	40.70	1.4976	4	-2 -7 1	61.91
1.0411		2-51	77.70				
1.841M		-2 -3 3	49.46	1.4881	4	070	62.35
1.8220M	10	2 0 2	50.02	1.4842+	6	4 3 0	62.53
1.8220M		2 1 2	50.02	1.4842+		4 0 0	62.53
1.8045M	6	-2 1 3	50.54	1.4736M	4	-3 2 3	63.03
1.8045M		-1 4 2	50.54	1.4736M		-2 -3 4	63.03
1.80.08	6	-1 2 3	50-65	1.4620	6	270	63.59
1.7785M	17	-1 -6 1	51.33	1.4575	7	3 1 2	63.81
1.7785M		-2 4 0	51.33	1.4532	6	0 0 4	64.02
1.7718M	17	-1 5 1	51.54	1.4512	5	3 - 3 1	64.12
1.7718M		1 6 0	51.54	1.4490	4	-4 1 2	64.23
	_		<b>Fo o t</b>	1.44.1.7	11	-2 -6 3	64-46
1.7491	5	0 -3 3	52.26	1. 44.004	7	-2-0 5	64.68
1.7466M	6	3 1 1	52.34	1.4400+	•	3 2 2	64.68
1.7466M		1 -5 1	52.34	1.4394	7	203	64.76
1.7343	8	-1 -4 3	52.74	1.4304	10		65.32
1.7249	6	1 -4 2	53.05	1.42/4+	14	+ + 0	03.32
1.7197	8	-2 -4 3	53.22	1.4274+		-4 -3 3	65.32
1.6979M	25	-3 -2 3	53.96	1.4096	3	-1 2 4	66+25
1.6979M		-3 -5 1	53.96	1.3967+	3	-1 -4 4	66.94
1.6738	2	2 3 2	54.80	1.3967+		3 3 2	66.94
1.6566+	16	3 -1 1	55.42				

Manganese Phosphate, Mn<sub>2</sub>P<sub>2</sub>O<sub>7</sub>

Sample It was prepared from a stoichiometric mixture of MnO <sub>2</sub> and P <sub>2</sub> O <sub>5</sub> .	CuKa <sub>l</sub> Intern	CuK $\alpha_1 \lambda$ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å						
Color	d (Å)	I		hkl		· 20 (°)		
Pinkish white								
Structure	5.166	8	1	1	0	17.15		
Monoclinic, $C2/m$ (12), $Z = 2$ , isostructural with	4.432	7	0	0	1	20.02		
Sc <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> (thortveitite). The structure of	4.294	З	0	2	0	20.67		
Mn <sub>2</sub> P <sub>2</sub> O <sub>7</sub> was determined by Lukaszewicz and	3.107	60	1	1	1	28.71		
Smajkiewicz [1961].	3.086	100	0	2	1	28.91		
Lattice constants of this sample:	2.944	60	-2	0	1	30.34		
a = 6.636(1) Å	2.618	18	1	З	0	34 . 22		
b = 8.584(1)	2.585	20	2	2	0	34.67		
c = 4.5457(9)	2.376	4	2	0	1	37.83		
$\beta = 102.78(1)^{\circ}$	2.348	2	-1	3	1	38.30		
a/b = 0.7731	2.217	3	0	e	2	40.66		
c/b = 0.6850	2.181	6	-1	1	2	41.37		
.,	2.171	20	1	З	1	41.56		
Volume	2.147	4	0	4	0	42.06		
252.55 Å <sup>3</sup>	2.093	6	З	1	0	43.19		
Density	2.078	15	2	2	1	43.52		
(calculated) 3 733 g/cm <sup>3</sup>	2.070	15	-3	1	1	43.69		
(carcurated) 5.755 g/cm	2.053	8	-2	0	2	44.08		
Reference intensity	1.971	З	0	2	2	46.02		
I/I = 1.50(6)	1.932	4	0	4	1	46.99		
Additional pattern	1.851	14	-2	2	2	49.18		
1. PDF card 3-555 [Dow Chemical Co.].	1.7708	4	-1	3	2	51.57		
	1.7519	1	3	1	1	52.17		
Reference	1.7333	4	-2	4	1	52.77		
Lukaszewicz, K. and Smajkiewicz, R. (1961). Rocz. Chem. 35, 741.	1.7227		3	3	0	53.12		
	1.7108	7	-3	З	1	53.52		
	1.6649	9	2	0	2	55.12		
	1.6591	8	1	5	0	55.33		
	1.6209	18	1	З	2	56.75		
	1.6175	11	4	0	0	56.88		
	1.5836	5	-1	5	1	58.21		
	1.5523	2	2	2	2	59.50		
	1.5418	3	0	4	2	59.95		
	1.5325	7	-4	2	1	60.35		
	1.5263	6	1	5	1	60.62		
	1.5175	5	З	з	1	61.01		
	1.4937	4	-3	З	2	62.09		
	1.4834	3	-2	4	2	62.57		
	1.4715	4	-4	0	2	63.13		
	1.4309	5	0	6	0	65.14		
	1.4224	З	4	0	1	65.58		
	1.3921	2	-4	2	2	67.19		
	1.3659	З	-1	5	2	68.66		
	1.3390	9	-1	З	3	70.24		

			0				-
Sample	СиКа	$1 \lambda = 1.540$	598 A;	tem	p. 2	5±1 °C	
equimolar amounts of $MnCO_3$ and $K_2TiO_3$ . The mix-	Internal standard Ag, $a = 4.08651 \text{ A}$						
ture was heated in a silver boat which was placed in a tube with N <sub>2</sub> current. The sample was then heated about 5 min. with a torch until the sample was red hot (≈900 °C).	d (Å)	I		hkl		20(°)	
	4.253	2	1	O	1	20.87	
Color	3.776	25	0	1	2	23.54	
Gray yellowish brown	2.785	100	1	0	4	32.11	
Structure	2.569	70	1	1	0	34.89	
Hexagonal $R_3$ (148) $7 = 6$ isostructural with	2.3811	4	C	0	6	37.75	
FeTiO <sub>2</sub> . The structure of FeTiO <sub>2</sub> , ilmenite, was							
determined by Barth and Posnjak [1934]. Shirane,	2.2620	30	1	1	3	39.82	
Pickart and Ishikawa [1959] confirmed the struc-	2.1985	4	0	2	1	41.02	
ture of MnTiO <sub>3</sub> by neutron diffraction.	2.1244	2	2	0	2	42.002	
• -	1.7460	40	1	2	4	40 • 1 4 62, 33	
Lattice constants of this sample:	1.1409	40	•	•	C	52+35	
$a = 5.1396(1) \text{ \AA}$	1.6710	5	2	1	1	54.90	
c = 14.2902(6)	1.6577	10	0	1	8	55.38	
	1.6378	3	1	2	2	56.11	
c/a = 2.7804	1.5220	35	2	1	4	60.81	
	1.4838	30	З	0	0	62.55	
Volume o							
326.91 A <sup>3</sup>	1.4496	2	1	2	5	64.20	
Prove the	1.3929	Э	2	0	8	67.15	
Jensity	1.3605	11	1	0 1	10	68.97	
(calculated) 4.596 g/cm <sup>2</sup>	1.3507	4	1	1	9	69.54	
Poforongo intensity	1.2849	e	2	2	0	73.67	
T/T = 1.5(1)		_	_	_	_		
forundum for the form	1.2593	3	Э	0	6	75.42	
Polymorphism	1.2403	2	2	2	3	70.79	
Syono et al. [1969] report the existence of a	1.2247	4	1 7	2	с 2	76.59	
high pressure magnetic phase of MnTiO3.	1.2023	5	0	2 1	2	75.69	
	1.2025	0	Ŭ			13003	
Additional patterns	1.1668	10	1	3	4	82.63	
1. PDF card 12-435 [Lee, 1955]	1.1307	6	2	2	E	85.88	
2. Portnov [1963]	1.0996	1	ō	4	2	88.94	
3. Posnjak and Barth [1934]	1.0892	7	2	1	10	90.02	
	1.0804	2	1	1 1	12	90.95	
References							
Barth, T. F. W. and Posnjak, E. (1934). Z. Kris-	1.0673	1	1	0	13	<b>\$2.40</b>	
tallogr. Kristallgeometrie Kristallphys.	1.0625	З	4	0	4	\$2.93	
Kristallonem. 88A, 265.	1.0157	З	3	1	8	98.65	
Lee, D. E. (1955). Stanford Univ. Publ, Univ.	•9989	1	2	2	9	100.91	
Portnov, A. M. (1963). Dokl. Akad. Nauk. SSSR	.9949	3	a	1 1	14	101.47	
$\frac{153}{100}$ , 187.	•9818	7	3	2	4	103.36	
Posnjak, E. and Barth, T. F. W. (1934). 2.	.9714	5	4	1	0	104.93	
Kristallogr. Kristallgeometrie Kristallphys.	•9615	1	2	3	5	106.48	
Chirana C Dickart S J and Johikawa V	•9526	2	0	0	15	107.92	
(1959). J. Phys. Soc. Jap. <u>14</u> , No. 10.	• 9517	1	4	1	3	108.07	
Syono, Y., Akimoto, S., Ishikawa, Y., and Endoh,	.9444	3	0	4	ε	169.30	
Y. (1969). J. Phys. Chem. Solids <u>30</u> , 1665.	.9342	5	1	3	10	111.09	
	.9279	4	2	0	14	112.23	
	.8994	7	4	1	ć	117.85	

Sample					
The NBS anne	sample wa by arc r aling at 1	ns prepared Melting in 1600 °C in v	by R. M. Wate vacuo four acuo for 4 ho	erstrat at times and urs.	+
Color Gray	metallic				
Struct Tetr Cr5B by Pa	ure agonal, I4 3. The st arthé et a	/mcm(140), 5 ructure of 6 al. [1955].	Z=4, isostruc α-Nb5Si3 was o	tural with letermined	
Lattice a = 0 c = 1	e constant 6.5698(3) 11.8877(8)	s of this sa Å	ample:		
c/a :	= 1.8094				
Volume 513.	10 Å <sup>3</sup>				
Density (cale	y culated) 7	.104 g/cm <sup>3</sup>			
Referen I/I	nce intens orundum <sup>=</sup>	ity 3.9(3)			
Three by Ki tempo β-Nb gonal 1900 ted l carbo	e modifica hapton [19 erature i 55i3, hig 1, W <sub>5</sub> Si3 t °C and 210 by Knaptor on is pre-	tions of Nb 55]. The c s tetragonal th temperatur ype. The tra 0°C. The the [1955] and for esent is her	5Si3 have been X-Nb5Si3, stat 1, Cr5B3 type re form is all ansition occur ird modificat: bund to exist xagonal, Mn55	n reported ole at low , and the lso tetra- rs between ion repor- when 1-2% Si <sub>3</sub> type.	
In so "Nb 3	ome litera Si <sub>2</sub> ."	ture the co	omposition is	given as	
Additio	onal patte PDF card 9	rn 9-222 [Parthé	é, 1955].		
Referen Knap Part Mon	nces ton, A. G. hé, E., I natsh. Che	(1955). Na лих, В., and m. <u>86</u> , 859.	ature <u>175</u> , 730 d Nowotny, H.	). . (1955).	
	CuKα <sub>1</sub> λ =	• 1.540598 A	; temp. 25±1	°C	
	Internal	standard Si	a = 5.43088	Å	
d (A	)	I	hkl	20(°)	
3.6	60	8	112	24.30	
3.2	83 71	2	200	27.14	
2.9	75	17	202	31.08	
2.8	54	25	211	31.32	
2.5	04	25	114	35.84	L
2.3	60 I 25	13	213	38.10	
4.3	6.5	1.0	660	JO . / U	

2.204

2.963

30

<1

204

222

d(A)	I	hk l	20(°)
2.077	40	310	43.54
1.982	16	006	45.75
1.962	1	312	46.24
1.848	1	215	49.26
1.831	<1	224	49.77
1.823	<1	116	50.00
1.802	<1	321	50.62
1.696	1	206	54.02
1.655	<1	323	55.47
1.642	1	400	55.97
1.5792	8	411	58.39
1.5488	4	330	59.65
1.5077	1	226	61.45
1.4982	2	332	61.88
1.4859	3	008	62.45
1.4780	16	413	62.82
1.4699	20	217,420	63.21
1.4464	<1	325	64.36
1.4376	9	404	64.80
1.4338	17	316	64.99
1.4158	<1	118	65.92
1.3731	13	334	68.25
1.3534	1	208	69.38
1.3170	<1	424	71.59
1.2646	2	406	75.05
1.2591	2	512	75.44
1.2513	2	228	75.99
1.2201	4	336	78.30
1.2135	2	521	78.81
1.2085	6	318	79.20
1.2045	5	219	79.51
1.1888	1	0•0•10	80.78
1.1820	5	514	81.34
1.1800	4	426	81.51
1.1660	12	523	82.70
1.1623	10	417	83.02
1.1519	1	1•1•10	83.94
1.1400	<1	442	85.02
1.1267	4	530	86.26
1.1178	2	2•0•10	87.12
1.0950	3	600	89.41
1.0854	<1	525	90.42
1.0818	<1	444	90.80
1.0534	<1	534	93.98
1.0448	2	428	95.00
1.0318	1	3·1·10	96.59
1.0276	1	604	97.12
1.0171	2	419	98.46
1.0141	3	2·1·11	98.85

40.92

6 з З

8

20(°)

12.46

17.65

25.09 26.50

28.11

35.37

35.79

36.81

37.66

38.02

39.80

40.18

41.12

43.86

51.21

52.29

53.21

54.58

54.86

58.14

58.32 58.87

59.44

61.98

64.05

64.49

65.00

65.55 65.79

67.02

67.43

69.92

70.83

71.62 74.87

75.99

76.47

76.97

78.34

78.60

79.22

81.34

81.74

82.49

82.73

84.21

84.70

85.83

86.55

86.94

Sample	CuKal	$\lambda = 1.5409$	598 Å;	tem	p. 25	±l °C
The sample was prepared by R. M. Waterstrat at NBS. Niobium and silicon placed in a copper crucible were are melted under argon. The	Inter	nal standar	d Si,	a =	5.43	088 Å
product was then rapidly cooled.	d (A)	I	ł	hkl		2
Color						·
Grav metallic	7.10	3	1	1	Ģ	12
Gray motarrat	5.921	2	2	0	0	17
at we have	3.546	6	2	2	0	25
Structure	3.361	25	2	1	1	26
Tetragonal, I4/mcm (140), Z=4 [Parthé, Schachner,	3.172	30	3	1	0	28
and Nowotny, 1955], isostructural with w5513. The						
structure of W <sub>5</sub> Si <sub>3</sub> was determined by Aronsson	2.536	30	0	0	2	35
[1955].	2.507	14	4	õ	0	35
	2.001	80	3	2	1	36
Lattice constants of this sample:	2.440	10		-	•	37
a = 10.0289(4) Å	2.387	14	<u>+</u>	±	2	31
c = 5.0698(4)	2.365	11	3	3	0	36
	2.263	40	2	0	2	39
c/a = 0.5058	2.243	55	4	2	0	40
	2.243	100	4	1	ĩ	61
Volume	2.193	100	4	+	-	
509.91 A <sup>3</sup>	2.0625	60	2	2	2	43
	1.7824	3	4	0	2	51
Density	1.7481	6	5	2	1	52
(calculated) 7.149 g/cm <sup>3</sup>	1.7000	,	5	2	•	5
	1.7200	1	5	2	2	5.
Reference intensity	1.6801	IL	4	2	2	5.
I/I = 1.22(15)	1.6721	1	6	0	e	54
corundum	1.5854	14	6	2	0	58
Polymorphism	1.5800	10	2	1	٦	58
Three modifications of Nb <sub>5</sub> Si <sub>3</sub> have been reported	1.5674	10	6	÷	ĩ	54
by Knapton [1955]. The $\alpha$ -Nb <sub>5</sub> Si <sub>3</sub> , stable at low	1.5674	1	5	-	-	50
temperatures, is tetragonal Cr <sub>5</sub> B <sub>3</sub> -type and the	1.5538	13	5		2	5
$\beta$ -Nb <sub>5</sub> Si <sub>3</sub> high temperature phase is reported here.	1.4961	10	5	4	1	0.
The $\alpha$ - $\beta$ transformation occurs between 1,900 and	1.4526	9	4	4	2	64
2100 °C. The third modification reported by many	1 44 37	1.8	٦	2	=	6
authors and found by Knapton [1955] to exist when	1.44.57	10	ی د	2	,	6
1-2% carbon is present is hexagonal Mn <sub>5</sub> Si <sub>3</sub> -type.	1.4330	11	-	2	-	6
	1.4229	14	5	3	2	0:
In some of the literature, McSia compounds have	1.4183	20	5	5	e	6:
been labelled "M <sub>3</sub> Si <sub>2</sub> ."	1.3953	18	6	O	2	6
	1.3878	30	4	1	з	6
Additional pattern	1 7447	11	6	2	2	6
1. PDF card 9-272 [Parthé, Nowotny, and Schmid,	1.3443	1	7	2	1	70
1955].	1.3293	1	<u>'</u>	2	-	
	1.3165	1		5	0	-
References	1.2672	8	0	0	4	
Aronsson, B. (1955). Acta Chem. Scand. 9, 1107.	1 0517	2	=	2	٦	7
Knapton, A. G. (1955). Nature London 175, 730.	1.2513	2	5	2		
Parthé, E., Nowotny, H., and Schmid, H. (1955).	1.2446	2	0	5	1	-
Monatsh, Chem, 86, 385,	1.2378	10	5	5	2	
Parthé, E., Schachner, H., and Nowotny, H. (1955).	1.2196	15	6	4	2	78
Monatsh. Chem. 86, 182.	1.2162	15	8	2	0	78
	1 00.00	1	7	4	1	7
	1.2002	1	6	6	•	
	1.1829	5	0		6	0.
	1.1772	5	3	+	4	8
	1.1684	6	_	3	2	8
	1.1656	4	1	5	0	8
	1-1489	4	5	4	з	8
	1.1435	14	8	3	1	8
	1 1 2 1 2	3	4	2	4	8
	1.1013	3	-	ó	2	0
	1.1237		0	0	2	0

d (Å)	I		hkl		20(°)
1.1169	5	3	3	4	87.21
1.1076	2	9	1	C	88.13
1.1033	14	4	2	4	88.56
1.0714	1	6	6	2	91.94
1.0681	1	7	2	3	92.31
1.0636	1	7	6	1	92.81
1.0405	2	8	5	1	95.52
1.0310	1	4	4	4	96.69
1.0256	7	8	4	2	97.37
1.0224	2	6	5	3	97.78
1.01 50	8	9	1	2	98.74
1.0130	3	7	7	0	99.00
1.0099	2	6	0	4	99.41
1.0028	2	8	6	0	100.37
• 99 82	3	9	4	1	101.01

Niobium Silicide,  $\beta$ -Nb<sub>5</sub>Si<sub>3</sub> - (continued)

Potassium Borate Hydroxide Hydrate,  $K_2B_40_5(0H)_4 \cdot 2H_20$ 

	•				
Sample	d (A)	I	hkl.		20(°)
The sample was made by slow evaporation from					20( )
aqueous solution at room temperature.	7 070	4.5	• •	~	
1	3.030	45	0 2	2	29.46
Color	3.019	40	3 2	1	29.57
Colorless	2.964	40	2 0	2	30.13
	2.945	60	4 0	0	30.33
Structure	2.922	45	0 4	1	30.57
Orthorhombic, $P_{2_1} 2_{1_2} (19)$ , $7 = 4$ . The structure				_	_
was studied by Marezio et al [1963]	2.891	50	2 1	2	30.91
was studied by Marchie et al. (1905).	2.872	35	4 1	0	31.12
Lattice constants of this cample.	2.833M	40	1 4	1	31.55
2 = 11785(3)	2.833M		2 4	0	31.55
a = 11.703(3) A	2.706	50	4 0	1	33.08
D = 12.917(3)					
C = 0.005(1)	2.698	40	2 2	2	33.18
(1 0 0104	2.683M	70	03	2	33.37
a/b = 0.9124	2.683M		4 2	0	33.37
c/b = 0.5315	2.650	20	4 1	1	33.80
	2.617M	45	2 4	1	34.23
Volume •					
1045.0 A <sup>3</sup>	2.617M		1 3	2	34.23
· · ·	2.585	7	3 0	2	34.68
Density	2.524	11	1 5	0	35.54
(calculated) 1.942 g/cm <sup>3</sup>	2.495	55	A 2	1	35.66
	2.495M	55	7 4	•	35.50
Reference intensity	20490M		5 4	0	32030
T/T = 0.20(1)					
corundum corundum	2.431	15	4 3	0	36.95
Additional matterna	2 • 39 9	6	3 2	2	37.46
Additional patterns	2.368M	18	1 5	1	37.97
1. PDF card 19-950 [Toledano, 1966]	2.368M		25	0	37.97
	2.344	12	34	1	38.37
References					
Marezio, M., Plettinger, H. A., and Zachariasen,	2.305	50	1 4	2	39.04
W. H. (1963). Acta Crystallogr. <u>16</u> , 975.	2.292	25	4 3	1	39.27
Tolédano, P. (1966). Bull. Soc. Chim. France 1966,	2.253	13	01	з	39.98
2302.	2.248	12	1 0	З	40.08
[·····································	2.236M	10	2 5	1	40.31
$CuK\alpha_1 \lambda = 1.540598 \text{ A}; \text{ temp. } 25\pm1 \text{ °C}$	2.2364		<u> </u>	~	40.71
0	2.230M	4.0	4 0	2	40.31
Internal standard Si, a = 5.43088 A	2.202	40	4 1	2	40.95
0	2.196	35	5 1	1	41.06
$d(A)$ I $hk\ell$ $2\Theta(^{\circ})$	2.157M	30	35	0	41.84
	2.157M		02	з	41.84
	2.132	20	2 0	З	42.36
	2.115	30	4 2	2	42.72
5.94 90 1 0 1 14.91	2.105	35	21	з	42.94
5.388 95 1 1 1 16.44	2.075	40	4 4	1	43.59
4.471 40 2 0 1 19.84	2.068	30	5 3	0	43.74
4.367 16 1 2 1 20.32	2.055	12	06	1	44.03
4.223 20 2 1 1 21.02	2.033	12	1 5	2	44.52
4.042 6 1 3 0 21.97	2.022+	36	1 6	1	44.78
3.759 35 3 1 0 23.65	2.022+		2 6	•	44.70
3.673 35 2 2 1 24.21	1.001	4.0	1 7	2	44 . 10
	1 + 7 7 1	40	1 3	3	40.02
3.648 45 0.3.1 24.38				~	
3.480M 25 1 3 1 25.58	1.985	35	4 3	2	45.66
3.480M 2.3.0 25.58	1.978	20	3 O	З	45.84
3.428 20 0.0 25.07	1.948	17	2 5	2	46.58
	1.942+	17	4 5	0	46.73
3.409 75 3 0 1 20.12	1.942+		ε 1	0	46.73
3.317 65 0 1 2 26.86	1.922	11	5 1	2	47.26
3.227 45 0 4 0 27.62	1.891	14	3 2	З	48.08
3.194 100 1 1 2 27.91	1.887M	14	€ 0	1	48.18
3.112 50 1 4 0 28.66	1.887M		36	0	48.18
3.102 50 2 3 1 28.76	1.869M	13	4 5	1	48.68
	1.869M		6 1	1	48.68
46	1.8392	7	4 4	2	49.52
	1.00072			-	

•

7

4 4 2

Sample The sample was obtained from the B. R. Elk & Co., Garfield, N.J. and was recrystallized from aqueous solution. Color Orange red Structure Triclinic, Z = 4 [Gossner and Mussgnug, 1930], [Klement and Schwab, 1960]. Lattice constants of this sample  $a = 7.468(2) \text{ \AA}$ b = 13.419(5)c = 7.391(3) $\alpha = 98.13(3)^{\circ}$  $\beta = 90.86(3)$  $\gamma = 96.23(3)$ a/b = .5565c/b = .5508Volume 728.5 A<sup>3</sup> Density (calculated) 2.682 g/cm<sup>3</sup> Polymorphism K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> transforms to a monoclinic form at about 250 °C. There is also a metastable monoclinic form at room temperature [Klement and Schwab, 1960]. Additional patterns 1. PDF card 12-300 [Inst. of Phys. Cardiff, Wales] References Gossner, B., and Mussgnug, F. (1930). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 72, 476. Klement, U., and Schwab, G. M. (1960). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 114, 170. CuK $\alpha_1$   $\lambda$  = 1.540598 A; temp. 25±1 °C Internal standard Si, a = 5.43088 A d(A) Ι hkl 20(°) **ī**10 6.79 10 13.02 6.59 12 020 13.42 6.04 10 011 14.65 5.30 8 021,101 16.70 5.13 14 101 17.27 5.09 14 111 17.40 4.949 17 111 17.91 4.873 30 111 18.19 4.682 6 120 18.94

20

4.516

111

$d(a)$ Ihkk $20(\circ)$ 4.45415 $1\overline{2}1$ $21,23$ 3.71130 $200$ $23.96$ 3.65755 $012,002$ $24.32$ 3.5535 $031$ $25.64$ 3.47385 $210$ $25.63$ 3.42820 $\overline{13}1$ $25.97$ 3.40120 $\overline{2}20,012$ $26.18$ 3.34740 $\overline{2}01,1\overline{3}1$ $26.61$ 3.300100 $040,2\overline{1}1$ $27.00$ 3.24216 $\overline{12}1$ $27.66$ 3.1837 $041$ $28.01$ 3.1416 $2\overline{2}1,1\overline{2}2$ $28.90$ 3.06530 $\overline{12}2$ $29.52$ 3.00935 $\overline{2}30$ $29.67$ 2.9469 $\overline{2}\overline{2}1$ $30.31$ 2.87435 $\overline{12}2$ $31.09$ 2.85625 $041,2\overline{3}1$ $31.29$ 2.7578 $\overline{13}2,221$ $34.35$ 2.60913 $2\overline{1}2,\overline{2}\overline{1}2$ $34.35$ 2.64016 $050$ $33.93$ 2.60913 $2\overline{1}2,\overline{2}\overline{1}2$ $34.35$ 2.47510 $\overline{2}\overline{2}2,300$ $36.26$ 2.43811 $212,003$ $36.84$ 2.40410 $\overline{3}20,150$ $37.38$ 2.38515 $\overline{15}1,310$ $37.38$ 2.47510 $\overline{2}\overline{2}2,1\overline{2}3$ $39.25$ 2.64014 $\overline{3}3,250$ $36.62$ 2.43811 $212,003$ $36.84$ 2.47716				
4.454       15 $1\overline{21}$ 19.92         4.182       6 $1\overline{21}$ 21.23         3.711       30       200       23.96         3.657       55 $0\overline{12},002$ 24.32         3.473       85 $2\overline{10}$ 25.63         3.428       20 $\overline{131}$ 25.97         3.401       20 $\overline{220},012$ 26.18         3.347       40       201, $\overline{131}$ 26.61         3.300       100       040,211       27.00         3.242       16 $\overline{211}$ 27.66         3.183       7 $0\overline{41}$ 28.01         3.141       6       221,122       29.52         3.067       12       220       28.90         3.065       30 $\overline{122}$ 29.52         3.009       35       230       29.67         2.946       9 $\overline{221}$ 30.31         2.856       25 $041, 2\overline{31}$ $31.29$ 2.757       8 $\overline{132}, 221$ $3.68$ 2.609       13 $212, \overline{212}$ $34.35$ 2.640       16       050 <th>d(Å)</th> <th>I</th> <th>hkl</th> <th>20(°)</th>	d(Å)	I	hkl	20(°)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4.454	15	121	19.92
	4.182	6	121	21.23
	3.711	30	200	23.96
	3.657	55	012,002	24.32
	3.553	5	031	25.04
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3.473	85	210	25.63
	3.428	20	131	25.97
	3.401	20	220,012	26.18
	3.347	40	201,131	26.61
	3.300	100	040,211	27.00
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3.242	16	102	27.49
	3.222	16	211	27.66
	3.183	7	041	28.01
	3.141	6	221,122	28.39
	3.087	12	220	28.90
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3.065 3.024 3.009 2.946 2.874	30 40 35 9 35	$     \begin{array}{r} 1 \overline{2} 2 \\     112,022 \\     230 \\     \overline{2} 21 \\     \overline{1} 22     \end{array} $	29.11 29.52 29.67 30.31 31.09
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2.856	25	041,231	31.29
	2.757	8	132,221	32.45
	2.711	6	231	33.01
	2.692	7	230	33.25
	2.640	16	050	33.93
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2.609	13	2Ī2,2Ī2	34.35
	2.575	13	141	34.81
	2.547	16	222,142	35.21
	2.540	18	151,241	35.31
	2.475	10	222,300	36.26
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2.438	11	212,003	36.84
	2.404	10	320,150	37.38
	2.385	15	151,310	37.68
	2.338	9	013,103	38.47
	2.301	11	321	39.12
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2.293	12	232,123	39.25
	2.273	8	033,250	39.62
	2.252	10	142,152	40.00
	2.193	12	151,133	41.12
	2.151	8	241,152	41.96
	2.132	10	142	42.37
	2.089	12	242	43.27
	2.061	18	213,330	43.90
	2.055	20	143	44.02
	2.047	20	160,250	44.21
	1.990	7	152,322	45.55
	1.905	8	162,133	47.69

Potassium Iodate, KIO3

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0

20(°)

14.11 14.11 19.86 19.86 24.19

24.19 24.40 24.40 28.13 28.38

31.58 31.58 31.80 31.80 34.41

34.86 34.86 37.35 37.35 37.71

37.71 37.82 37.82 40.29 40.37

45.18 45.18 45.46 45.52 45.57

47.92 47.92 48.05 49.52 49.52

50.02 50.02 50.12 50.12 50.23

51.75 51.75 52.08 52.08 52.45

52.45 56.37 56.37 56.71 56.71

Sample	$CuK\alpha_1 \lambda = 1.540598 A; temp. 25\pm1 °C$					
The sample was reagent material from Fisher Scientific Co., Bloomfield, N.J.	Inte	rnal stand	ard Ag, a	a = 4.08651 A		
Color Colorless	d (Å)	I	hkl		20	
Structure	6.27M	1	0'-1	1	14	
	6.27M		-1 0	1	14	
Triclinic, $PI(1)$ , $Z = 4$ , pseudo-monoclinic and a	4.467+	45	1 -1	1	10	
distorted perovskite-type. The structure was	4.467+	40	-1 1	i	10	
refined by Hamid [1973]. Much work has been done	7.676+	,	-1 1		13	
on the symmetry problems of KIO <sub>3</sub> and a summary was given by Crane [1972].	3.0704	•		0	24	
	3.0/0+		0 1	1	24	
Lattice constants of this sample:	3.645+	1	-1 2	0	24	
a = 7.708(1) Å	3.645+		-2 1	0	24	
h = 7.722(2)	3.170	100	0 0	2	28	
c = 7.689(2)	3.142	80	0 -2	2	28	
$\alpha = 109.25(2)^{\circ}$						
R = 109.25(2)	2.831+	1	-1 -2	1	31	
p = 100.35(2)	2.831+		-2 -1	1	31	
Y = 109.37(2)	2.812+	1	-1 -2	2	31	
// 0.0000	2.812+		-2 1	2	31	
a/b = 0.9982	2.604	4	1 1	1	34	
c/b = 0.9975				•		
The NBS data could be indexed only with this	2.572M	6	1'=3	1	34	
triclinic cell, refined from the one derived by	2.572M		-3 1	1	34	
Hamid [1973].	2.406+	1	2 1	0	37	
	2.406+		1 2	0	37	
Volume	2.384+	1	-1 0	3	37	
355 9 A <sup>3</sup>						
555.5 A	2.384+		-2 3	0	37	
Depaitu	2.377+	1	0 -2	3	37	
(a a l a b a b a d) = 2.004 a (a a 3)	2.377+		-3 2	1	37	
(calculated) 3.994 g/cm°	2.237	35	2 -2	2	40	
m Annual fra	2.232	30	-2 2	2	40	
Polymorphism						
Between -200 °C and +250 °C there are at least 5	2.005+	15	-1 3	1	45	
phase changes. The room temperature triclinic	2.005+		-1 -3	1	45	
symmetry becomes monoclinic at 72.5 °C and rhom-	1.994	11	3 -3	1	45	
bohedral at 212 °C [Hamid, 1973; Salje, 1973].	1.991	12	1 -3	3	45	
	1.989	13	-3 3	1	45	
Additional pattern				•		
1. PDF card 1-776 [Hanawalt et al., 1938].	1.897M	16	-1 -1	4	47	
	1.897M		-4 2	1	47	
References	1.892	11	-1 -2	<u>م</u>	48	
Crane, G.R. (1972). J. Appl. Crystallogr. <u>5</u> , 360.	1.839M	16	2 2	0	49	
Hamid, S.A. (1973). Z. Kristallogr. Kristallgeo-	1.830M		2 0	2	40	
metrie Kristallphys. Kristallchem. 137, 412.	1.003.914		2 0	2		
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K.	1 8224	30	- 1 2	•	50	
(1938). Ind. Eng. Chem. Anal. Ed. 10, 457.	1.0224	50	-4 2	0	50	
Salje, E. (1973). Z. Kristallogr. Kristallgeome-	1.022+	76	-2 4	0	50	
trie Kristallphys. Kristallchem. 137. 1.	1.819+	35	2 -4	2	20	
	1.819+		0 =2	4	50	
	1.815	18	-2 0	4	50	
	1.765+	1L	1 3	0	51	
	1.765+		30	1	51	
	1.755+	1L	-4 0	1	52	
	1.755+		-2 3	2	52	
	1.743M	1L	-4 3	1	52	
	1.743M		0 -3	4	52	
	1.6309+	1∟	4 -3	1	56	
	1.6309+		-4 -1	2	56	
	1.6219M	1L	-3 1	4	56	
	1.6219M		-4 2	3	56	

# Potassium Iodate, $KIO_3$ - (continued)

d (Å)	I	hkl	20(°)
1.5874M	12	0 4 0	58.06
1.5874M		4 0 0	58.06
1.5738	10	-4 4 0	58.61
1.5701	5	0 - 4 4	58.76
1.5222M	1L	-4 1 4	60.80
1.5222M		-2 -1 5	60.80
1.5017+	2	1 3 1	61.72
1.5017+		3 1 1	61.72
1.4893	5	-5 1 1	62.29
1.4848M	6	-1'-1 5	62.50
1.4848M		3 -5 1	62.50
1.4802M	5	-5 1 3	62.72
1.4802M	_	-1 -3 5	62.72
1.4185	9	4 - 2 2	65.78
1.4153M	11	-4 -2 2	65.95
1.4153M		-2 -4 2	65.95
1.4070M	7	-2 -4 4	66.39
1.4070M		-4 4 2	66.39
1.3552	2	-3 -3 1	69.28
1.3440M	3	1'=3 5	69.94
1.3440M		3-5 3	69.94
1.3019	1L	2 2 2	72.55
1.2871	2	2'-6 2	73.52
1.2846	з	-6 2 2	73.69
1.2441M	3	-5-1 1	76.51
1.2441M		-1 -5 1	76.51
1.2321	2	-1 -5 5	77.39
1.2029M	7	2 4 0	79.64
1.2029M		4 2 0	79.64
1.1935	6	-6 0 2	60.39
1.1910+	е	-6 4 0	80.60
1.1910+		-4 6 0	80.60
1.1884M	7	-6 4 2	E0. E1
1.1884M		0'-4 6	80.81
1•1851M	4	-4 0 6	£1.08
1.1851M		-2 -4 6	81.08

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Sample		red by besting	a leled molar	d(Å)	I	h	kl		20(°)
The sample	was "prepa	Pred by heating							
followed by	rogrindi	ng molting at	about 500 °C	4.247	19	1	1	2	20.90
TOTTOwed D	y regrindi	then bested at	$225 ^{\circ}C$ for a	3.962M	9	0	2	2	22.42
The ground	glass was	then heated at	525 °C 101 a	3.962M		2	0	2	22.42
weekena.				3.877	55	3	2	1	22.92
				3.850	80	4	0	0	23.08
Color				and the second s					
Colorless				3.748	4	1	4	0	23.72
				3.552	25	4	0	1	25.05
Structure				3.520	25	2	2	2	25.28
Orthorhombi	ic, Pcab (6	1), $Z = 8$ . The	is agrees with	3.456	35	2	4	0	25.76
Mahama et a	al. [1977]	but is a diffe	erent form of	3.437	100	0	з	2	25.90
the space	group that	an reported by	y Brunel-Laügt						
[1977].				3.388	9	з	з	1	26.28
				3.348	30	3	1	2	26.60
Lattice const	ants of th	is sample:		3.235M	60	2	4	1	27.55
a = 15.4160	(4) Å	-		3.235M		4	2		27.55
b = 15.465	(5)			3.130M	7	3		2	27.000
c = 9.225(	(3)			5.15.50	,	د	5	2	20041
0 51225	(5)			7 1704		-	~	~	00 41
a/b = 0.996	59			3.139M		-	4	2	28.41
a/D = 0.990	50			3.088	4	3	4	0	28.89
C/D = 0.596	55			2.963M	25	0	4	2	30.14
				2.963M		1	1	з	30.14
Volume				2.928M	60	З	4	1	30.51
2199.1 A <sup>3</sup>									
				2.928M		4	З	1	30.51
Density		2		2.906	30	4	1	2	30.74
(calculated	a) 3.632 g/o	cm <sup>5</sup>		2.875	35	5	1	1	31.08
				2.859	30	з	з	2	31.26
Polymorphism				2.81 OM	45	1	2	з	31.82
There is a	second pha	ase which is t	cetragonal re-						
ferred to a	as K2PbP401	2, stable below	v 537° [Mahama	2.810M		2	1	з	31.82
et al., 197	77].			2.766	9	2	4	2	32.34
				2.731	25	4	4	0	32.77
Additional pa	attern			2.680	6	2	2	3	33.41
1. Mahama	et al. [19	771		2.618	5	4	4	1	34.22
	00 un (1)				5	-	-	•	34022
References				2.60.24	7	,	7	2	74.44
Brunol-Louis	t Mand	Cuitol J -C	(1977) Acta	2 60 24	'		,	7	74 44
Druner-Daug	$g_{c}$ , $H_{c}$ and $g_{c}$	27	(1977). Acta	2.5674	50	0	-	2	34.44
CIYSLAIIC Mahama T	Jyr. <u>535</u> , 9	J/. T-ümt M	ad December als	2.5074	50	-	-	2	34.92
Manama, 1.	, Brunel	Laugt, M., an	a Averbuch-	2.507+	•	3	4	2	34.92
Poucnot,	MT. (19	//). C. R. Ad	cad. Sci. Ser.	2.54.3M	8	5	3	I	35+20
$C \underline{284}, 68$	31.						_		
				2.543M		1	e	0	35.26
		0		2.499M	30	2	З	З	35.90
CuKα <sub>1</sub>	$\lambda = 1.54059$	98 A; temp. 25±	:1 °C	2.499M		3	2	З	35.90
				2.475	8	6	0	1	36.26
Intern	al standard	d Ag, a = 4.086	51 Å	2.445M	5	2	6	0	36.73
d(A)	I	hkl	20 (°)	2.445M		6	1	1	36.73
				2.403	4	4	0	-	37.39
			-	2.363	12	2	6	ĩ	38.05
7.70	10	200	11.49	2.7064	16	2	0	^	39.03
7.03	55	1 1 1	12.58	2.3000	10		4	~	39.03
6.89	45	1 2 0	12.83	2.300M		3	0	0	39.03
5.91	ЗC	2 0 1	14.98			_	-		
5.53M	50	1 2 1	16.02	2.299M	25	3	5	2	39.16
				2 • 29 9M		2	4	3	39.16
5.53M		2 1 1	16.02	2.258	4	1	1	4	39.90
4.609	6	C 0 2	19.24	2.231	10	6	З	1	40.40
4.416	20	C 1 2	20.09	2.222	12	6	1	2	40.56
4.308	25	3 1 1	20.60						
4.277	45	3 2 0	20.75	2.189M	12	1	2	4	41.21
		5 2 0	20015	2.189M		2	1	4	41.21
•				2.182	10	З	4	З	41.35
				2.158M	13	2	6	2	41.82
				2.158M		1	5	з	41.82

d (Å)	I	hk	٤	20(°)
2.142	13	4	6 0	42.15
2.125M	12	5	51	42.51
2.125M		2	2 4	42.51
2.120	12	7	2 0	42.62
2.096	12	5	23	43.13
2.088M	13	4	61	43.30
2.088M		1	34	43.30
2.070	12	2	7 1	43.70
2.064	11	7	2 1	43.83
2.059	13	6	32	43.94
2.042	6	4	4 3	44.33
2.031M	10	2	3 4	44.58
2.031M		З	2 4	44.58
1.993	е	0	7 2	45.47
1.981+	19	З	7 1	45.76
1.981+		0	4 4	45.76
1.974	15	5	5 2	45.94
1.934+	ç	5	6 1	46.95
1.934+		0	8 0	46.95
1.915M	12	7	4 0	47.45
1.915M		2	63	47.45
1.886	4	8	0 1	48.22
1.876M	ç	4	7 1	48.49
1.876M		2	e o	48.49
1.873M	10	7	4 1	48.58
1.873M		8	1 1	48.58
1.848+	6	0	5 4	49.26
1.848+		З	4 4	49.26
1.843	8	з	63	49.41
1.820M	З	6	6 0	50.09
1.820M		1	1 5	50.09
1.796M	е	5	2 4	50.81
1.796M		2	0 5	50.81
1.782+	12	1	2 5	51.21
1.782+		2	1 5	51.21
1.771M	25	8	3 1	51.55
1.771M		1	8 2	51.55
1.748M	12	2	7 3	52.28
1.748M		2	25	52.28

Potassium Lead Phosphate,  $K_2Pb(PO_3)_4$  - (continued)

Sample The sample was prepared by adding H <sub>2</sub> SeO <sub>4</sub> to a solution of K <sub>2</sub> CO <sub>3</sub> and PbCO <sub>3</sub> , thus co-precipita- ting K <sub>2</sub> SeO <sub>4</sub> and PbSeO <sub>4</sub> . The solution was dried and the solids were heated for 17 hrs. at 600°C.	
Color Vivid pale yellow	
Structure Hexagonal, $R\overline{3}m$ (166), $Z = 3$ , isostructural with Ba <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> and many double sulfates, chromates, and selenates [Schwarz, 1966]. The structure of (NH <sub>4</sub> ) <sub>2</sub> Pb(SO <sub>4</sub> ) <sub>2</sub> was studied by Møller [1954].	
Lattice constants of this sample: a = 5.7059(7) A c = 21.134(3)	
c/a = 3.7039	
Volume . 595.90 Å <sup>3</sup>	
Density (calculated) 4.776 g/cm <sup>3</sup>	
Additional patterns 1. PDF card 19-972 [Schwarz, 1966].	
References Møller, C. K., (1954). Acta Chem. Scand. <u>8</u> , 81. Schwarz, H., (1966). Z. Anorg. Allg. Chem. <u>344</u> , 214.	

CuKa	$\lambda = 1.54$	0598 A; temp. 25	±1 °C
Inte	rnal stand	ard Ag, $a = 4.08$	651 Å
d (Å)	I	hkl	20 (°)
7.04	35	003	12.56
4 82	5	101	18 40
4.480	45	012	19 80
3, 613	3	104	24.62
3.212	100	015	27.75
2.854	75	110	31.32
2.645	25	113	33,86
2.579	13	107	34.76
2.456	1	021	36.55
2.408	<1	202	37.32
2.351	4	009	38.26
2.332	3	018	38.58
2.239	6	024	40.25
2,218	7	116	40.65
2.133	30	205	42.35
1,944	30	1•0•10	46.70
1,913	2	027	47.50
1.861	1	211	48,91
1.840	6	122	49.51
1.813	2	119	50.29
1,805	3	208	50.53
1.762	2	0.0.12.214	51.85
1.709	20	125	53.58
1,6470	10	300	55.77
1.6058	10	0.2.10	57.33
1,5886	3	217	58.01
1.5441	<1	1•0•13	59.85
1,5250	1	128	60.68
1,4984	2	1•1•12	61.87
1.4922	<1	306	62.16
1,4436	1	0•1•14	64.50
1,4264	6	220	65.37
1.4090	2	0.0.12	66.28
1.3997	13	2•1•10	66.78
1.3586	2	312,0•2•13	69.08
1.3484	<1	309	69.68
1.3391	<1	1•2•11	70.23
1.3035	6	315	72.45
1.2629	9	1.1.15	75.17
1.2476	<1	137	76.26
1.2260	<1	2.1.13	77.85
1.2165	<1	318	78.57
1.2025	2	404	79.67
1.1855	1	045	81.05
1.1742	3	0.0.18	81.99
1.1495	4	1•3•10	84.15

Sample The sample was prepared from stoichiometric	CuK $\alpha_1 \lambda = 1.540598 \text{ Å}; \text{ temp. } 25\pm1 \text{ °C}$						
amounts of KOH and $MoO_3$ ground together and heated for 15 minutes at 450 °C. The material was	Inte	rnal stand	ard Ag,	a =	= 4.08	8651 Å	
heated at 900 °C for a few minutes then allowed to cool.	d (A)	I		hkl		20(°)	
Color	6.789	5	-1	0	1	13.03	
Vellowish white	5.676	19	1	0	1	15.60	
Terrowish white	5.566	12	2	0	0	15.91	
Structure	5.336	14	1	1	0	16.60	
Monoclinic, $I2/m$ (12), $Z = 4$ , isostructural with $K_2WO_{12}$ . The structure was determined concurrently	4.699	40	0	1	1	18.87	
by Gatehouse and Leverett [1969] and by Koster,	3.828	30	-2	1	1	23.22	
Kools and Rieck [1969].	3.700	18	C	0	2	24.03	
	3.609	14	-3	0	1	24.65	
Lattice constants of this sample:	3.396	70	-2	0	2	26.22	
a = 11.3406(9)  Å b = 6.0814(5)	3.169	100	3	1	0	28.14	
c = 7.5393(7)	3.087	6	Е	0	1	28.90	
$\beta = 101.07(1)^{\circ}$	3.042	55	0	2	0	29.34	
	2.918	65	1	1	2	30.61	
a/b = 1.8648	2.840	6	2	0	2	31.48	
c/b = 1.2397	2.780	ç	4	0	0	32.17	
Volume	2.776	6	-1	2	1	32.22	
510.28 A <sup>3</sup>	2.680	4	1	2	1	33.41	
	2.669	3	2	2	0	33.55	
Density	2.627	3	-3	1	2	34.10	
(calculated) 3.100 g/cm <sup>3</sup>	2.534	1	-4	1	1	35.40	
Reference intensity	2.464	2	-4	0	2	36.44	
$I/I_{correction} = 2.5(1)$	2.349	3	0	2	2	38.28	
Corunaun	2.325	2	-3	2	1	38.70	
Polymorphism	2.316	2	1	0	3	38.85	
Van den Akker et al. [1969] report two other polymorphic phases of $K_2MoO_4$ with transition	2.280	13	0	1	3	39.38	
points above 305° and above 440°.	2.2663	50	-2	2	2	39.74	
	2.2314	4	3	1	2	40.39	
Additional patterns	2.0911	2	5	1	0	43.23	
1. PDF card 24-880 [Kools et al., 1970]	2.0431	12	4	0	2	44.30	
2. Gatehouse and Leverett [1969]	2.0274	4	5	0	1	44.00	
References	1.9932	2	2	1	3	45.47	
Gatehouse, B. M. and Leverett, P. (1969). J.	1.9796	25	-5	1	2	45.80	
Chem. Soc. <u>A</u> , 849.	1.9546	3	0	3	1	46.42	
Kools, F. X. N. M., Koster, A.S., and Rieck, G.D.	1.9365	5	-1	2	-	46.88	
(1970). Acta Crystallogr. <u>B26</u> , 1974. Koster, A.S., Kools, F. X. N. M., and Rieck, G.D.	1.9134	2	=4	2	2	47.48	
(1969). Acta Crystallogr. <u>B25</u> , 1704.	1.0744	•	- 0	-	3	48.02	
Van den Akker, A. W. M., Koster, A. S., and	1.9547	12	-2	3	1	40.08	
Rieck, G. D. (1970). J. Appl. Cryst. <u>3</u> , 389.	1.8427	12	1	2	7	49.00	
	1.8156	4	2	2	1	50.21	
	1.0150	5	2	5	•	20021	
	1.8112	4	-5	2	1	50.34	
	1.7995	14	=1	1	4	50.69	
	1.7789	14	3	3	0	51.32	
	1.7309	11	1	3	2	52.85	
-	1.6961	12	4	2	2	54.02	
	1.6869	3	5	2	1	54.34	
	1.6621	4	2	0	4	55.22	
	1.6574	4	6	1	1	55.39	
	1.62.96	1	4	1	3	56.42	
	1.6071	3	З	2	3	57.28	

I

d (A)	I		hkl		20(°)
1.5901	4	-2	2	4	57.95
1.5834	7	6	2	Ó	58.22
1.5723	4	-5	2	3	58.67
1.5662	Э	0	З	3	58.92
1.5502	2	-6	2	2	59.59
1.5481	2	З	З	2	59.68
1.5434	З	6	0	2	59.88
1.5286	2	-5	1	4	60.52
1 • 52 02	7	0	4	0	60.89
1.4827	6	-4	2	4	62.60
1.4711	2	-7	0	з	63.15
1.4678	2	1	4	1	63.31
1.4591	10	- 2	1	5	63.73
1.4563	11	-5	З	2	63.87
1.3878	5	-2	4	2	67.43
1.3804	6	-8	1	1	67.84

Potassium Molybdenum Oxide,  $K_2^{MOO}_4$  - (continued)

Sample The sample was purified by slowly evaporating a water solution of the salt at room temperature. This material is known as Rochelle salt. The d(A) sample was reagent material from J. T. Baker Ι Chemical Company, Phillipsburg, N.J. Color 7.14 5 Colorless 6.22 13 6.11 16 Structure 5.95 25 Orthorhombic,  $P2_12_12$  (18), Z = 4. The structure 5.70 7 of Rochelle salt was studied by Beevers and Hughes, [1941]. 5.48 95 5.16 4 Lattice constants of this sample: 4.694 8 a = 11.899(3) Å 4.567 25 b = 14.279(3)4.371 17 c = 6.229(2)4.306 40 a/b = 0.83334.120 9 c/b = 0.43623.828 9 3.784 30 Volume 3.687 40 1058.3 A<sup>3</sup> 3.573 7 Density 3.469 7 (calculated) 1.771 g/cm<sup>3</sup> 3.419 З 3.343 9 Additional pattern 3.258 17 1. PDF card 11-851 [Amendola, A., Polytechnic Inst. of Brooklyn, 1959] 3.193 20 3.118 5 Reference 3.102 7 Beevers, C. A. and Hughes, D. J. (1941). Proc. 3.060 12 Roy. Soc. Ser. A, 177, 251. 3.030 55 2.998 16 2.976 12 2.949 18 2.912 35 2.855 10 2.776M 40 2.776M 2.737 100 2.709 30 2.683 40 2.652 14

Potassium Sodium Tartrate Hydrate, C<sub>4</sub>H<sub>4</sub>KNaO<sub>6</sub>·4H<sub>2</sub>O

a(b)	т	hb	,	2 (0)
u (n/	-	••••	C C	2 ( )
2.316M		3 2	2	38.86
2.302	35	1 4	2	39.10
2.297	36	A A	-	36.37
2.207	50		Ň	39.37
2.250	8	5 2	0	39.90
2.222M	19	06	1	40+57
				:
2.222M		5 0	1	40.57
2.196	9	5 1	1	41.07
2.184M	17	1 6	1	41.31
2.184M		2 4	2	41.31
2.171	6	3 5	1	41.57
20171	U	5 5		41404
0.100	•		~	40.40
2.120	2	4 1	2	42.48
2.081	15	26	1	43.44
2.058M	7	4 5	C	43.96
2.058M		4 2	2	43.96
2.040	6	36	C	44.38
2.026	1.6	1 1	٦	44.70
2.020	7			44.07
2.014		5 3	1	44.97
1.994	11	0 2	3	45+46
1.955	ć	4 5	1	46.40
1.940	8	36	1	46.78
1.938	7	0 7	1	46.84
1.915	4	1 7	1	47.45
1.8804	10	6 0	-	48.14
1 88.04	10	5 6		40 14
1.00 9/		5 4	-	40.14
1.875M	17	5 1	2	48.52
1.875M		6 1	1	48.52
1.858M	8	35	2	49.00
1.858M		4 6	0	49.00
1.843M	5	27	1	49.42
1.843M	-	4 4	2	49.42
1 1040			-	43442
1 0004			•	40.00
1.029M	18	5 5	0	49.82
1.829M		5 2	2	49.82
1.825M	20	62	1	49.92
1.825M		3 1	З	49.92
1.812	7	2 3	З	50.32
1.785	7	0 8	С	51.12
1.7814	8	3 3	3	51.24
1 7014	0	2 2	1	51 04
1.781M		4 0	1	51.24
1.757M	4	5 3	2	52.00
1.757M		63	1	52.00

Potassium Sodium Tartrate Hydrate,  $C_4H_4KNaO_6 \cdot 4H_2O$  - (continued)

### Sample

The sample was prepared by heating a 1:1 molar mixture of SrCrO<sub>4</sub> and  $K_2$ CrO<sub>4</sub> at 450 °C for 15 hrs., and at 700 °C for 2 hrs. The product was then reground and reheated to 750 °C for 15 hrs.

#### Color

Vivid green yellow

#### Structure

Hexagonal, R3m (166), Z = 3, isostructural with Sr<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of (NH<sub>4</sub>)<sub>2</sub>Pb(SO<sub>4</sub>)<sub>2</sub> was determined by Møller [1954].

```
Lattice constants of this sample:

a = 5.6782(3) A

c = 21.027(2)
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```
c/a = 3.7031
```

```
Volume
```

```
587.13 A<sup>3</sup>
```

```
Density
```

(calculated) 3.375 g/cm<sup>3</sup>

Reference Intensity I/I = 2.97 (16)

```
Additional Patterns
1. PDF card 19-994 [Schwarz, 1966].
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References

```
Møller, C. K. (1954). Acta Chem. Scand. 8, 6.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. <u>345</u>,
230.
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Internal standard Ag, a = 4.08651 A d (A) 20(°) Ι hkl 6 003 7.02 12.60 19.90 4.458 13 012 3.591 1 104 24.77 3.508 2 006 25.37 3.198 100 015 27.88 2.840 90 110 31.48 113 34.03 2.632 11 2.564 107 34.96 5 2.396 5 202 37.51 2.338 5 009 38.47 2.227 6 024 40.47 2.207 6 116 40.86 42.56 2.122 35 205 1.933 25 1.0.10 46.97 1.830 2 122 49.78 2 119 50.54 1.804 50.78 1.796 2 208 1.753 2 214,0.0.12 52.13 1.7002 20 125 53.88 1.6392 300 56.06 10 7 0•2•10 1.5977 57.65 , 1.5802 217 58.35 1 1.5088 1 2.0.11 61.40 1.1.12 1.4911 1 62.21 1.4848 306 1 62.50 1.4197 11 220 65.72 1.4017 2 0.0.15 66.67 1.3925 13 2•1•10 67.17 1.3524 2 312 69.44 1.3156 1 226 71.68 1.2973 72.85 6 315 1.2568 9 1.1.15 75.60 1.2416 1 76.69 137 1.2133 1 229 78.82 1 80.12 1.1969 404,3.0.12 1.1800 2 045 81.51 1.1443 5 1•3•10 84.62 2.0.17 1.1050 <1 88.39 1.1028 1 324,2•2•12 88.61 1.0896 5 235 89.97 1.0733 3 410,2.1.16 91.73 1.0654 5 3.0.15 92.61 1.0611 2 4.0.10 93.09 1.0340 1 0•4•11 96.31 1.0280 2 0.1.20 97.06 0.9974 3 2•2•15 101.12 .9941 3 3•2•10 101.59 .9666 1 054,2.0.20 105.68 .9576 1 505 107.10 1 330,1•3•16 .9463 108.98 .9381 1 1.0.22,333 110.40 .9150 3 4 • 1 • 12, 1 • 2 • 20+ 114.67

CuK $\alpha_1$   $\lambda$  = 1.540598 A; temp. 25±1 °C

Sample The sample was prepared by treating a slurry of $K_2CO_3$ and $SrCO_3$ in water with a 40% solution of $H_2SeO_4$ , drying, grinding and heating to about 500 °C for 1/2 hour. It was then further heated at about 500 °C for 50 hours.	d (
Color Colorless	4.
Structure Hexagonal, $R\overline{3}m$ (166), Z = 3, isostructural with Sr <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> and many other double sulfates and selenates [Schwarz, 1966]. The structure of (NH <sub>4</sub> ) <sub>2</sub> Pb(SO <sub>4</sub> ) <sub>2</sub> was studied by Møller [1954].	3. 3. 2. 2.
Lattice constants of this sample: a = 5.6846(6) A c = 21.105(3)	2. 2. 2.
c/a = 3.7127 Volume 590.64 Å <sup>3</sup>	2.
Density (calculated) 3.810 g/cm <sup>3</sup>	1.
Additional patterns 1. PDF card 19-995 [Schwarz, 1966].	1.
References Møller, C. K. (1954). Acta Chem. Scand. <u>8</u> , 81. Schwarz, H. (1966). Z. Anorg. Allg. Chem. <u>344</u> , 214.	1.
	1. 1. 1.

Cu	$\kappa \alpha_1 \lambda = 1.540598$	BA; temp.	25±1 °C
In	ternal standard	Si, a = 5	.43088 Å
d (Å)	I	hkl	20(°)
7.036	16	003	12.57
4.795	6	101	18.49
4.465	19	012	19.87
3.599	5	104	24.72
3.516	3	006	25.31
3.203	100	015	27.83
2.842	80	110	31.45
2.636	12	113	33.97
2,572	5	107	34.85
2.398	1	202	37.48
		-	
2.345	1	009	38.36
2.231	2	024	40.39
2.211	1	116	40.77
2.126	30	205	42.48
1.939	20	1.0.10	46.82
1.907	1	027	47.66
1.832	2	122	49.73
1.800	2	208	50.68
1.759	2	0.0.12	51,95
1.756	2	214	52.05
1 702	17	125	53 90
1.703	17	200	53.80
1.040	o 7	300	50.02
1.6023	) / 1	0-2-10	57.47
T.2031	. 1	217	58.25
1.5128	5 I		61.22
1.4956	5 2	1•1•12	62.00
1.4214	8	220	65.63
1.4073	3	0.0.15	66.37
1.3958	3 9	2•1•10	66.99
1.3548	3 1	0•2•13	69.30
1.3180	) <1	226	71, 53
1.2992	6	315	72.73
1 2612	6	1•1•15	75.29
1 2436	, i	137	76.55
1 2001		3•0•12	79.85
1 1914		045	81 37
1 1/65		1.3.10	84.45
T. 1402	. 4	T 2.TO	04.45

Sample The sample was prepared by grinding together stiochiometric amounts of Rb <sub>2</sub> CO <sub>3</sub> , BaCO <sub>3</sub> and MoO <sub>3</sub> and heating to 700 °C for 18 hours. This was followed by regrinding and reheating to 700 °C for several hours.
Color Colorless
Structure Hexagonal, R3m (166), Z = 3. The similarity of the cell size, powder pattern, and chemistry of Rb <sub>2</sub> Ba(MoO <sub>4</sub> ) <sub>2</sub> , Sr <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> , K <sub>2</sub> Pb(SO <sub>4</sub> ) <sub>2</sub> (palmier- ite) and (NH <sub>4</sub> ) <sub>2</sub> Pb(SO <sub>4</sub> ) <sub>2</sub> strongly suggests an isostructural relationship. The structure of (NH <sub>4</sub> ) <sub>2</sub> Pb(SO <sub>4</sub> ) <sub>2</sub> was studied by Møller [1954].
Lattice constants of this sample: a = 6.0851 (4) A c = 22.017 (2) c/a = 3.6182
Volume 706.01 Å <sup>3</sup>
Density (calculated) 4.432 g/cm <sup>3</sup>
References Møller, C. K. (1954). Acta Chem. Scand. <u>8</u> , 81.

CuKa <sub>l</sub>	$\lambda = 1.540598$	8 A; temp. 25	5±1 °C
Interr	al standard	W, a = 3.16	5524 Å
d (Å)	I	hkl	20 (°)
7.35	3	003	12.03
4.751	6	012	18.66
3.378	100	015	26.36
3.043	75	110	29.33
2.812	3	113	31.80
2.702	2	107	33.13
2.564	2	202	34.96
2.447	1	009	36.69
2.441	1	018	36.79
2.377	2	024	37.82
2.343	2	116	38.39
2.260	25	205	39.85
2.0313	19	1.0.10	44.57
1.9602	1	122	46.28
1.8344	3	0.0.12	49.66
1.8152	19	125	50.22
1.7562	9	300	52.03
1.6892	7	0•2•10	54.26
1.6826	4	217	54.49
1.5216	7	220	60.83
1.4768	10	2•1•10	62.88
1.4674	4	0.0.15	63.33
1.3874	5	315	67.45
1.3218	5	1•1•15	71.29
1.2621	2	045	75.23
1.2176	4	1•3•10	78.49
1.1657	3	235	82.72
1.1500	2	410	84.11
1.1305	2	4.0.10	85.90
1.1286	3	327	86.08
1,1263	3	3.0.15	86.30
1.0776	1	0.1.20	91.26
1.0595	2	3•2•10	93.28
1.0564	2	2.2.15	93.63
1.0251	1	505	97.43
1.0158	2	2.0.20	98.63
1.0141	2	330	98.86

Rubidium Chromium Oxide,  $Rb_2Cr_20_7$ 

Sample	CuKa <sub>l</sub>	$\lambda = 1.5405$	98 Å; temp. 25±	1 °C
to a solution of $Rb_2CO_3$ to which a drop of HCl	Inter	nal standar	d W, a = 3.165	24 Å
with ethanol.	d(Å)	I	hkl	20(°)
Color	6.847	3	200	12.92
Vivid vellow	5 404	6	011	16 39
vivia yellow	5.404	5	<u>,</u> ,,	17.20
	5.098	3		17.38
Uptical data	4.954	3	<u>+</u> ++	17.89
Biaxial (+), $N_{\alpha} = 1.688$ , $N_{\gamma} = 1.790$ , 2V is medium.	4.331	1	211	20.49
	4.164	6	211	21.32
Structure	3.917	11	310	22.68
Monoclinic, $P2_1/n(14)$ , $Z = 4$ . The structure was	3.847	20	002	23.10
determined by Löfgren [1971].	3.800	30	020	23.39
	3,666	20	120	24 26
Lattice constants of this cample.	5.000	20	120	24.20
Dattice constants of this sample:	2 550	10		25 00
a = 13./11(2) A	3.559	10	- 311	25.00
b = 7.599(2)	3.432	90	202,012	25.94
c = 7.700(2)	3.419	100	400,311 +	26.04
$\beta = 93.36(2)^{\circ}$	3.371	3	112	26.42
	3.326	30	121,220	26.78
a/b = 1.8043		•••	101,000	20170
c/b = 1.0133	3.271	40	202	27.24
	3,133	25	212	28.47
Volume	3,124	11	410	28 55
	2 002	11	201	20.00
800.85 A	3.083	9	221	28.94
	3.020	18	221	29.55
Density			_	
(calculated) 3.209 g/cm <sup>3</sup>	2.949	4	411	30.28
	2.923	4	320	30.56
	2,840	з	411	31,47
	2.010	2	210	21 77
	2.014	5	512	31.77
	2.763	2	321	32.38
Polymorphism				
The existence of at least four modifications of	2.698	13	321	33.18
Rb <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> was reported by Löfgren and Waltersson,	2.676	12	312	33.46
[1971]. Three forms exist at room temperature	2.633	6	402,122	34.02
and are obtainable from aqueous solution.	2 629	5	501	34 08
trialinia form isostructural with one form of	2.625	2	510	24 80
K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> , a monoclinic form isostructural with a	2.376	2	-	54.60
second form of K2Cr2O7, and a monoclinic form	2.544	18	103,420	35.25
isostructural with $(NH_{\rm h})_2Cr_2O_7$ . The fourth is a	2.484	17	402,511	36.13
quenchable high temperature form of unknown	2,446	2	421	36.72
structuro	2 414	- 7	112	37 22
structure.	2.414	,	113	37.22
	2.407	8	031	37.33
Additional patterns				
1. PDF card 26-1363 [Löfgren, 1971]	2.383	16	421	37.72
	2.377	17	131,230	37.81
References	2.369	15	322,113	37.95
Löfaren P (1971) Acta Chem Scand 25 44	2 328	3	213	38 64
Löfgren, P. and Waltersson, K. (1971). Acta	2.282	5	231,600	39.46
Chem. Scand. <u>25</u> , 35.				
	2.220	3	520	40.60
	2.214	7	330	40.72
	2.196	5	512,313	41.07
	2.164	9	422	41.70
	2,161	15	521	41.77
	51101	20	-	
	2.144	3	331	42.12
	2.134	4	611	42.31
	2,116	5	032,123	42.70
	2 111	3	331	42 80
	2.111	5	100	42.00
	2.083	3	123	43.41

d (Å)	I	hkl	20(°)
2.058	6	223	43.97
2.037	4	430	44.45
2.014	6	602	44.98
2.002	13	232,223	45.27
1.985	3	431	45.66
1.963	4	522,323	46.22
1.957	3	620	46.37
1.948	6	612	46.59
1.929	3	413,503	47.08
1.922	5	701,004	47.25
1.894	6	710	48.00
1.879	4	204	48.41
1.869	5	701,513	48.67
1.864	5	711,014	48.83
1.844	4	<b>4</b> 23,041	49.38
1.830	8	240	49.79
1.824	10	214,531 +	49.97
1.815	6	711	50.24
1.795	2	Ī33	50.82
1.779	5	622	51.32
1.768	8	513,423	51.66
1.738	1	720,712	52.62
1.710	4	613,622	53.56
1.7005	8	532,333 +	53.87
1.6767	5	721,414	54.70
1.6624	3	242,712	55.21
1.6505	3	811	55.64
1.6397	3	631,523	56.04
1.6338	3	324,441	56.26
1.6177	2	613	56.87
1.6118	2	811	57.10
1.6000	1	703	57.56
1,5600	2	820	59.18
1.5472	3	730	59.72

Rubidium Chromium Oxide,  $Rb_2Cr_20_7$  (continued)

Sample The sample was prepared by adding HIO <sub>3</sub> to a solution of PheCO2	CuK $\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C					
301411011 01 102/003.				<u> </u>		
Color	d (A)	I	ł	nkl		20(°)
001011035						
Structure	4.539	17	1	0	1	19.54
Hexagonal, R3m (160), Z=3, distorted perovskite	3.212	100	0	1	2	27.75
structure [Bousquet et al., 1967]. The struc-	3.205	95	1	1	0	27.81
ture of RbIO3 has been determined by Alcock	2.631	2	0	0	З	34.05
[1972].	2.271	35	2	0	2	39.65
Lattice constants of this sample:	2.033	3	1	1	з	44.53
a = 6.413(4) Å	2.029	3	2	1	1	44.63
c = 7.8920(8)	1.860	13	1	0	4	48.93
	1.853M	30	1	2	2	49.14
c/a = 1.2306	1.853M		3	0	0	49 • 14
Volume	1.6079	7	0	2	4	57.25
260 37 Å <sup>3</sup>	1.6035	9	2	2	Ó	57.42
200.3, 11	1.5186	2	0	1	5	60.96
Density	1.5135	2	3	0	3	61.19
(calculated) 4.614 g/cm <sup>3</sup>	1.4372	10	2	1	4	64.82
Reference intensity	1.4346	13	3	1	2	64.95
I/I = 6.6(8)	1.3726	1	2	0	5	68.28
corundum	1.3692	1	2	2	З	68.47
Additional pattern	1.3156	1	0	0	6	71.68
1. PDF card 20-997 [Bousquet et al., 1967]	1.3094	2	0	4	2	72.07
References	1.2615	1	1	2	5	75.27
Alcock, N. W. (1972). Acta Crystallogr. B28.	1.2575	1	З	2	1	75.55
2783.	1.2171	3	1	1	6	78.53
Bousquet, J., Rivière, R., and Remv, J. C.	1.2138	7	1	З	4	78.78
(1967). C. R. Acad. Sci. Ser. C <u>265</u> , 712.	1.2122M	9	2	З	2	78.91
	1.2122M		4	1	0	78.91
	1.1352	2	4	0	4	85.46
	1.1022	1	3	1	5	88.67
	1.1006	1	4	1	3	88.84
	1.0726	2	3	0	6	91.81
	1.0695	4	5	0	2	92.15
	1.0167	2	2	2	6	98.52
	1.0142	2	4	2	2	98.84
	.9671	2	1	5	2	105.59
	.9258	1	6	0	0	112.61

Sample The sample was prepared by heating MoO <sub>3</sub> and com- bining it with PbCO <sub>3</sub> and Rb <sub>2</sub> CO <sub>3</sub> . The mixture	CuK $\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å				
was heated to 700 °C, then ground and heated at 700 PC for 15 hours.	å d (A)	I	hł	cl.	20 (°)
Color					12 24
001011055	7.23	11	2		12.24
Structure	6.67	11	-2	0 1	13.20
Monoglinia C contored (Webband and Coloughi	5.342	1	2	0 1	16.58
Monoclinic, C-centered [Hubbard and Sadowski,	5.090	2	0	0 2	17.41
similar to that of palmierite, K <sub>2</sub> Pb(SO <sub>4</sub> ) <sub>2</sub> .	4•719M	13	1	1 1	18.79
	4.719M		-2	0 2	18.79
Lattice constants of this sample:	3.778+	2	3	1 0	23.53
a = 14.905(5) A	3.778+		-3	1 1	23.53
b = 6.070(3)	3.697	1	-4	0 1	24.05
c = 10.477(3) $\beta = 103.55(3)^{\circ}$	3.607	1	1	12	24.66
	3.346+	100	3	1 1	26.62
a/b = 2.4555	3.346+		-4	0 2	26.62
c/b = 1.7260	3.184	1	4	0 1	28.00
	3.029	85	-1	1 3	29.47
Volume	2.794M	7	-3	1 3	32.01
921.52 A <sup>3</sup>					
	2.794M		1	1 3	32.01
Density	2.671M	2	-5	1 1	33.52
(calculated) 5.031 g/cm <sup>3</sup> , assuming $Z = 4$	2.671M		4	0 2	33.52
the second se	2.617	2	5	1 0	34.24
Reference Hubbard, C. R. and Sadowski, L. (1977). Private	2.606	2	0	22	34.38
communication.	2.414+	1L	6	0 0	37.21
	2.414+		5	1 1	37.21
	2.361	2	-4	0 4	38.09
	2.323	3	3	1 3	38.74
	2.245	30	2	0 4	40.13
	2.100	1	4	2 1	41.02
	2 140	1	5	1 2	42.00
	2 0000	18	-7	1 1	45.10
	2.009M	10	6	0 2	45.10
	1.975	1	-2	2 4	45.91
	1.951 M	2	3	1 4	46.50
	1.951M		0	2 4	46.50
	1.888+	1L	-7	1 3	48.17
	1.888+		5	1 3	48.17
	1.8065M	15	3	3 1	50.48
	1.8065M		-3	3 2	50.48
	1.8021	19	-5	1 5	50.61
	1.7525	7	-7	1 4	52.15
	1.7463	9	-2	0 6	52.35
	1.7153	1	8	0 1	53.37
	1.6724+	7	-5	3 1	54.85
	1.6724+		-8	0 4	54.85
	1.6571	1	5	1 4	55.40
	1.5139	6	-2	2 6	61.17
	1.4645M	10	-8	2 4	63.47
	1.4645M	2	5	1 5	63.47
	1.4492	2	10	0 0	66 20
	1.4088M	1	-10	0 4	66.00
	1.4088M	_	7	1 4	60.29
	1.3798	7	-5	3 5	67.87

Sample	CuKa <sub>1</sub> $\lambda$ = 1.540598 Å; temp. 25±1 °C									
$CrO_3$ were dissolved in water and evaporated	Internal standard Ag, a = 4.08651 Å				651 Å					
for 4 hours, reground and briefly heated to 850 °C where it had melted.	d (Å)	I	]	hkl	20(°)					
Color	7.28	1	0	03	12.14					
Vivid yellow	4.852	2	1	0 1	18.27					
Ctructure	3.676	2	1	0 4	24.19					
Structure Howagonal $P_{2m}$ (166) 7 = 2. It is isostruc-	3.283	100	0	1 5	27.14					
tural with $Sr_3(PO_4)_2$ and many double chromates,	2.674	70	1	1 0	31.09					
sulfates and selenates [Schwarz, 1966]. The	2.473	1L	0	2 1	36.30					
structure of (NH4)2PD(SO4)2 was studied by	2.426M	8	0	09	37.02					
Møller [1954].	2.426M		2	0 2	37.02					
Tattice constants of this couple.	2.395	. 2	0	18	37.53					
a = 5.7455(5)Å	2.263	8	0	2 4	39.80					
c = 21.854(2)	2.255	10	1	16	39.94					
/ 2.0027	2.161	35	2	0 5	41.76					
c/a = 3.8037	2.0007	25	1	0 10	45.29					
11 - 1	1.8547M	1	1	1 9	49.08					
624.75 Å <sup>3</sup>	1.8547M		1	2 2	49.08					
	1.8445	1	0	1 11	49.37					
Density	1.8203	1L	0	0 12	50.07					
(calculated) 3.911 g/cm <sup>3</sup>	1.7279	17	1	2 5	52.95					
	1.6585	10	З	0 0	55.35					
<pre>Reference intensity I/I_corundum = 3.7(3)</pre>	1.6421	6	0	2 10	55.95					
	1.6107	1L	2	1 7	57.14					
Additional pattern	1.5094	2	з	0 6	61.37					
1. PDF card 19-1093 [Schwarz, 1966].	1.4569	2	0	0 15	63.84					
	1.4366	8	2	2 0	64.85					
Møller, C. K. (1954). Acta Chem. Scand. <u>8</u> , 81.	1.4253	11	2	1 10	65.43					
Schwarz, H. (1966). Z. Anorg. Allg. Chem. <u>344</u> ,	1.3160	6	з	1 5	71.65					
41.	1.2996	8	1	1 15	72.70					
	1.1974	З	0	2 16	80.05					
	1.1671	4	1	3 10	82.60					
	1.1052	3	2	1 16	88.37					
	1.0946	2	з	0 15	89.45					
	1.0856	2	4	1 0	90.40					
	1.0666	2	1	3 13	92.47					
			_							
Sample				d (Å)	I		hkl		20(°)	
-----------------------	---------------------	---------------------------	-----------------------	---------	--------------	---	-----	---------	--------	--
Prepared	by dissol	ving $4.5 \text{ g Rb}_2$	SO4 in 10 ml		•• •• •• •••					
water, a	dding 0.5	$g SrCl_2 \cdot 2H_2O$ d	ropwise with		-					
stirring,	and then	stirring for 8	days at room	1 7072	5	2	1	1	50.32	
temperatu	ad there	product was such	tion-illtered	1.7949	1	2	õ	12	50.83	
[Accordin	a to Schwai	$r_z$ 19661	cting paper.	1.7230	1	2	1	4	53.11	
[ACCOLUM	ig to Schwal	[2, 1900].		1.6755	15	1	2	5	54.74	
Color										
Colorless	;			1.6056	10	0	2	10	57.34	
Charles haven				1.69.39	10	3	0	0 -7	57.44	
Structure	D3- (166)			1.5660M	1	2	1	7	58.93	
Hexagonal	, R3m (166)	J, Z = 3, 1SOSTI	ructural with	1.5195	11	2	õ	11	50.93	
and selen	ates [Schwa	arz, 1966].	The structure		•-	-	v	••	00.92	
of $(NH_4)_2$	Pb(SO4) 2 Wa	as studied by Mg	øller [1954].	1.5097	16	1	1	12	61.36	
				1.5075	16	1	2	8	61.46	
Lattice con	stants of t	this sample:		1.4674	1	0	1	14	63.33	
a = 5.55	43(1)A			1.4645	2	3	0	6	63.47	
c = 21.57	2(1)			1.4382	2	0	0	15	64.77	
c/a = 3.8	838			1.3901	15	2	1	10	67.30	
-,				1.3330M	2	1	2	11	70.60	
Volume				1.3330M		З	0	9	70.60	
576.34 A <sup>3</sup>				1.2985	1L	1	0	16	72.77	
				1.2955M	11	2	2	6	72.97	
Density	1) 2 005	, 3		1 20554			-		70.07	
(calculat	ea) 3.895 g	g/cm <sup>o</sup>		1 2900	10	1	3	4	72.97	
Poforonco i	ntongitu			1.2748	10	-	4	10	74.19	
T/T	= 5 1(2)	•		1.2015	1	2	2	q	79.75	
' <sup>'</sup> corund	um = 5.1(2)	,		1.1759M	1	č	2	16	81.85	
Additional	pattern				-	-				
1. PDF c	ard 19-1095	5 [Schwarz, 1966	5].	1.1759M		1	2	14	81.85	
				1.1582	2	0	4	5	83.38	
References				1.1346	4	1	3	10	85.52	
Møller, C	. K. (1954)	. Acta Chem. S	Scand. <u>8</u> , 81.	1.1049	1	1	0	19	88.40	
Schwarz,	н. (1966).	Z. Anorg. Allo	g. Chem. <u>344</u> ,	1.0705	5	3	0	15	92.03	
41.				1.0691	4	2	З	5	92.19	
				1.0525	2	0	1	20	94.09	
CuKal	$\lambda = 1.54059$	98 A; temp. 25±	1 °C	1.0498	4	4	1	0	94.41	
			0	1.0405	1	1	2	17	95.52	
Intern	al standard	d W, $a = 3.165$	24 A	1.0076	1	4	1	6	\$9.72	
0 (7)	T	1- 1- 0	20 (8)							
u (A)	T	nkt	20(*)	.9989	З	2	2	15	100.91	
				.9841	2	2	0	20	103.02	
				•9824	3	3	2	10	103.28	
4.699	4	1 0 1	18.87	.9634	1	1	1	21	106.17	
3.594M	1	0 0 6	24.75	.9512	1	0	5	1	108.52	
3.594M		1 0 4	24.75	0483	1	•	3	16	108.64	
3.212	100	0 1 5	27.75	. 6380	1	5	õ	5	110.25	
2.779	65	1 1 0	32.19	.9277	2	1	2	20	112.27	
2 50 4	••		74 55	.9256	2	3	3	ō	112.65	
2.394	1	1 0 7	34.55							
2.352	<b>4</b> 8	0 1 9	38.24	k						
2.348	ç	202	36.31							
2.197M	20	1 1 6	41.04							
0.000										
2.197M	25	0 2 4	41.04							
1.9682	25	1 0 10	45.01							
1.8965	1	0 2 7	47.93							
1.8145	5	1 1 9	50.24							

Sodium Acetate Hydrate,  $C_2H_3Na0_2 \cdot 3H_2O_2$ 

Sample	CuKa <sub>l</sub> $\lambda$ = 1.540598 A; temp. 25±:				5±1 °C	
Chemical and Dye Corp., New York.	Internal standard Si, a = 5.430				3088 Å	
Color	d (Å)	I		hkl		20(°)
001011005					_	
Optical data	7.72	55	1	1	0	11.45
Biaxial (-), $N_{0} = 1.448$ , $N_{1} = 1.484$ , 2V is very	6.94	е	-1	1	1	12.75
large. " Y	5.73	1	2	0	0	15+45
	5.41	8	1	1	1	16.37
Structure Monoclinic, C2/c (15), Z = 8 [Kálmán, 1965;	5.227	20	C	2	0	16.95
Mannan and Rahaman, 19721.	4.834	2	0	0	2	18.34
	4.653	40	-1	1	2	19.06
Lattice constants of this sample:	3.943	40	-2	2	1	22.53
a = 12.358(3) Å	3.869	5	2	2	0	22.97
b = 10.450(3) c = 10.414(2)	3.708	10	1	1	2	23.98
$\beta = 111, 75(2)^{\circ}$	3.593	16	3	1	0	24.76
$\beta = 111.75(2)$	3.549	20	0	2	2	25.07
a/b = 1.1926	3.470	é	-2	2	2	25.65
a/b = 0.0066	3.317	13	2	2	1	26.86
C/D = 0.9966	3.277	2	-1	1	3	27.19
Volume	3,250	5	-1	7	1	27.34
1249.0 A <sup>3</sup>	3.166	11	- +	~	•	29.16
	3.100	10	1	7	1	20.10
Density	3.052	100	-4	~	•	29.24
(calculated) 1.447 g/cm <sup>3</sup>	2.895	5	-1	E	2	30.86
Ň	2.869	10	4	ο	0	31.15
	2.744M	16	0	2	з	32.61
Additional methown	2.744M		1	1	З	32.61
Additional patterns	2.708	12	2	2	2	33.05
<ol> <li>PDF card 24-1045 [Ranawait et al., 1938]</li> <li>PDF card 28-1030 [Technische Physische District Delta 1026]</li> </ol>	2.659	30	-3	3	1	33.68
Dienst, Delit, Holland, 1976]	2.610	6	0	4	0	34.33
Defense	2.601	6	-2	0	4	34.45
References	2.554	7	-3	З	2	35.11
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K.	2.524	14	Ō	4	1	35.54
(1938). Ind. Eng. Chem. Anal. Ed. <u>10</u> , 457. Kálmán, A. (1965). Acta Crystallogr. <u>19</u> , 853.	2.498	5	3	1	2	35.92
Mannan, K.M. and Rahaman, Md. O. (1972). Acta	2.455	20	- 1	З	3	36.58
Crystallogr. <u>B28</u> , 320.	2.420	11	0	õ	4	37.12
	2.391	20	-5	1	2	37.58
	2.346	7	3	3	1	38.33
	2.319	3	-4	0	4	38.80
	2.262	5	4	2	1	39.82
	2.243	8	5	1	С	40.18
	2.218	6	2	2	3	40.65
	2.204	8	1	3	3	40.92
	2.143	1	4	0	2	42.13
	2.122	10	-4	2	4	42.58
	2.072	e	-2	4	3	43.66
	2.057+	7	-5	1	4	43.98
	2.057+ 2.031	17	1	5 4	0 3	43.98
	2.001	1	-5	з	1	45.28
	1.983	4	4	2	2	45.72
	1.932M	A	4	4	0	47-00
	1.932M	U	-5	3	3	47.00
	1.915	1	-6	2	2	47.44

d (Å)	I	hkl		20(°)
1.887	6	-6 2	1	48.18
1.877M	7	-6 0	4	48.47
1.877M		-4 4	3	46.47
1.871	8	-6 2	3	48.63
1.865	4	1 3	4	48.78
1.850	6	-4 2	5	49.20
1.813	5	0 2	5	50.28
1.808	6	4 4	1	50.42
1.797M	8	-5 3	4	50.78
1.797M		62	C	50.78
1.7785	12	5 3	1	51.33
1.7660	3	-6 2	4	51.72
1.7416	2	0 6	0	52.50
1.7285M	4	4 2	3	52.93
1.7285M		-2 0	6	52.93
1.6652	1L	6 2	1	55.11
1.6378M	3	0 6	2	56.11
1.6378M		-5 3	5	56.11
1.6154	5	-5 1	6	56.96
1.6112	5	0 0	6	57.12
1.5909M	6	-5 5	2	57.92
1.5909M		5 1	3	57.92
1.5829	3	4 0	4	58.24
1.5780+	1	-4 4	5	58.44
1.5780+		3 3	4	58.44

Sodium Acetate Hydrate,  $C_2H_3Na0_2 \cdot 3H_20$  - (continued)

Sodium Aluminum Sulfate Hydrate (Soda alum),  $NaAl(SO_4)_2 \cdot 12H_2O_4$ 

Sample	CuK $\alpha_1$ $\lambda$ = 1.540598 A; temp. 25±1 °C					±l °C
The sample was prepared by slow evaporation of	Internal standard Si a = 5 43099 A					٥
a 1:1 molar aqueous solution of $Na_2SO_4$ and	Inter	nal standar	d Si,	a =	5.43	088 A
$Al_2(SO_4)_3$ at room temperature.	0	_				20 (0)
	d (A)	I		hkl		20(0)
Color		-				
Colorless						
	7.05	7	1	1	1	12.55
Structure	6.100	2	2	0	O	14.51
Cubic, Pa3 (205), $Z = 4$ [Lipson, 1935]. The	5.457	4	2	1	0	16.23
structure was confirmed by Haussuni (1961).	4.985	4	2	1	1	17.78
Lattice constants of this cample.	4.314	100	2	2	o	20.57
$r_{2} = 12.214(1)$		_	~	~		
a = 12.214(1) R	4.000	3	2	2	1	21.84
Volume	3.081	4	5	1	1	24.10
1822 0 <sup>3</sup>	3.520	14	2	2	2	20.24
1022.0 A	3.307	4	3	2	2	20.29
Density	3.203	0	3	2	+	27.01
(calculated) 1.670 g/cm <sup>3</sup>	3.054	5	^	2	•	20.22
(0410414004) 11010 3) 011	2.962	35	4	1	õ	30.15
Reference intensity	2.902	11	7	-	ĩ	31.02
I/I = 2.6(3)	2.733	2	ے م	2	ċ	32.74
-/ corundum	2.666	2	4	2	ĩ	33,59
Additional pattern	2.000	2	•	2	-	55.59
1. PDF card 1-397 [Hanawalt et al., 1938]	2.603	1	з	٦	2	34.43
	2.493	6	4	2	2	36.00
References	2.395	6	4	-	1	37.53
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K.	2.351	ĩ	5	1	i	38.25
(1938). Ind. Eng. Chem. Anal. Ed. 10, 457.	2.268	4	5	ō	2	39.71
Haussühl, S. (1961). Z. Kristallogr. Kristall-			-	•	_	
geometrie Kristallphys. Kristallchem. 116 371.	2.229	2	5	2	1	40.44
Lipson, H. (1935). Proc. Roy. Soc. London,	2.159	2	4	4	ō	41.80
A151, 347.	2.127	5	5	2	2	42.47
	2.095	2	4	з	з	43.15
	2.063	2	5	З	1	43.85
	2.0361	1	6	0	0	44.46
	2.0065	2	6	1	0	45.15
	1.9808	6	6	1	1	45.77
	1.9314	4	6	2	0	47.01
	1.9077	7	6	2	1	47.63
	1.8417	2	6	2	2	49.45
	1.8203	1	6	З	C	50.07
	1.8008	2	6	3	1	50.65
	1.7625	1	4	4	4	51.83
	1.7447	1	6	3	2	52.40
		_	-		-	57.00
	1.7264	1	5	4	<del>د</del> .	53.00
	1.7108	1	<u>'</u>	2	1	55.52
	1.6722	1 7	ć	~	1	55.32
	1.6195	1	7	2	2	56.84
	1.0105	-	'	2	2	50.04
	1.5004	1	7	٦	1	57.94
	1.5641	1	6	5	0	59.01
	1.5512	i	6	5	1	59.55
	1.5150	1	8	1	0	61.12
	1.4705	1	8	2	1	63.18
	1.4400	3	8	2	2	64.68
	1.4299	1	8	З	0	65.19
	1.4197	1	8	З	1	65.72
	1.3655	1	8	4	0	68.68
	1.3170	1L	9	2	1	71.59

Sample	d (A)	I	h	nkl	2⊖(°)
The sample was made by heating a 1:2:2 molar					
mixture of Na <sub>2</sub> CO <sub>2</sub> , CaCO <sub>2</sub> and (NH <sub>1</sub> ) <sub>2</sub> HPO <sub>1</sub> to					
900 °C, grinding and reheating to 650 °C for 18	2.701	55	0	0 2	33,14
hours. This material is also called rhena-	2.660	80	0	3 1	33.66
nite [Ando and Matsuno, 1968].	2.437	2	2	2 1	36.86
	2.423	5	1	1 2	37.08
Color	2.329	10	0	2 2	38.62
Colorless					
	2.272	15	2	з о	39.63
Structure	2.200	35	з	1 0	41.00
Orthorhombic, Pnam (62), $Z = 4$ , isostructural	2.171	8	1	4 0	41.56
with $\beta$ -K <sub>2</sub> SO <sub>4</sub> [Bredig, 1942]. The structure was	2.115	7	2	0 2	42.72
studied by Bredig [1942].	2.062	7	2	1 2	43.88
Lattice constants of this sample:	2.036	11	З	1 1	44.47
a = 6.797(1) A	2.031	13	З	2 0	44.58
b = 9.165(2)	2.015	30	1	4 1	44.95
c = 5.406(1)	1.940	12	1	32	46.79
0 0 7414	1.921	35	2	2 2	47.28
a/b = 0.7416					
c/b = 0.5899	1.900M	10	З	2 1	47.84
	1.900M		2	4 0	47.84
Volume	1.8196	3	3	30	50.09
336.8 A*	1.7695M	6	1	50	51.61
Densites	1.7695M		0	1 3	51.61
(coloriand) 2 117 g/cm <sup>3</sup>					
(calculated) 3.11/ g/cm <sup>2</sup>	1.7395	11	2	32	52.57
Defense intensity	1.7058	9	З	1 2	53.69
reference intensity	1.6996	11	4	0 0	53.90
corundum = I.I(I)	1.6710	2	4	1 0	54.90
Additional matterna	1.6290	1	1	2 3	56.44
Additional patterns					
2 DDE card 3-762 [Predig 1942]	1.6136	3	2	5 0	57.03
2. FDF Card 5-762 [Dredry, 1942].	1.5931M	5	4	2 0	57.83
Polymorphicm	1.5931M		2	0 3	57.83
Above about 650° R-NaCaPO, transforms to an 0	1.5689	6	2	1 3	58.81
form [Bredig 1942: Ando and Matsuno 1968]	1.5526	12	0	33	59.49
TOTM. (Breaty, 1942, Ando and Macsuno, 1900).			_		
References	1.5443	9	3	4 1	59.84
Ando, J. and Matsuno, S. (1968), Bull, Chem.	1.5275M	2	0	6 0	60.57
Soc. Jap. 41. 345.	1.5275M	_	4	2 1	60.57
Bredig, M. A. (1942), J. Phys. Chem. 46, 744.	1.4853	5	4	3 0	62.48
Klement, R. and Dibn, P. (1938). 7. Anorg.	1.4808	6	1	5 2	62.69
Alla, Chem. $240.40$ .			_		<i>( ( ( ( ( ( ( ( ( (</i>
hilly: chair. <u>110</u> , 101	1.4370	6	1	6 1	64.83
	1.4319	9	4	3 1	65.09
$CuK\alpha_1 \lambda = 1.540598 \text{ Å}; \text{ temp. } 25\pm1 \text{ °C}$	1.4210	5	4	1 2	65.65
	1.3930M	I	4	6 0	67.11
Internal standard W. $a = 3.16524$ Å	1.3930M		3	1 3	67+11
	1 39 61	-		<b>4</b> -	<b>() (</b> )
$d(\tilde{A})$ I $hk\ell$ 20(°)	1.3001	5	1	4 3	67.52
	1.3030	5	3	4 2	67.65
	1 3497	(	0	0 4 c 1	69.48
	1 3206	4	2	0 1	09.00
5.460 7 1 1 0 16.22	1.3290	4	0	6 2	/0.81
4.653 5 0 1 1 19.06					
3.837 45 1 1 1 23.16					
3.795 25 1 2 0 23.42					
3.397 7 2 0 0 26.21					
3.189 1L 2 1 0 27.96					
3.109 5 1 2 1 28.69					
2.875 5 2 0 1 31.08					
2.787 12 1 3 0 32.09					
2.745 100 2 1 1 32.60					

Sample The sample was obtained from the City Chemical Corporation, N.Y.
Color Deep orange yellow
Structure Hexagonal, $R\overline{3}m$ (166), Z = 3. The structure was determined by Okaya et al. [1957].
Lattice constants of this sample: a = 7.8105(4)  Å c = 14.885(1)
c/a = 1.9058
Volume . 786.41 A <sup>3</sup>
Density (calculated) 2.559 g/cm <sup>3</sup>
Reference intensity I/I <sub>corundum</sub> = 0.81(6)
Additional pattern 1. PDF card 12-444 [Shrier, priv. comm.]
References Okaya, Y., Pepinsky, R., Takeuchi, Y., Kuroya, H.

Okaya, Y., Pepinsky, R., Takeuchi, Y., Kuroya, H., Shimada, A., Gallitelli, P., Stemple, N., and Beevers, A., (1957). Acta Crystallogr. <u>10</u>, 798.
Shrier, College of Engineering, Rutgers University New Brunswick, N. J. (private communication).

CuKα <sub>1</sub> λ	= 1.540598	8 Å; t	emp	. 25±	1 °C
Internal	standard	W, a	=	3.165	24 Å
d (Å)	I	h	kl		20(°)
6.155	85	1	0	1	14.38
5.004	90	1	1	2	17.71
3.904	60	-	2		22.00
3.261	8	1	6	4	27.33
5.201	U	•	Ŭ		21.00
3.078	100	2	0	2	28.99
2.726	4	ō	1	5	32.83
2.519	15	2	1	1	35.61
2.504	85	0	2	4	35.84
2.481	11	0	Ċ	6	36.17
			_	_	
2.419	95	1	2	2	37.14
2.235	4	2	0	5	40.32
2.1078	90	2	1	4	42.81
1.9522	40	2	2	0	44.00
1.9522	40	۷	2	v	40.40
1.9400	7	1	2	5	46.79
1.8618	4	1	З	1	48.88
1.8179M	12	з	1	2	50.14
1.8179M		2	2	з	50.14
1.8005	25	0	2	7	50.66
		-		_	
1.7945	20	c	1	8	50.84
1.6752	18	1	3	4	54.75
1.6539	14	3	0	0	54.98
1.6349	4	2	1	7	56.22
1:0049	-	2	•	•	50.22
1.6304	4	2	0	8	56.39
1.5432	11	з	2	1	59.89
1.5397	11	4	0	4	60.04
1.5195	3	2	3	2	60.92
1.5039	18	1	2	8	61.62
1 4757	1.6	^	,	~	62.07
1.41.40	14	4	1	2	65.97
1.4068	4	1	3	7	66.40
1.3624	2	ō	2	10	68.86
1.3335	9	3	0	9	70.57
1.3311	9	5	0	2	70.72
1.3237	7	4	0	7	71.17
1.3212	6	3	1	8	71.33
1.3918	12	3	3	0	72.50
1.2004	4	۷	+	10	13.31
1.2711	7	0	5	4	74.60
1.2684	7	4	1	6	74.79
1.2596M	5	4	2	2	75.40
1.2596M		З	З	З	75.40
1.2562	5	2	0	11	75.64
1 0515	_	~			75 09
1.2515	3	0	4	12	76.78
1.2310	2	5	0	5	77-41
1.2088	2	2	4	4	79.17
1.1989	2	1	5	2	79.96
1.1917	4	2	З	8	80.54
1.1821	з	1	1	12	81.33
1.1549	5	5	1	4	83.67

Sample	d (Å)	I	hk	l		2⊖(°)
The sample was a natural mineral from Sweetwater County, Wyoming, (U. S. National Museum #117729)					-	26.74
	2.510	12	3	1	2	32 . 74
Color	2.4/2	20		1	2	36.74
Colorless	2.426	13	-2	Ō	2	37.02
	2.254	30	-6	õ	4	39.96
Structure			Ŭ	•		
Monoclinic, I2/a (15), Z=4 [Brown et al., 1949].	2.185M	2	5	1	2	41.29
A partial structure determination was done by	2.185M		7	1	0	41.29
Candlin [1956].	2.146	5	-7	1	2	42.08
	2.116	2	-6	1	з	42.69
Lattice constants of this sample:	2.057	7	4	0	4	43.99
a = 20.106(4) A						
b = 3.492(1)	2.040M	18	4	1	3	44.36
C = 10.333(2)	2.040M		-8	1	1	44.36
$\beta = 103.05(2)^{-1}$	2.029	30	8	0	2	44.62
-/h - 5 7577	1.995	8	-8	0	4	45.42
a/b = 2.9590	1.964	9	- 5	1	4	46•18
				_	_	
Volume	1.959	10	10	0	0	46.31
706.7 Å <sup>3</sup>	1.885	7	7	1	2	48.23
	1.854M	2	3	1	4	49.11
Density	1.854M	-	-9	1	2	49.11
(calculated) 2.124 g/cm <sup>3</sup>	1.8480	3	9	T	0	49021
	1 9059	-	£	0	4	50 50
Reference intensity	1.7785	10	-2	1	5	51.33
I/I = 0.96(2)	1.7425	16	-10	1	1	52.47
corunaum	1.7197+	4	=2	0	6	53.22
Additional pattern	1.7197+	-	-1	2	1	53.22
1. PDF card 11-643 [Pabst, 1959].			-	_	-	
	1.6883	2	5	1	4	54.29
References	1.6806	4	-6	1	5	54.56
Brown, C.J., Peiser, H. S., and Turner-Jones, A.	1.6618	14	2	1	5	55.23
(1949). Acta Crystallogr. <u>2</u> , 167.	1.6516	5	-6	0	6	55.60
Candlin, R. (1956). Acta Crystallogr. 9, 545.	1.6354	З	9	1	2	56.20
Pabst, A. (1959). Amer. Mineral. <u>44</u> , 274.						
	1.6325M	З	12	0	0	56.31
0	1.6325M		10	1	1	56.31
$CuK\alpha_1 \lambda = 1.540598 \text{ A}; \text{ temp. } 25\pm1 \text{ °C}$	1.5977	8	-5	2	1	57.65
	1.5949M	9	8	1	З	57.76
Internal standard S1, a = 5.43088 A	1.5949M		2	0	e	57.76
a(n) T $b(n)$ $20(2)$		-	0	•		50 17
	1.5846	3	3	0	4	50 - 17
	1.5573M	2	- 1	2	2	59629
•	1.5319M	1	-1	1	6	60.38
9.77 45 2 0 0 9.04	1 53104	1	-1	2	3	60.38
4.892 55 4 0 0 18.12	1.00100		-	-	5	00000
4.113 2 2 0 2 21.59	1.5184M	Я	_ =	1	6	60.97
	1.5184M	Ŭ		2	2	60.97
2 1 1 0 25.91	1.4921	2	-7	2	1	62.16
3,261 6 6 0 0 07 77	1.4344M	2	0	2	4	64.96
3-196 20 -2 1 1 27.89	1.4344M	-	-14	0	2	64.96
3.167 4 4 0 2 28.15						
3.071 80 -6 0 2 20.05	1.4214M	1	12	1	1	65.63
	1.4214M		8	2	0	65.63
	1.3991	9	14	0	0	66.81
2.785 6 1 1 2 32.11						
2.759 14 -3 1 2 32.42						
2.647 100 4 1 1 33.84						
2.608 4 5 1 0 34.36						
2.582 8 -2 0 4 34.72						

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hkl

212

121

221

211

122,102

302

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130,112

312

131

221

213,231

122

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311,032

232

223

412

040

231

400

141

323

421 422

241

204

240

104,142

214

302

042,114

502,423

314

232,512

511,432

404

142

324 150

522

521 433

151

523,424

341,134

504 514,252 20(°)

25.95

26.62

26.88

28.64

29.19

29.81

30.71

30.80

31.41

31.57

33.36

34.71

35.23

36.58

37.82

38.12

38.72

38.87

39.16

40.05

40.17

41.07 41.56

42.00

42.58

43.63

44.18

44.25

45.20

45.31

45.73

46.27

46.54

46.66

47.60

48.21

49.21

49.58 49.93

50.61

50.86 51.37

51.89

53.22

53.37

54.62 54.79

55.77

Sample				å d(Å)	I
The sample	was prepar	ced by melting	a 3:1 molar		
mixture of	Na2SO4 a	and MgSO4 at a	bout 800 °C.	3.431	100
This was	tollowed k	by heating for	15 hrs. at	3.346	8
450 °C, gr	inding and	reheating ag	ain for 15	3.314	3
hrs. at 45	0 °C. As t	chis phase bo	th melts and	3.114	75
dissolves	incongruer	itly, it is d	ifficult to	3.057	50
prepare pu	re and set	veral weak peak	s of impuri-		
ties were	present. 1	The strongest	of these was	2,995	50
at 25.05°	$(2\theta)$ and ha	ad an intensity	of about 9.	2.909	70
				2.901	50
Color				2.846	60
Colorless				2.832	60
Charles have been				0.004	05
Structure				2.684	25
Monoclinic	$P2_1/c(14)$	(1), Z = 2. T	he structure	2.582	40
was determ	ined by Fi	ischer and Hell	ner [1964].	2.545	11
				2.455	25
Lattice cons	tants of th	his sample:		2.377	11
a = 9.781(2)	2) A				
b = 9.196(2)	2)			2.359	12
c = 8.197(	2)			2.324	12
$\beta = 113.61$	(2) °			2.315	14
(1 - 1 - 0.5	2.5			2.299	12
a/b = 1.06	36			2.250	13
c/b = .891	4				
				2.243	14
volume 3				2.196	10
675.5 A°				2.171	18
Desired have				2.149	9
Density	1) 0 607	/ 3		2.122	5
(calculate	a) 2.687 g,	/cm°			-
<b>D C</b>				2.073	6
Reference in	tensity			2.048	4
1/1 corundu	m = 0.64(5)			2.045	3
				2.004	8
Additional p	attern	[No.1		2.000	4
I. PDF Ca	ra 21-1138	[Madsen, 1966]	•	1 000	4
Defenences				1.982	4
Fischer	and H	llnow E (l	064) 7040	1.961	12
rischer,	and ne	TTHET' P. (T	904). Acta	1.950	15
Madson B	M (1966)	DI G Ceol	Surv Prof	1.945	T2
Pap 550	R 125	. 0. 5. 6601.	Surv. Fror.	1.909	0
	<u>, 125.</u>			1 886	14
CuKa	$\lambda = 1.540$	598 A: temp. 25	+1 °C	1.850	12
Curtor	x 1.010.	by the compt by	-1 0	1 837	17
Inter	nal standau	rd Ag, a = 4.08	651 Å	1.825	35
		iu iig) u 1100		1,802	5
d(A)	I	hkl	20(°)	11000	J.
				1.794	6
8,94	9	100	9.89	1.777	8
5.81	20	011	15.25	1,761	9
4,595	12	020	19.30	1.720	11
4.478	5	200	19.81	1.7153	10
4,241	25	211	20.93	111100	
				1.6789	11
4.090	20	102,120	21.71	1,6741	8
4.032	95	210	22.03	1,6470	2
3,917	70	021	22.68	210110	
3.754	15	002	23.68		
3.477	25	012	25.60		

Sample The sample was prepared by heating a stoichio- metric mixture of Sr(OH) <sub>2</sub> and V <sub>2</sub> O <sub>5</sub> at 1100 °C, cooling to 900 °C and holding for 15 hrs. It was then ground and annealed at about 800°C for a few minutes.
Color Colorless
Structure Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with Sr <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> and other similar phosphates, vana- dates and arsenates [Durif, 1959]. The struc- ture of Sr <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> was determined by Zachariasen [1948].
Lattice constants of this sample: a = 5.6197(2) A c = 20.103(2) c/a = 3.5772
Volume 549.81 Å <sup>3</sup>
Density (calculated) 4.464 g/cm <sup>3</sup>
<pre>Additional patterns 1. PDF card 19-1289 [Lubin and Rittershaus,     Gen. Tel. and Electronics, N. Y. (1966)] 2. Durif [1959]</pre>
References Durif, A. (1959). Acta Crystallogr. <u>12</u> , 420. Zachariasen, W. H. (1948). Acta Crystallogr. <u>1</u> , 263.

CuK $\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C								
Interr	Internal standard W, $a = 3.16524 \stackrel{\circ}{A}$							
d (Å)	I	hkl	20(°)					
6.69	1	003	13.22					
4.731	2	101	18.74					
3.494	2	104	25.47					
3.098	100	015	28.79					
2.810	85	110	31.82					
2.591	<1	113	34.59					
2.416	<1	021	37.18					
2.365	7	202	38.02					
2.232	7	009,018	40.37					
2.190	7	024	41.19					
2.153	4	116	41.92					
2.082	40	205	43.43					
1.858	25	1.0.10,027	49.00					
1.8319	<1	211	49.73					
1.7487	3	119,208	52.27					
1.7279	1	214	52.95					
1.6724	25	125	54.85					
1.6222	12	300	56.70					
1.5500	12	0•2•10,217	59.60					
1.4844	1	128	62.52					
1.4602	1	306	63.68					
1.4047	10	220	66.51					
1.3770	1	0.1.14	68.03					
1.3570	12	2.1.10	69.17					
1.3403	T	0•0•15	70.16					
1.3124	1	309	71.88					
1.2797	6	315	74.02					
1.2367	<1	2•0•14	77.05					
1 1 1 9 9 9	6	T.T.T2	79.12					
1.1092	T	229,310	80.74					
1.1826	<1	404	81.29					
1.1645	3	045	82.83					
1.1319	1	1•2•14	85.77					
1.1209	4	1•3•10	86.82					
1.0899	1	324	89.94					
1.0758	2	235	91.45					
1.0620	2	410	92.99					
1.0407	1	4.0.10,327	95.49					
1.0334	3	3.0.12	96.39					
1.0169	<1	1•3•13	98.49					
1.0124	<1	416	99.08					

Sample	CuKo
The sample was precipitated by adding an aqueou solution of lead acetate to a concentrated solu tion of Tl <sub>2</sub> SO <sub>0</sub> .	15 1- Inte
2.4.	d (A)
Color	
Colorless	
Champana .	7.34
Here $P_{2m}$ (166) $7 = 3$ is set tructure with	4.759
$Sr_{2}(PO_{1})_{2}$ and many other double sulfates an	a 4.462
chromates [Schwarz, 1966]. The structure c (NH4) <sub>2</sub> Pb(SO4) <sub>2</sub> was studied by Møller [1954]	of 3.648
	3.271
Lattice constants of this sample:	2.812
$a = 5.626(1) \tilde{A}$	2.647
c = 22.047(3)	2.448
c/a = 3.9188	2.401
	2.378
Volume	2.229
604.36 A <sup>3</sup>	2.131
Donaitu	2.008
(calculated) 6.661 g/cm <sup>3</sup>	1.9264
	1.8533
Reference intensity	1.8480
$1/1_{\rm corundum} = 9.3(4)$	1.7469
Additional nattern	1.6988
1. PDF card 20-1262 [Schwarz, 1966]	1.0340
	1.4984
References	1.4699
Møller, C. K., (1954). Acta Chem. Scand. 8, 81	. 1.4134
Schwarz, H., (1966). Z. Anorg. Allg. Chem. <u>344</u>	1.3540
41.	1.3025
	1.2920
	1,2533

CuKa	$\lambda = 1.54059$	8 A;	te	mp. 2	25±1 °C
Inte	rnal standard	l Si,	a	= 5.4	13088 Å
d (Å)	I		hkl		20(°)
_					
7.34	2	0	0	3	12.05
4.759	20	1	0	1	18.63
4.402	5	0	1	4	19.88
3.649	9		0	~	24.19
3.048	19	1	U	4	24.30
3.271	100	0	1	5	27.24
2.812	50	1	1	0	31.80
2.647	З	1	0	7	33.84
2.448	6	0	0	9	36.68
2.401	3	0	1	8	37.43
		~	•	~	77 00
2.378	4	2	0	2	37.80
2.229	15	0	2	4	40.43
2.131	18	2	0	5	42.38
2.008	17	1	0	10	45.12
1.9264	1	0	2	7	47.14
1.8533	9	0	1	11	49.12
1.8480	7	1	1	9	49.27
1.7469	2	2	1	4	52.33
1.6988	12	1	2	5	53.93
1.6346	7	0	2	10	56.23
1.4984	2	0	1	14	61.87
1.4699	2	õ	ò	15	63.21
1.4134	7	2	1	10	66.05
1.3540	2	3	0	- 9	69.35
1.3025	6	1	1	15	72.51
	·	-	-		
1.2920	1	3	1	5	73.20
1.2533	1	0	1	17	75.85
1.1969	2	1	2	14	80.12
1.1521	3	1	3	10	83.92
1.1288	2	1	0	19	86.06
			-		

```
Sample
  The sample was precipitated by adding a solu-
  tion of Sr(NO_3)_2 to a concentrated solution of
  T1_2SO_4.
Color
  Colorless
Structure
  Hexagonal, R\overline{3}m (166), Z = 3, isostructural with
  Sr_3(PO_4)_2 and many other double chromates and
  sulfates [Schwarz, 1966]. The structure of
  (NH4)2Pb(SO4)2 was studied by Møller [1954].
Lattice constants of this sample:
  a = 5.5811(4) A
  c = 22.198(3)
  c/a = 3.9774
Volume
  598.81 Å<sup>3</sup>
Density
  (calculated) 5.728 g/cm<sup>3</sup>
Additional pattern
  1. PDF card 19-1339 [Schwarz, 1966].
References
  Møller, C. K. (1954). Acta Chem. Scand. 8, 81.
  Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344,
    41.
```

CuK $\alpha_1 \lambda = 1.540598 \text{ Å}; \text{ temp. } 25\pm1 \text{ °C}$						
Int	ternal standar	d W, $a = 3.165$	24 Å			
d (Å)	I	hkl	20 (°)			
7.39	14	003	11.96			
4.724	9	101	18.77			
4.436	20	012	20.00			
3.645	11	104	24.40			
3.270	100	015	27.25			
2.791	45	110	32.04			
2.651	10	107	33.78			
2.610	5	113	34.33			
2.466	5	009	36.40			
2.407	6	018	37.33			
2.361	8	202	38.08			
2.228	8	116	40.45			
2.217	8	024	40.66			
2.123	16	205	42.55			
2.018	19	1.0.10	44.89			
1,922	3	027	47.26			
1.848	7	119	49.26			
1.822	2	208,211	50.03			
1.803	3	122	50.59			
1.736	2	214	52.69			
1.689	10	125	54.27			
1.634	5	0•2•10	56.24			
1.6105	5 5	300,1.0.13	57.15			
1.5826	5 3	217	58.25			
1.5418	3 3	1.1.12	59.95			
1.5259	9 1	128	60.64			
1.5068	3 <1	0.1.14	61.49			
1.4797	7 2	0.0.15	62.74			
1.4768	3 2	306	62.88			
1.4105	5 6	2.1.10	66.20			
1.3953	3 3	220,0•2•13	67.02			
1.3715	5 <1	223	68.34			
1.3489	) 1	309	69.65			
1.3307	7 <1	312	70.74			
1.3075	5 5	1.1.15	72.19			
1.2834	1 3	315	73.77			
1.2346	5 <1	137	77.21			

## Sample

The sample of tin arsenide was prepared from a mixture of tin and arsenic in the atomic ratio of 3:2. The mixture was heated in an evacuated tube at 750°C for 20 minutes, then ground, sealed again in an evacuated tube and annealed at 350°C. It was ground again and annealed at 325°C for 17 hours.

```
Color
```

Metallic gray

## Structure

Hexagonal, R3m (166), Z = 3. The structure was proposed by Hägg and Hybinette [1935] and confirmed by Eckerlin and Kischio [1968] who gave the formula above. There was excellent agreement between a powder pattern calculated from their structure, and the experimental data given here. Earlier, the formula was assumed to be  $Sn_3As_2$ .

Lattice constants of this sample: a = 4.0896(3) Åc = 36.079(3)

$$c/a = 8.822$$

Volume 522.56 Å<sup>3</sup>

```
Density
(calculated) 6.442 g/cm<sup>3</sup>
```

Additional pattern 1. PDF card 3-0664 [Hägg and Hybinette, 1935]

References

```
Eckerlin, P. and Kischio, W. (1968). Z. Anorg.
Allg. Chem. <u>363</u>, 1.
Hägg, G. and Hybinette, A. G. (1935). Phil.
Mag. 20, 913.
```

CuKa <sub>l</sub>	$\lambda = 1.54059$	98 Å;	ten	np. 2	5±1 °C
Intern	nal standard	łw,	a =	= 3.1	6524 Å
a (X)	I		hk		2θ ( <sup>°</sup> )
6.02	1L	0	0	6	14.71
4.006	1L	0	0	9	22.17
3.524	1	1	0	1	25.25
3.477	1	0	1	2	25.60
3.296	1	1	0	4	27.03
3.181	8	0	1	5	28.03
3.006	5	0	0	12	29.70
2.918	100	1	0	7	30.61
2.789	1	0	1	8	32.07
2.526	1L	1	0	10	35.51
2.406M	1	0	1	11	37.35
2.406M		0	0	15	37.35
2.983	25	0	1	14	43.40
2.045	25	1	1	C	44.26
2.005	1L	0	0	18	45.19

d (Å)	I	hkl	20(°)
1.932	1	1 0 16	47.79
1.821M	1	1 1 9	50.05
1.821M	1	0 1 17	50.05
1.7770	11	0 2 4	52.62
1 7170	-	0 0 21	57.29
1.7179	5	0 0 21	53.20
1.6912	4	1 1 12	54.19
1.0744M	12	0 2 7	54.78
1.6744M		1 0 19	54.78
1.6084	1L	0 1 20	57.23
1.5037	11	0 0 24	61.63
1.4599	6	2 0 1 4	63.69
1.4344	1L	0 1 2 3	64.96
1.3923	1L	0 2 16	67.18
1.3601	1L	2 0 17	68.99
1.3365M	1L	1 0 25	70.39
1.3365M		0 0 27	70.39
1.3157M	5	1 2 5	71.67
1.3157M		1 1 21	71.67
1.2958M	5	2 1 7	72.95
1.2958M	•	0 2 1 9	72.95
1 20 24	5	0 1 26	73.17
1.2924	5	1 1 20	70.03
1.2100M	2	1 1 24	79.03
1.2100M		1 0 20	79.03
1.2026	1	0 0 30	79.00
1.1880	4	1 2 14	80.84
1.1808	2	300	81.44
1.1742M	1L	2 0 23	81.99
1.1742M		0 1 29	81.99
1.1512	1L	2 1 16	84.00
1.1326M	1L	309	85.71
1.1326M		1 2 17	85.71
1.1189M	1L	0 2 25	87.01
1.1189M		1 1 27	87.01
1.1058	1L	1 0 31	88.31
1.0990	1L	3 0 12	89.00
1.0932	1	0 0 33	89.60
1.0922	1	2 0 26	89.70
1.0418	1	0 2 28	95.36
1.0366	11	1 1 30	95.99
1.0224	1	2 2 0	97.77
1.0100	11	1 2 27	09.70
1.0102M	IL	2 2 2 3	90.32
1.0182M		2 0 29	90.32
.9897	1	V 1 35	102.22
.9729	1	3 0 21	104.70
. 9078	2	2 2 12	105.48
.9648	2	1 3 7	105.96
• •9640	2	1 1 33	106.08

Aluminum Plutonium, Al<sub>2</sub>Pu

Structure Hexagonal,  $P6_3/mmc(194)$ , Z = 6. The structure was determined by Larson, Cromer and Stambaugh [1957]. Atom positions 12 aluminum 12(k) 6 aluminum 6(h) 4(f)4 plutonium 2(b) 2 plutonium [ibid.] Polymorphism There are altogether 4 polymorphs: a-rhombohedral, β-rhombohedral, the hexagonal form described here, and cubic. The transformations occur at 915+3 °C, 127+3 °C, and 1210+3 °C, respectively [Runnalls and Boucher, 1965]. Lattice constants a = 6.083 Åc = 14.411c/a = 2.3691(published values: a = 6.083 A, c = 14.410 [Runnalls, 1965]) Volume 。 461.8 A<sup>3</sup> Density (calculated) 6.967 g/cm<sup>3</sup> Thermal parameters Isotropic: aluminum B = 0.977; plutonium B = 0.366 [Larson et al., 1957]. Scattering factors Al<sup>0</sup> [International Tables, 1962] Pu<sup>0</sup> [Larson, Cromer and Roof, 1963] Scale factor (integrated intensities)  $\gamma = 0.356 \times 10^{-3}$ Additional pattern 1. PDF card 8-201 [Runnalls, 1956] References International Tables for X-ray Crystallography, (The Kynoch Press, Birmingham, III (1962). Eng.) p. 202. Larson, A. C., Cromer, D. T. and Stambaugh, C. K. (1957). Acta Crystallogr. <u>10</u>, 443. Larson, A. C., Cromer, D. T. and Roof, R. B., Jr. (1963). Acta Crystallogr. 16, 835. Runnalls, O.J.C. (1956). Can. J. Chem. 34, 133. Runnalls, O.J.C. and Boucher, R. R. (1965). J. Nucl. Mater. 15, 57.

	Calculated	Pattern	(Pea	ak he	eights)
d (Å)	I		hkl		$2\Theta(^{\circ}) \circ \\ \lambda = 1.540598A$
A 046				1	17.02
4.940	100	1	õ	2	20.88
3.548	100 x 100	1	ñ	4	25.08
3.042		1	1	0	29.34
2.072	. 50	1	-	~	30.04
2.972	. 50	•	5	*	30:04
2.590	25	2	0	1	34.60
2.528	3 5	1	0	5	35.48
2.474	55	2	0	2	36.28
2.401	. 35	0	0	6	37.42
2.310	65	2	0	З	38.96
2.126		2	•	•	42.49
1 070	40	2	1	7	42.40
1.044	- 10	2		-	45.50
1 010	5	2	1	3.	40.00
1.005	25	2	1	6	47.04
1.885	40	1	1	0	40.24
1.839	20	2	1	з	49.52
1.756	15	3	0	0	52.04
1.743	3 20	2	1	4	52.46
1 • 7 0 4	5	1	0	8	53.74
1.638	3 1	2	1	5	56.10
1.622	2 5	2	0	7	56.70
1.550	1	1	1	8	59.60
1.532	2 5	1	0	9	60.38
1.521	20	2	2	0	60.86
1.487	10	2	0	8	62.40
1.454	5	З	1	1	64.00
1.432	2 10	3	1	2+	65.10
1.417	15	3	0	6	65.84
1.398	3 10	3	1	З	66.88
1.390	5	1	0	10	67.30
1.368	3 10	2	0	9	68.52
1.354	5	3	1	4	69.34
1.336	5 5	2	1	8	70.44
1.311	1	4	0	1	71.94
1.303	3 1	З	1	5+	72.50
1.296	5 5	4	0	2	72.96
1.285	5 20	2	2	6	73.68
1.270	) 5	4	0	з	74.68
1.264	5	2	0	10	75.08
1.248	5 5	2	1	9	76.24
1.237	5	۵	0	4	77.04
1.204	. 1	3	2	1	79.52
1.201	5	0	0	12	79.80
1.198	1	4	0	5	80.04
1.192	2 5	3	2	2+	80.54
		_	-	_	00.10
1.172	5	3	2	3	82.18
1.167	5	2	1	10	82.58

Γ		Calculated	Pattern	(Int	egr	ated)
F		_				
	a (A)	I		hkl		$2\Theta$ (°) $\lambda = 1.540598A$
	4.948	50	1	0	1	17.91
	3.550	100	1	0	4	20.07
	3.042	95	1	1	õ	29.34
	2.974	55	1	0	4	30.02
1	2.591	30	2	0	1	34. 59
	2.529	5	1	õ	5	35.47
	2.474	65	2	ō	2	36.28
	2.402	40	0	0	6	37.41
	2.324	1	1	1	4	38 • 71
	2.310	75	2	0	з	38.97
	2.126	45	2	0	4	42.48
	1.972	15	2	1	1	45.98
	1.944	5	2	0	5	46.68
	1.919	20	2	1	2	47.33
	1.917	10	1	0	7	47.37
	1.885	45	1	1	6	48.24
	1.839	25	2	1	3	49.52
	1.756	20	3	0	0	52.04
	1.743	20	2	1	4	52.47
	1.704	5	1	0	8	53.73
	1.638	5	2	1	5	56.10
	1.622	: 10	2	0	7	56.70
	1.550	1	1	1	8	59.60
	1.532	5	1	0	9	60.37
	1.521	25	2	2	0	60.87
	1.487	10	2	0	8	62.40
	1.454	5	3	1	1	64.00
	1.432	10	3	1	2	65.12
	1 44 31	10	2	-	1	05+12
	1.418	15	3	0	6	65.83
	1.398	10	3	1	3	66.88
	1.368	10	2	0	10	68.52
	1.354	10	3	1	4	69.35
	1 776	-			~	70.47
	1.330	5	2	1	1	70+43
	1.296	5	4	0	2	72.96
	1.285	30	2	2	6	73.67
	1.270	10	4	0	З	74.67
	1.264	10	2	0	10	75-08
	1.248	5	2	ĩ	9	76.24
	1.237	5	4	0	4	77.03
	1.204	1	3	2	1	79.52
	1.201	5	0	0	12	79.80
	1.198	1	4	0	5	80.04
	1.192	5	3	2	2	80.52
	1.192	5	3	1	7	80.55
	1.172	5	3	2	3	82.18
	1.167	5	2	1	10	82.57

Aluminum Plutonium, Al<sub>3</sub>Pu - (continued)

```
Calculated Pattern (Peak heights)
Structure
 Cubic, Pm3m (221), Z = 1, isostructural with CsCl
 and AlRu [Obrowski, 1960].
                                                           d (A)
                                                                         Ι
                                                                                     hkl
                                                                                                  20(°)
                                                                                             \lambda = 1.540598A
Atom positions
 1(a)
         l aluminum
 1(b)
          l rhenium
                                                           2.88
                                                                        80
                                                                                  1
                                                                                      0
                                                                                          0
                                                                                                 31.04
                                                           2.04
                                                                       100
                                                                                  1
                                                                                      1
                                                                                          0
                                                                                                 44.46
Lattice constant
                                                           1.66
                                                                        20
                                                                                  1
                                                                                     1
                                                                                         1
                                                                                                 55.20
 a = 2.88 A [ibid.]
                                                           1.44
                                                                        15
                                                                                  2
                                                                                      0
                                                                                          0
                                                                                                 64.68
                                                           1.29
                                                                        25
                                                                                  2
                                                                                     1
                                                                                          0
                                                                                                 73.46
Volume
 23.89 A<sup>3</sup>
                                                           1.18
                                                                        25
                                                                                  2
                                                                                     1
                                                                                                 81.86
                                                                                          1
                                                           1.02
                                                                        10
                                                                                  2
                                                                                      2 0
                                                                                                 98.32
Density
                                                                                  2
                                                            .960
                                                                        15
                                                                                      2 1+
                                                                                                106.72
  (calculated) 14.82 g/cm<sup>3</sup>
                                                            •911
                                                                        15
                                                                                  3
                                                                                     1 0
                                                                                                115.52
                                                                                                125.02
                                                            .868
                                                                        10
                                                                                  З
                                                                                      1
                                                                                          1
Thermal parameters
 Isotropic: aluminum B = 1.0, rhenium B = 0.5
                                                                         5
                                                                                  2 2 2
                                                                                                135.80
                                                            .831
                                                            .799
                                                                         10
                                                                                  3 2 0
                                                                                                149.32
Scattering factors
 Al<sup>0</sup> [Cromer and Mann, 1968]
 Re<sup>0</sup> [International Tables, 1974]
Scale factor (integrated intensities)
 \gamma = 2.186 \times 10^{-3}
References
 Cromer, D. T. and Mann, J. B. (1968).
                                                Acta
   Crystallogr. <u>A24</u>, 321.
```

International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.

Obrowski, W. (1960). Naturwissenschaften, 47, 14.

	Calculated	Pattern	(Integrated)					
d (Å)	I		hkl		20(°) $\lambda = 1.540598Å$			
2.88 2.04 1.66 1.44 1.29 1.18 1.02 .960 .960	75 100 20 15 25 30 10 5 15	1 1 2 2 2 3 2 2	0 1 1 0 1 1 2 0 2	0 0 1 0 0 1 0 0 1	31.03 44.45 55.20 64.68 73.46 81.86 98.31 106.72 106.72			
•868 •831 •799	15 10 25	3 3 2 3	1 2 2	1 2 0	115.52 125.02 135.80 149.31			

Aluminum Rhenium,  $Al_{12}Re$ 

Structure $(204)$ $7 = 2$ is structure with $1 = 1$	Calculated Pattern (Peak heights)					
The structure was determined by Walford [1964].	d (Å)	I	ł	nkl	λ	20(°) ° = 1.540598A
Atom positions						
24(g) 24 aluminum						
2(a) 2 rhenium [ibid.]	5.32	100	1	1	0	16.66
	3.764	13	2	0	0	23.62
Lattice constant.	3.072	44	2	1	1	29.04
a = 7.5275(5) A	2.6605	4	2	2	0	33.66
(published value 7.5270(5) A [ibid.])	2.3805	47	3	1	0	37.76
Volume	2.1732	21	2	2	2	41.52
426.53 A <sup>3</sup>	2.0120	47	З	2	1+	45.02
	1.8821	7	4	0	0	48.32
Density	1.7743	9	4	1	1+	51.46
(calculated) 3.971 g/cm <sup>3</sup> (measured) 3.90 g/cm <sup>3</sup> [Walford, 1964]	1.6829	3	4	2	0+	54.48
	1.6051	2	3	з	2	57.36
Thermal parameters	1.5364	8	4	2	2	60.18
Isotropic: aluminum $B = 1.0$ ; rhenium $B = 0.5$	1.4764	15	4	з	1+	62.90
	1.3743	5	1	2	5+	68.18
Scattering factors	1.3307	2	4	4	ō	70.74
Al <sup>0</sup> , Re <sup>0</sup> [Forsyth and Wells, 1959]		-			-	
-, -, -,,,,	1.2911	9	0	з	5	73.26
Scale factors (integrated intensities)	1.2545	5	6	0	0+	75.76
$y = 1.375 \times 10^{-3}$	1.2211	13	5	3	2+	78.22
I/I (calculated) 8.28	1.1902	1	0	2	6+	80.66
-/ Corundum	1.1616	3	5	4	1+	83.08
Additional pattern						
1. PDF card 18-55 [d'Alte da Veiga, Cavendish	1.1348	1	6	2	2	85.50
Lab., Cambridge, Eng. ]. It gives a space	1.1099	5	6	З	1+	87.90
group Im3m which is apparently an error and	1.0646	8	5	4	3+	92.70
incompatible with intensities calculated in	1.0440	2	0	4	6+	95.10
Im3.	1.0244	4	7	2	1+	97.52
References	1.0058	2	6	4	2+	99.96
Forsyth, J.B. and Wells, M. (1959). Acta Crystal-	.9884	1	0	З	7+	102.40
logr. 12, 412.	.9560	3	7	З	2+	107.36
Walford, L. K. (1964). Acta Crystallogr. 17, 57.	.9265	4	1	4	7+	112.48
	.9128	2	6	4	4+	115.10
	.8997	5	з	5	6+	117.78
	•8871	5	8	2	2+	120.52
	.8750	6	1	З	8+	123.36
	.8523	3	2	5	7+	129.32
	.8313	1	9	1	0+	135.84
	.8213	з	2	4	8+	139.40
	.8117	5	1	6	7+	143.24
	•8024	1	6	6	4	147.46

Aluminum	Rhenium,	A1,_Re	<u>-</u> =	(continued)
----------	----------	--------	------------	-------------

Cal	culated Pa	ttern	(Inte	egr	ated)
d(Å)	I	1	hkl		20 (°)
					$\lambda = 1.540598A$
5.32	100	1	1	0	16.64
3.764	14	2	0	0	23.62
3.073	50	2	1	1	29.03
2.6614	5	2	2	0	33.65
2.3804	52	3	1	0	37.76
2.3804	З	0	1	З	37.76
2.1730	26	2	2	2	41.52
2.0118	51	3	2	1	45.03
2.0118	8	1	2	3	45.03
1.8819	9	4	0	0	48.32
1.7742	2	з	з	0	51.46
1.7742	10	4	1	1	51.46
1.6832	2	4	2	0	54.47
1.6832	1	0	2	4	54.47
1.6049	3	3	3	2	57.37
1.5365	10	4	2	2	60.17
1.4763	9	4	з	1	62.90
1.4763	1	5	1	0	62.90
1.4763	4	0	1	5	62.90
1.4763	7	1	3	4	62.90
1.3743	1	5	2	1	68.18
1.3743	5.	1	2	5	68.18
1.3307	2	4	4	0	70.74
1.2910	1	4	З	З	73.27
1.2910	11	0	3	5	73.27
1.2546	4	6	0	0	75.76
1.2546	З	4	4	2	75.76
1.2211	14	5	З	2	78.22
1.2211	З	6	1	1	78.22
1.2211	2	2	3	5	78.22
1.1902	1	0	2	6	80.66
1.1615	2	5	4	1	83.09
1.1615	2	1	4	5	83.09
1.1348	2	6	2	2	85.50
1.1099	6	6	3	1	87.90
1.1099	1	1	з	6	87.90
1.0865	1	4	4	4	90.30
1.0645	5	5	4	3	92.70
1.0645	2	7	1	0	92.70
1.0645	4	3	4	5	92.70
1.0439	2	0	4	6	95.11
1.0439	2	6	4	0	95.11
1.0244	1	6	З	З	97.52
1.0244	1	1	2	7	97.52
1.0244	4	7	2	1	97.52
1.0059	1	6	4	2	99.95
1.0059	1	2	4	6	99.95
.9884	1	0	3	7	102.40
.9560	1	6	5	1	107.37
•9560	2	1	5	6	107.37

d (Å)	I		hk	2	$20(°)$ $\lambda = 1.540598A$
.9560	2	7	з	2	107.37
.9266	1	5	5	4	112.47
.9266	2	8	1	1	112.47
.9266	2	7	4	1	112.47
.9266	2	1	4	7	112.47
.9128	2	6	4	4	115.10
.8997	1	6	5	З	117.78
.8997	7	З	5	6	117.78
.8871	3	6	6	0	120.53
.8871	6	8	2	2	120.53
.8751	з	7	5	0	123.35
•8751	5	1	З	8	123.35
.8751	1	8	З	1	123.35
•8751	1	7	4	З	123.35
•8751	1	3	4	7	123.35
.8635	1	6	6	2	126.28
.8523	5	2	5	7	129.32
•8523	1	7	5	2	129.32
.8313	2	9	1	0	135.84
.8313	1	8	3	3	135.84
.8213	4	8	4	2	139.40
.8213	4	2	4	8	139.40
•8117	2	1	2	9	143.24
•8117	2	7	6	1	143.24
•8117	1	6	5	5	143.24
.8117	4	9	2	1	143.24
.8117	5	1	6	7	143.24
.8024	4	6	6	4	147.46

Aluminum Rhodium, AlRh

Structure	Calcu
Cubic, Pm3m (221), $Z = 1$ , isostructural with CsCl. This composition is the rhodium-rich end member. At the other end of the range, the aluminum-rich phase has the composition $Al_{1,146}$ Rh <sub>.854</sub> and a lattice constant a = 2.968 [Ferro et	d (A)
al., 1964].	2.98
	2.107
Atom positions	1.490
l(b) l rhodium	1.333
Lattice constant	1.217
a = 2.980 A	1.054
Volume	.993
26.46 Å <sup>3</sup>	.898
Density	.860
(calculated) 8.149 g/cm <sup>3</sup>	.826
Thermal parameters Isotropic: aluminum B = 1.0; rhodium B = 0.5	•796
Scattering factors	Calc
Al <sup>0</sup> [Cromer and Mann, 1968] Rh <sup>0</sup> [International Tables, 1974]	d (Å)
Scale factor (integrated intensities) $\gamma = 1.344 \times 10^{-3}$	
	2.98
References	2.107
Cromer, D. T. and Mann, J. B. (1968). Acta	1.490
Ferro, R., Rambaldi, G., and Capelli, R. (1964).	1.333
Natur, Rend. 36, 491.	1.217
International Tables for X-ray Crystallography,	1.054
IV (1974). (The Kynoch Press, Birmingham, Eng.)	•993
p. 100.	•993
	•942

	Calculated	Pattern	(Pea	k hei	ghts)
å(Å)	I		hkl	λ	20(°) = 1.540598
2.98	55	1	0	0	29.96
2.10	7 100	1	1	0	42.88
1.72	0 10	1	1	1	53.20
1.49	0 15	2	0	0	62.26
1.33	3 15	2	1	0	70.62
1.21	7 25	2	1	1	78.56
1.05	4 10	2	2	0	93.96
.99	3 5	2	2	1+	101.70
.942	2 10	3	1	0	109.66
•89	8 5	3	1	1	118.04
.86	0 5	2	2	2	127.12
.82	6 5	3	2	0	137.50
	6 20	2	2	1	150.56

	Calculated	Pattern	(In	tegr	ated)
d(A)	I		hkl		20(°) $\lambda = 1.540598A$
2.98	50	1	0	0	29.96
2.107	100	1	1	0	42.88
1.721	10	1	1	1	53.19
1.490	15	2	0	0	62.26
1.333	15	2	1	0	70.62
1.217	30	2	1	1	78.57
1.054	10	2	2	0	93.96
.993	1	3	0	0	101.70
.993	5	2	2	1	101.70
.942	15	3	1	0	109.65
•899	5	3	1	1	118.03
•860	5	2	2	2	127.13
•827	10	3	2	0	137.50
•796	55	3	2	1	150.56

```
Structure
  Cubic, Pm3m (221), Z = 1, isostructural with
  CsCl [Edshammar, 1966].
Atom positions
         l aluminum
  1(a)
  1(b)
               1 ruthenium
Lattice constant
  a = 2.95 Å [ibid.]
Volume
25.67 Å<sup>3</sup>
Density
  (calculated) 8.28 g/cm<sup>3</sup>
Thermal parameters
  Isotropic: aluminum B = 1.0; ruthenium B = 0.5.
Scattering factors
  Al<sup>0</sup> [Cromer and Mann, 1968]
  Ru<sup>0</sup> [International Tables, 1974]
Scale factor (integrated intensities)
  \gamma = 1.377 \times 10^{-3}
References
  Cromer, D. T. and Mann, J. B. (1968). Acta
    Crystallogr. A24, 321.
  Edshammar, L.-E. (1966). Acta Chem. Scand. 20,
    427.
  International Tables for X-ray Crystallography,
IV (1974). (The Kynoch Press, Birmingham,
    Eng.) p. 100.
```

-	Calculated	Pattern	(Pea	ak he	eights)
å (Å)	I		hkl		$2\Theta(^{\circ})$ ° $\lambda = 1.540598A$
2.95 2.09 1.70 1.48 1.32 1.20 1.04	55 100 10 15 10 25 10 3 5	1 1 2 2 2 2 2 2	0 1 1 0 1 1 2 2	0 0 1 0 0 1 0	30.28 43.34 53.78 62.96 71.44 79.52 95.22 103.14
•933 •933 •889 •852 •818 •788	3     10       3     5       2     5       3     5       3     25	3 3 2 3 3	1 1 2 2 2	0 1 2 0 1	111.32 120.00 129.52 140.60 155.38

	Calculated	Pattern	(Int	cegr	ated)
d(Å)	I		hkl		$2\Theta(°)$ $\lambda = 1.540598 Å$
2.95 2.09 1.70 1.47 1.32	50 100 10 15 15	1 1 1 2 2	0 1 1 0 1	0 0 1 0 0	30.27 43.34 53.78 62.96 71.45
1.20 1.04 .983 .983 .933	30 10 3 1 5 5 3 15	2 2 3 2 3	1 2 0 2 1	1 0 0 1 0	79.53 95.22 103.14 103.14 111.32
•889 •852 •818 •788	5 5 3 10 3 65	3 2 3 3	1 2 2 2	1 2 0 1	120.00 129.52 140.60 155.38

Structure	Ca	alculated 1	Pattern	(Pea	ık he	eights)
with $Al_6Mn$ . The structure was determined by Edshammer [1968].	d (Å)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
Atom positions						
4(c) 4 ruthenium	4.9295	100	1	1	0	17.98
8(e) 8 aluminum(1)	4.4803	42	0	0	2	19.80
8(f) 8 aluminum(2)	4.3206	16	1	1	1	20.54
8(g) 8 aluminum(3) [ibid.]	3.7418	26	2	0	0	23.76
	3.3166	66	1	1	2	26.86
Lattice constants	7.3797	22	•	2	•	27 10
a = 7.4886(4) A	3.0796	22		2	1	27.18
D = 0.5503(3)	2.8734	24	2	2	2	31.10
C = 0.9010(3)	2.5546	5	1	1	3	35.10
(published values: $a = 7.4882(4)$ b = 6.5559(3)	2.4663	12	2	2	õ	36.40
c = 8.9605(5) [Edshammar, 1968]).	0.7700		-		•	30.56
0	2.3329	2	3	1		38.50
CD cell: a=7.4886(4)A, b=8.9610(5), c=6.5563(3),	2.2570	27	3	1	-	39.90
sp. gp. $Bmmb(63)$ ; $a/b = 0.835/$ ; $c/b = 0.7316$	2.2078	22		2	-	40.22
11 June	2.1603	63	2	2	2	41.78
439.96 Å <sup>3</sup>	201000	00	5	-	-	41010
	2.0980	30	1	3	0	43.08
Density	2.0688	66	3	1	2	43.72
(calculated) 3.970 g/cm <sup>3</sup>	2.0396	55	1	1	4+	44.38
	1.9013	13	2	2	3+	47.80
Thermal parameters Isotropic [Edshammar, 1968]	1.0/13	'	4	0	0	48.00
	1.8497	9	0	2	4	49.22
Scattering factors	1.8385	2	3	1	3	49.54
Al <sup>0</sup> , Ru <sup>0</sup> [Cromer and Mann, 1968]	1.7276	5	4	0	2	52.96
	1.7168	4	1	3	3	53.32
Scale factors (integrated intensities) $\gamma = 0.343 \times 10^{-3}$	1.6582	9	2	2	4	55.30
I/I (calculated) 2.15	1.6440	1	3	3	0	55.88
corunaum	1.6392	2	0	4	0	56.06
References	1.6259	3	4	2	0	56.56
Cromer, D. T. and Mann, J. B. (1968). Acta	1.6159	8	3	1	4+	56.94
Crystallogr. A24, 321. Edshammar, LE. (1968). Acta Chem. Scand. 22,	1.5726	2	0	2	5	58.00
2374.	1.5434	5	З	3	2	59.88
	1.5309	6	1	3	4	60.42
	1.5281	11	4	2	2	60.54
	1.4934	3	0	0	6	62.10
	1.4810	9	2	4	1	62.68
	1.4601	3	5	1	0	63.68
	1.4364	1	4	0	4+	64.86
	1.4278	5	4	2	3+	65.30
	1.4239	7	2	4	2	65.50
	1.4212	5	3	1	5	65.64
	1.3872	5	2	0	6+	67.46
	1.3627	3	1	3	5	68.84
	1.3416	4	2	4	3	70.08
	1.3229	5	0	4	4	71.22
	1.3159	4	4	2	4	71.66
	1.3124	3	5	1	З	71.88
	1.2776	8	2	2	6+	74.16
	1.2579	6	3	1	6	75.52
	1.2481	4	6	0	0+	76.22
	1.2355	5	5	3	0	77.14

Aluminum Ruthenium,  $Al_6Ru$  - (continued)

d (Å)	I	]	hkl	λ	20(°) = 1.540598Å
1.2232	9	5	1	4+	78.06
1.2216	6	4	4	1	78.18
1.2167	4	1	З	6	78.56
1.2039	1	4	2	5	79.56
1.2024	1	6	0	2	79.68

	Calculated	Pattern	(Int	egr	ated)
d (Å)	I		hkl		$20(^{\circ})$ $\lambda = 1.540598A$
4.932	9 100	1	1	0	17.97
4.480	5 43	0	0	2	19.80
4.321	4 16	1	1	1	20.54
3.744	3 28	2	0	0	23.74
3.316	6 72	1	1	2	26.86
3.278	1 21	o	2	0	. 27.18
3.078	6 9	0	2	1	28.98
2.873	1 27	2	0	2	31.10
2.555	1 6	1	1	3	35.09
2.466	4 14	2	2	0	36.40
2.332	8 2	3	1	0	38.56
2.257	6 32	3	1	1	3990
2.240	2 24	0	0	4	40.22
2.207	9 24	0	2	3	40.84
2.160	7 76	2	2	2	41.77
2.097	9 36	1	З	0	43.08
2.069	2 80	З	1	2	43.71
2.042	7 23	1	З	1	44.31
2.039	8 51	1	1	4	44.38
1.901	9 11	2	2	З	47.79
1.900	0 7	1	З	2	47.84
1.872	1 9	4	0	0	48.59
1.849	6 11	0	2	4	49.22
1.838	6 2	3	1	3	49.54
1.727	4 6	4	0	2	52.97
1.716	8 5	1	з	З	53.32
1.658	3 11	2	2	4	55.36
1.644	3 1	3	3	0	55.87
1.639	1 2	0	4	0	56.06
1.625	7 3	4	2	0	56.57
1.617	3 3	3	3	1	56.89
1.615	8 9	3	1	4	56.94
1.612	3 1	0	4	1	57.08
1.572	5 3	0	2	5	58.66
1.0743	0 0	3	3	2	24.91
1.539	3 1	0	4	2	60.06
1.531	36	1	З	4	60.40
1.528	2 11	4	2	2	60.54
1.493	5 4	0	0	6	62.10
1.480	9 12	2	4	1	62.69

d (Å)	I		hkl		20(°) $\lambda = 1.540598A$
1.4601	۵	5		0	63.69
1.4499	1	2	2	5	64.19
1.4366	1	Ā	0	4	64.85
1.4294	2	1	1	6	65.22
1.4279	5	4	2	З	65.29
1.4237	6	2	4	2	65.51
1.4212	3	3	1	5	65.64
1.3883	2	5	1	2	67.40
1.3872	6	2	0	6	67.46
1.3627	4	1	3	5	68.84
1.3416	5	2	4	з	70.09
1.3228	7	0	4	4	71.23
1.3158	5	4	2	4	71.67
1.3118	1	5	1	З	71.92
1.2784	2	1	5	1	74.11
1.2775	G	2	2	6	74.16
1.2578	8	3	1	6	75.53
1.2481	5	6	ō	õ	76.22
1.2473	1	2	4	4	76.28
1.2354	7	5	3	0	77.14
1.2239	۵	5	з	1	78.01
1.2232	ġ	5	1	Ā	78.06
1.2217	4	4	Ā	1	78.18
1.2167	4	1	3	6	78.56
1.2041	1	4	2	5	79.54
1.2023	1	6	0	2	79.68

Structure	Ca
Orthorhombic, Pnma(62), $Z = 4$ , isostructural with Ni <sub>2</sub> Si and AlHo <sub>2</sub> , from powder data, [Buschow and van der Goot, 1971].	d (Å)
Atom positions From geometric considerations, the atomic positions used were those for AlHo <sub>2</sub> . All atoms were located in positions 4(c).	5.474 4.813 4.567 3.901
Lattice constants a = 6.654  Å	3.767
b = 5.193	3.119
c = 9.632 °	2.892
(published value for c was 9.631 A [Buschow	2.801
and van der Goot, 1971])	2.731
	2.090
CD cell: $a = 6.654 \text{ A}, b = 9.632, c = 5.193,$	2.596
sp. gp. $Pnam(62)$ ; $a/b = 0.6908$ ; $c/b = 0.5391$	2.527
Volume	2.421
332 8 Å <sup>3</sup>	2.310
552.0 //	2.264
Density	
(calculated) 6.540 g/cm <sup>3</sup>	2.161
	2.075
Thermal parameters	1.995
Isotropic: samarium B = 0.5; aluminum	1.951
B = 1.0	1.952
Scattering factors	1.884
Al <sup>0</sup> [International Tables, 1962]	1.850
Sm <sup>0</sup> [Cromer and Mann, 1968]	1.825
	1.806
Scale factor (integrated intensities) $y = 0.180 \times 10^{-3}$	1.743
,	1.726
References	1.707
Buschow, K.H.J. and van der Goot, A.S.	1.661
(1971). J. Less-Common Metals <u>24</u> , 117.	1.630
Cromer, D. T. and Mann, J. B. (1968). Acta	1.039
Crystallogr. A24, 321.	1.632
araphy III (1962) (The Kunoch Press	1.605
Birmingham England) p 202	1.587
brintingnam, bigrana, p. 202.	1.583
	1.573
	1.556
	1.535
	1.524
	1.516
	1.505
	1 404
	1.494
	1.477
	1.446
	1.421
	1.400

	Calculated	Pattern	(Peal	k hei	ghts)
d (Å)	I		hkl	λ	20(°) = 1.540598A
5.474 4.813 4.567 3.901 3.767	1 15 20 45	1 0 0 1 1	0 0 1 0 1	1 2 1 2	16.18 18.42 19.42 22.78 23.60
3 • 1 19 2 • 892 2 • 801 2 • 731 2 • 690	35 15 30 100 75	1 1 2 0 2	1 0 1 1	2 3 0 3+ 1	28.60 30.90 31.92 32.76 33.28
2.596 2.527 2.421 2.310 2.264	45 5 1 10 5	0 1 2 2 1	2 1 1 0 0	0 3 2 3 4	34.52 35.50 37.10 38.96 39.78
2.161 2.075 1.995 1.951 1.932	15 5 1 5	3 1 3 2 1	0 1 1 0 2	1+ 4 1 4 3	41.76 43.58 45.42 46.52 47.00
1.884 1.850 1.825 1.806 1.743	20 5 1 1 5	2 1 3 0 1	2 0 1 1	2 5 3 5 5	48.28 49.20 49.94 50.50 52.46
1.726 1.707 1.661 1.651 1.639	10 5 10 5 5	2 1 3 1 4	2 2 3 0	3 4 1 1 1	53.02 53.66 55.26 55.64 56.06
1.632 1.605 1.587 1.583 1.573	5 1 5 5	3 0 2 1 4	0 0 1 3 0	4 6 5 2 2	56.34 57.36 58.06 58.24 58.66
1.556 1.535 1.524 1.516 1.505	20 5 10 10	3 2 0 2 4	1 3 3 3	4 0 3 1 2+	59.34 60.22 60.74 61.06 61.58
1•494 1•485 1•477 1•446 1•421	10 1 1 1	1 1 4 2 4	1 3 0 0	6 3 3 6 3	62.06 62.48 62.86 64.38 65.66
1.400 1.393 1.386 1.383 1.375	5 1 5 5 1	4 2 4 3 1	2 1 2 2 3	0+ 6 1 4 4	66.74 67.16 67.52 67.72 68.12
1.366 1.347 1.345	1 1 1	0 1 4	2 0 2	6 7 2	68.68 69.74 69.88

Aluminum Samarium,  $AlSm_2$  - (continued)

С	alculated	Pattern	(In	tegr	ated)
d (Å)	I		hkl		$20(^{\circ})$ $\lambda = 1.540598A$
5.475	,	,	0	1	16.18
4.916	1		Š	-	10.10
4.010	1	0	0	2	18+41
4.571	20	0	1	1	19.40
3.901	25	1	0	2	22.78
3.768	55	1	1	1	23.59
3.119	45	1	1	2	28.59
2.892	20	1	0	3	30.90
2.801	35	2	1	0	31.92
2.737	50	2	0	2	32.69
2.731	100	0	1	3	32.77
2.690	95	2	1	1	33.28
2.596	60	0	2	0	34.52
2.526	10	1	1	З	35.50
2.422	1	2	1	2	37.10
2.310	15	2	0	3	38.95
2.264	10	1	0	4	39.78
2.162	1.0	1	2	2	41.75
2.161	15	3	5	1	41.76
2.111	10	2	,	-	42.01
2 076	-	2	1	5	42.01
2.070	5	•	•	*	43.57
1.995	5	З	1	1	45.41
1.951	5	2	0	4	46.52
1.932	10	1	2	3	47.00
1.884	30	. 2	2	2	48.27
1.878	1	3	1	2	48.42
					17.25
1.850	10	1	0	5	49.20
1.825	1	3	0	3	49.94
1.806	1	0	1	5	50.49
1.743	5	1	1	5	52.45
1.726	15	2	2	3	53.01
1.707	5	1	2	4	53.66
1.704	1	0	3	1	53.76
1.667	1	2	0	5	55.04
1.663	5	4	0	0	55.17
1.661	10	3	2	1	55.25
1.650	5	1	з	1	55.64
1.639	5	4	0	1	56.06
1.631	5		õ	Δ	56.35
1.605	5	0	õ	6	57.35
1.587	5	2	ĩ	5	58.06
	J	-	•	5	50.00
1.584	1	4	1	0	58.19
1.582	5	1	3	2	58.27
1.572	1	4	0	2	58.67
1.563	5	4	1	1	59.05
1.561	5	1	0	6	59.16
1.560	5	2	2	4	59.20
1.556	25	3	1	4	59.33
1.536	5	2	З	0	60.22
1.524	15	0	3	3	60.74
1.516	15	2	3	1	61.06

d (Å)	I		hkl		$2\Theta(\circ)$ $\lambda = 1.540598A$
1.507	10	1	2	5	61.48
1.505	10	Ā	1	2	61.58
1.495	10	1	1	6	62.05
1.493	1	-	2	3	62.12
1.485	1	1	7	7	62.48
1.405	•	•	5	5	02+40
1.477	1	4	0	з	62.87
1.446	-	2	õ	6	64.39
1.421	5	4	1	3	65.67
1.403	, i	2	5	5	66.61
1.401	-	~	2	~	66 73
1+401	5		~	U	00.13
		-		-	66 74
1.401	1	3		5	60.74
1.393	5	2	1	6	67.15
1.386	5	4	2	1	67.52
1.381	5	3	2	4	67.78
1.375	1	1	3	4	68.13
1.365	5	0	2	6	68.69
1.347	1	1	0	7	69.73
1.345	1	4	2	2	69.88

Aluminum Samarium, AlSm<sub>3</sub>

Structure (ubic, $Pm3m(221)$ , $Z = 1$ , isostructural with AuCua	Cal	culated Pat	ttern	(Pea	k heig	ghts)
AlCe <sub>3</sub> and AlLa <sub>3</sub> , from powder data [Iandelli, 1959].	d(Å)	I	ł	nkl	λ	20(°) = 1.540598Å
Atom positions						
l(a) l aluminum				10000		
3(c) 3 samarium	4.897	20	1	0	0	18.10
	3.464	20	1	ĩ	0	25.70
Lattice constant	2.829	100	1	1	1	31.60
a = 4.901 A [Iandelli, 1959]	2.451	50	2	0	0	36.64
	2.191	10	2	1	0	41.16
Volume						
117.7 A <sup>3</sup>	2.001	5	2	1	1	45.28
	1.732	30	2	2	0	52.80
Density	1.634	5	2	2	1+	56.26
(calculated) 6.743 g/cm <sup>3</sup>	1.550	5	3	1	0	59.60
	1.478	30	3	1	1	62.84
Thermal parameters						
Isotropic: aluminum $B = 1.0$ , samarium $B = 0.5$	1.415	10	2	2	2	65.98
	1.359	1	3	2	0	69.04
Scattering factors	1.310	5	3	2	1	72.04
Al <sup>o</sup> [Cromer and Mann, 1968]	1.225	5	4	0	0	77.90
Sm <sup>°</sup> [International Tables, 1974]	1.189	1	3	2	2+	80.78
Scale factor (integrated intensities)	1.155	1	4	1	1+	83.64
$\gamma = 0.737 \times 10^{-3}$	1.124	10	З	з	1	86.48
	1.096	10	4	2	0	89.32
References	1.069	1	4	2	1	92.16
Cromer, D.T. and Mann, J.B. (1968). Acta Crystal- logr. A24, 321.	1.000	10	4	2	2	100.70
Iandelli, A. (1959). Physical Chemistry of	.980	1	4	3	0+	103.60
Metallic Solutions and Intermetallic Compounds,	.961	1	4	3	1+	106.54
Vol. 1. (HMSO, London), 3F. p. 2.	•943	10	5	1	1+	109.50
International Tables for X-ray Crystallography,	.910	1	4	3	2+	115.64
IV (1974). (The Kynoch Press, Birmingham, Eng.), p. 100.	.895	1	5	2	1	118.82
	.866	5	4	4	0	125.52
	.853	1	4	4	1+	129.08
	•841	1	4	3	3+	132.82
	.828	15	5	З	1	136.82
	.817	10	4	4	2+	141.14
	•795	1	5	3	2+	151.34
	trade and the second second					

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Aluminum Samarium,  $AlSm_3$  - (continued)

	Calculated	Pattern	(Int	egr	ated)
d (Å)	I		hkl		$20(^{\circ})$ ° $\lambda = 1.540598A$
A . 901	20	1	0	0	18.09
3.466	15	1	1	ŏ	25.69
2.830	100	1	1	1	31.59
2.451	50	2	ō	ō	36.64
2.192	10	2	1	ō	41.15
2.001	5	2	1	1	45.29
1.733	35	2	2	0	52.79
1.634	1	3	0	0	56.27
1.634	5	2	2	1	56.27
1.550	5	3	1	0	59.61
1.478	40	3	1	1	62.84
1.415	10	2	2	2	65.98
1.359	1	3	2	0	69.04
1.310	5	3	2	1	72.04
1.225	5	4	0	0	77.91
1.189	1	4	1	0	80.79
1.189	1	3	2	2	80.79
1.155	1	4	1	1	83.64
1.124	15	3	3	1	86.49
1.096	15	4	2	0	89.32
1.069	1	4	2	1	92.15
1.045	1	3	3	2	94.99
1.000	10	4	2	2	100.70
•980	1	4	3	0	103.60
•961	1	4	3	1	106.53
.961	1	5	1	0	106.53
•943	10	5	1	1	109+51
•943	5	3	3	3	109.51
•910	1	5	2	0	115+64
•910	1	4	3	2	115.64
.895	1	5	2	1	118.83
•866	5	4	4	0	125.52
•853	1	5	2	2	129.08
•853	1	4	4	1	129.08
•841	1	5	3	0	132.83
.841	1	4	3	З	132.83
•828	25	5	3	1	130.82
•817	15	4	4	2	141.13
.817	5	6	0	0	141.13
•806	1	6	1	0	145.90
.795	5	5	3	2	151.33
.795	1	6	1	1	151.33

Aluminum Samarium, Al<sub>2</sub>Sm

```
Structure
  Cubic, Fd3m(227), Z = 8, a Laves phase, iso-
  structural with Cu<sub>2</sub>Mg [Harris et al., 1965].
Atom positions
   8(a) 8 samarium
          16 aluminum
  16(d)
  origin at 43m [ibid.]
Lattice constant
  a = 7.9423 \text{ Å}
  (published value: 7.9258 kX [ibid.])
Volume
  501.00 Å<sup>3</sup>
Density
  (calculated) 5.418 g/cm<sup>3</sup>
Thermal parameters
  Isotropic: aluminum B = 1.0, samarium B = 0.5.
Scattering factors
  Al<sup>0</sup> [Cromer and Mann, 1968]
  Sm<sup>0</sup> [International Tables, 1974]
Scale factor (integrated intensities)
  \gamma = 0.583 \times 10^{-3}
References
  Cromer, D. T. and Mann, J. B. (1968).
                                                Acta
    Crystallogr. A24, 321.
  Harris, I. R., Mansey, R. C. and Raynor, G. V.
    (1965). J. Less-Common Metals 9, 270.
  International Tables for X-ray Crystallography,
    IV (1974). (The Kynoch Press, Birmingham,
    Eng.) p. 100.
         Calculated Pattern (Peak heights)
   d(A)
                  Ι
                              hkl
                                            20(°)
```

					$\lambda = 1.540598A$
4.581	70	1	1	1	19.36
2.8083	100	2	2	0	31.84
2.3939	95	3	1	1	37.54
2.2929	5	2	2	2	39.26
1.9853	5	4	0	0	45.66
1.8220	15	3	З	1	50.02
1.6211	30	4	2	2	56.74
1.5286	25	5	1	1+	60.52
1.4042	.15	4	4	0	66.54
1.3426	10	5	З	1	70.02
1.2557	10	6	2	0	75.68
1.2113	10	5	З	З	78.98
1.1974	1	6	2	2	80.08
1.1463	1	4	4	4	84.44
1.1121	5	7	1	1+	87.68
1.0614	15	6	4	2	93.06
1.0339	15	7	З	1+	96.32
•9927	1	8	0	0	101.78
.9703	1	7	З	З	105.10
•9360	10	8	2	2+	110.76

å (Å)	I	hkl	λ	20(°) = 1.540598A
•9171	10	7 5	1+	114.26
•8879	5	8 4	0	120.34
•8718	5	7 5	3+	124.16
•8467	5	6 6	4	130.96
•8326	5	9 3	1	135.40
•8106	5	8 4	4	143.72
•7982	5	7 5	5+	149.60
•7788	15	8 6	2+	163.04

_	Calculated	Pattern	(Int	egr	ated)
d (Å)	I		hkl		$20(^{\circ})$ $\lambda = 1.540598A$
A 595	60	1	,	1	10.74
4.505		1	-	-	21.04
2.000		2	-		37 63
2.394	+7 100	3	-	-	37.00
2.292		2	2	2	39.20
1.985	50 10	4	0	0	43.03
1.822	21 15	3	З	1	50.02
1.621	12 35	4	2	2	56.74
1.528	35 20	5	1	1	60.52
1.528	85 5	З	3	3	60.52
1.404	20	4	4	0	66.55
1.342	25 10	5	з	1	70.03
1.255	58 15	6	2	0	75.67
1.211	12 10	5	З	З	78.99
1.197	73 1	6	2	2	80.08
1+146	54 1	4	4	4	84.43
1.112	21 5	5	5	1	87.68
1.112	21 5	7	1	1	87.68
1.061	13 15	6	4	2	93.07
1.034	40 10	7	з	1	96.31
1.034	•0 5	5	5	З	96.31
.992	28 5	8	0	0	101.77
.970	3 1	7	з	з	105.10
•936	50 5	8	2	2	110.76
.936	50 5	6	6	0	110.76
•917	71 10	7	5	1	114.27
•917	71 1	5	5	5	114.27
.888	80 5	8	4	0	120.33
.871	18 5	9	1	1	124.16
.871	18 5	7	5	з	124.16
.846	57 10	6	6	4	130.96
.832	26 15	9	З	1	135.40
-810	06 20	8	4	4	143.71
.795	32 5	7	7	1	149.60
.798	32 5	9	3	3	149.60
•798	82 5	7	5	5	149.60
	88 25	10	2	0	163-05
.776	38 45	8	6	2	163-05
• / / 6	40	0	0	6	103100

Aluminum Samarium, Al<sub>3</sub>Sm

Structure Hexagonal, $P6_3/mmc(194)$ , Z = 2, isostructural with Ni <sub>3</sub> Sn and Mg <sub>3</sub> Cd [Buschow and van Vucht, 1965]. It is unstable above 1055° [ibid.].
Atom positions 2(c) 2 samarium 6(h) 6 aluminum with $x = 0.857$ , $y = 0.714These are the positions given by Murray [1956]for Al3Th; the parameters were modified slight-ly because of the substitution of Sm for Th.$
Lattice constants a = 6.380(3)  Å c = 4.597(4) [Buschow and van Vucht, 1965]
c/a = 0.7205
Volume 162.1 A <sup>3</sup>
Density (calculated) 4.740 g/cm <sup>3</sup>
Thermal parameters Isotropic: aluminum B = 0.75; samarium B = 1.0
Scattering factors Al <sup>0</sup> Sm <sup>0</sup> [International Tables, 1962]
Scale factor (integrated intensities) $\gamma = 0.461 \times 10^{-3}$
References Buschow, K.H.J. and van Vucht, J.H.N. (1965). Philips Res. Rep. 20, 15. International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England) pp. 202, 211. Murray, J.R. (1956). J. Inst. Metals <u>84</u> , 1663.
Calculated Pattern (Peak heights)
$d(\hat{A}) \qquad I \qquad hk\ell \qquad 20(^{\circ}) \\ \bar{\lambda} = 1.540598\hat{A}$
5.521 25 1 0 0 16.04
<b>3.189 50 1 1 0 1 25.18</b>
<b>2.763 25 2 0 0 32.38</b> <b>2.367 90 2 0 1 37.98</b>
2.299         20         0         0         2         39.16           2.122         5         1         0         2         42.56

2.088

1.901

1.865

1.842

1.767

1.710

1.595

1.546

10

20

15

5

10

1

15

10

2

2

1

1 0

1 1

1 2

3 0 0

2 0 2

301

2 2 0 2 1 2

٥ ( ( ) ( )		1	- 1= 0		20(8)
u (A)	L		IKX		$\lambda = 1.540598A$
1.532	1	٦	1	0	60.36
1 476	Ē			2	62.00
1 4 5 4	5			3	64 00
1.434	15	5		-	64.00
1.437	5	3	0	2	64.82
1.381	1	4	0	0	67.78
1.340	10	2	0	з	70.18
1.323	10	4	0	1	71.22
1.311	10	2	2	2	72.00
1.275	1	3	1	2	74.34
1.236	5	2	1	з	77.14
1.222	5	з	2	1	78.16
1.206	5	4	1	0	79.42
1.184	1	۵	0	2	81.18
1.149	1	õ	õ	4	84.18
1 105	1	Ē	ő	~	
1.105	1	5	v	U	00.30
1.084	5	з	1	3	90.62
1.081	5	1	1	4	90.88
1.074	1	5	0	1	91.60
1.068	5	4	1	2	92.34
1-063	1	3	÷.	0	02.94
	•	3	Ĭ	Ŭ	52004
1.061	1	2	0	4	93.10
1.044	1	4	2	0	95.08
1.026	5	4	0	З	97.32
1.018	5	4	2	1	98.32
1.007	1	2	1	4	99.82
.996	1	5	0	2	101.32
.992	1	5	1	ā	101.82
.977	5	7	2	3	104.12
.075	1	3	2	~	104.40
070	Ē	5	1	- <b>T</b>	104+40
.970	5	5	•		105.14
•965	5	3	3	2	105.92
•951	1	4	2	2	108.24
•932	5	2	2	4	111.40
•921	1	6	0	0	113.54
•919	1	3	1	4	113.82
011	1	5	5	2	115.44
•911	1		-	5	115,08
.908	1	4	5	6	116.29
.907	1	1	0	5	110.20
.891	1	4	5	1	119.04

43.30

47.80

48.80

49.44

51.70

53.56

57.76

59.78

d(Å)       I       hkl $20(°)$ $\lambda = 1.540598Å$ 5.525       25       1       0       1       6.03         3.534       100       1       0       1       25.18         3.534       100       1       0       1       27.95         2.763       25       2       0       32.38         2.368       95       2       0       1       37.97         2.299       20       0       0       2       39.16         2.122       5       1       0       43.29         1.901       25       2       1       47.80         1.865       20       1       1       2       48.79         1.842       10       3       0       49.45         1.767       10       2       0       5.56         1.595       15       2       2       5.76         1.532       1       3       1       63.99         1.454       15       3       1       63.99         1.454       15       3       1       63.99         1.454       15       2       3       70.18		Calculated	Pattern	(Int	tegr	ated)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	d (A)	I		hkl		20 (°)
5.525 $25$ $1$ $0$ $16.03$ $3.534$ $100$ $1$ $0$ $1$ $25.18$ $3.190$ $50$ $1$ $10$ $27.95$ $2.763$ $25$ $2$ $0$ $32.38$ $2.368$ $95$ $2$ $0$ $1$ $37.97$ $2.299$ $20$ $0$ $2$ $39.16$ $2.122$ $5$ $1$ $0$ $43.29$ $1.901$ $25$ $2$ $1$ $47.80$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.842$ $10$ $3$ $0$ $49.45$ $1.767$ $10$ $2$ $0$ $57.76$ $1.532$ $1$ $3$ $1$ $60.35$ $1.437$ $5$ $3$						$\lambda = 1.540598A$
5.625 $25$ $1$ $0$ $16.03$ $3.534$ $100$ $1$ $0$ $1$ $25.18$ $3.190$ $50$ $1$ $1$ $0$ $27.95$ $2.763$ $25$ $2$ $0$ $32.38$ $2.366$ $95$ $2$ $0$ $1$ $37.97$ $2.299$ $20$ $0$ $2$ $39.16$ $2.122$ $5$ $1$ $0$ $43.29$ $1.901$ $25$ $2$ $1$ $47.80$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.842$ $10$ $3$ $0$ $49.45$ $1.767$ $10$ $2$ $2$ $57.76$ $1.546$ $10$ $2$ $1$ $2$ $59.78$ $1.532$ $1$ $3$ $0$ $64.82$ $1.437$ $5$ $3$ $2$ $64.82$ $1.340$ $15$ $2$ $0$ $370.18$ $1.323$ $10$ $71.22$ $1.310$ $15$ <						
3.534 $100$ $1$ $0$ $1$ $25.18$ $3.190$ $50$ $1$ $1$ $0$ $27.95$ $2.763$ $25$ $2$ $0$ $32.38$ $2.368$ $95$ $2$ $0$ $1$ $37.97$ $2.299$ $20$ $0$ $0$ $2$ $39.16$ $2.122$ $5$ $1$ $0$ $2$ $42.57$ $2.088$ $15$ $2$ $1$ $4$ $43.29$ $1.901$ $25$ $2$ $1$ $4$ $4$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.842$ $10$ $3$ $0$ $49.45$ $1.767$ $10$ $2$ $0$ $2$ $51.69$ $1.710$ $1$ $3$ $0$ $49.45$ $1.757$ $15$ $2$ $2$ $0$ $1.532$ $1$ $3$ $1$ $63.99$ $1.434$ $15$ $3$ $1$ $63.99$ $1.4477$ $5$ $1$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $37.18$ $1.323$ $10$ $4$ $0$ $71.122$ $1.310$ $15$ $2$ $2$ $72.01$ $1.225$ $1$ $3$ $1$ $79.42$ $1.340$ $15$ $2$ $1$ $74.33$ $1.225$ $5$ $2$ $1$ $74.33$ $1.225$ $5$ $2$ $1$ $74.33$ $1.222$ $10$ $3$ $2$ $74.33$ $1.222$ $10$ $3$ $2$ $1$	5.525	25	1	0	0	16.03
3.190 $50$ $1$ $1$ $0$ $27.95$ $2.763$ $25$ $2$ $0$ $0$ $32.38$ $2.366$ $95$ $2$ $0$ $1$ $37.97$ $2.299$ $20$ $0$ $0$ $2$ $39.16$ $2.122$ $5$ $1$ $0$ $2$ $42.57$ $2.088$ $15$ $2$ $1$ $0$ $43.29$ $1.901$ $25$ $2$ $1$ $1$ $47.80$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $10$ $2$ $1$ $2$ $57.76$ $1.532$ $1$ $3$ $1$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $2$ $1.437$ $5$ $3$ $0$ $2$ $1.437$ $5$ $3$ $0$ $2$ $1.437$ $5$ $3$ $0$ $2$ $1.4477$ $5$ $1$ $0$ $4$ $1.477$ $5$ $1$ $0$ $7.18$ $1.437$ $5$ $2$ $0$ $3$ <td>3.534</td> <td>100</td> <td>1</td> <td>0</td> <td>1</td> <td>25.18</td>	3.534	100	1	0	1	25.18
$2.763$ $25$ $2$ $0$ $32.38$ $2.368$ $95$ $2$ $0$ $1$ $37.97$ $2.299$ $20$ $0$ $0$ $2$ $39.16$ $2.122$ $5$ $1$ $0$ $2$ $42.57$ $2.088$ $15$ $2$ $1$ $4$ $43.29$ $1.901$ $25$ $2$ $1$ $4$ $47.80$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.842$ $10$ $3$ $0$ $49.45$ $1.767$ $10$ $2$ $0$ $2$ $51.69$ $1.770$ $1$ $3$ $0$ $1.595$ $15$ $2$ $2$ $57.76$ $1.546$ $10$ $2^{\circ}$ $1$ $2$ $1.532$ $1$ $3$ $1$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $2.849$ $1.437$ $5$ $3$ $0$ $1.437$ $5$ $3$ $0$ $2$ $1.381$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $1.323$ $10$ $4$ $1$ $71.22$ $1.310$ $15$ $2$ $2$ $72.01$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.235$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.66$ $5$ $4$ $10$ <td< td=""><td>3.190</td><td>50</td><td>1</td><td>1</td><td>0</td><td>27.95</td></td<>	3.190	50	1	1	0	27.95
2.366 $95$ $2$ $0$ $1$ $37.97$ $2.299$ $20$ $0$ $0$ $2$ $39.16$ $2.122$ $5$ $1$ $0$ $2$ $42.57$ $2.088$ $15$ $2$ $1$ $1$ $43.29$ $1.901$ $25$ $2$ $1$ $1$ $47.80$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.842$ $10$ $3$ $0$ $49.45$ $1.767$ $10$ $2$ $0$ $2$ $51.69$ $1.710$ $1$ $3$ $0$ $1.595$ $15$ $2$ $2$ $0$ $1.546$ $10$ $2.1$ $2$ $59.78$ $1.532$ $1$ $3$ $1$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $1.454$ $15$ $3$ $1$ $63.99$ $1.4437$ $5$ $3$ $0$ $2$ $1.361$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $1.323$ $10$ $4$ $0$ $1$ $1.225$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.330$ $15$ $2$ $2$ $72.01$ $1.225$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$	2.763	25	2	0	0	32.38
$2.299$ $20$ $0$ $0$ $2$ $39.16$ $2.122$ $5$ $1$ $0$ $2$ $42.57$ $2.088$ $15$ $2$ $1$ $4$ $43.29$ $1.901$ $25$ $2$ $1$ $4$ $47.80$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.842$ $10$ $3$ $0$ $49.45$ $1.767$ $10$ $2$ $0$ $2$ $51.69$ $1.710$ $1$ $3$ $0$ $49.45$ $1.595$ $15$ $2$ $2$ $57.76$ $1.546$ $10$ $2^{\circ}$ $1$ $2$ $1.532$ $1$ $3$ $1$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $2.64.82$ $1.381$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $1.340$ $15$ $2$ $0$ $1.323$ $10$ $4$ $0$ $1.323$ $10$ $4$ $0$ $1.225$ $1$ $3$ $1$ $1.225$ $1$ $3$ $2$ $1.340$ $15$ $2$ $2$ $1.340$ $15$ $2$ $2$ $1.340$ $15$ $2$ $0$ $1.225$ $1$ $3$ $70.18$ $1.323$ $10$ $4$ $0$ $1.225$ $1$ $3$ $77.15$ $1.222$ $10$ $3$ $2$ $1$ $1.149$ $1$ $0$ $4$ $1.149$ $1$ $0$ </td <td>2.368</td> <td>95</td> <td>2</td> <td>0</td> <td>1</td> <td>37.97</td>	2.368	95	2	0	1	37.97
2.299 $20$ $0$ $0$ $2$ $39.16$ $2.122$ $5$ $1$ $0$ $2$ $42.57$ $2.088$ $15$ $2$ $1$ $0$ $43.29$ $1.901$ $25$ $2$ $1$ $1$ $47.80$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.767$ $10$ $2$ $0$ $2$ $51.69$ $1.770$ $1$ $3$ $0$ $49.45$ $1.595$ $15$ $2$ $2$ $57.76$ $1.595$ $15$ $2$ $2$ $57.76$ $1.532$ $1$ $3$ $1$ $60.35$ $1.477$ $5$ $1$ $0$ $67.79$ $1.437$ $5$ $3$ $0$ $2$ $1.437$ $5$ $3$ $0$ $2$ $1.381$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $1.323$ $10$ $4$ $0$ $1$ $1.225$ $1$ $3$ $1$ $74.33$ $1.225$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $78.16$ $1.222$ $10$ $3$ $2$ $78.16$ $1.222$ $10$ $3$ $2$ $78.16$ $1.225$ $5$ $4$ $0$ $88.39$ $1.084$ $5$ $3$ $1$ $3$ $1.084$ $5$						
2.1225102 $42.57$ $2.088$ 15210 $43.29$ $1.901$ 25211 $47.80$ $1.865$ 20112 $48.79$ $1.865$ 20112 $48.79$ $1.865$ 20112 $48.79$ $1.865$ 20112 $48.79$ $1.842$ 1030 $49.45$ $1.767$ 10202 $51.69$ 15220 $1.595$ 15220 $1.546$ 102'12 $59.78$ $1.532$ 13160.35 $1.477$ 5103 $1.477$ 5103 $1.431$ 15203 $1.431$ 15203 $1.381$ 14067.79 $1.340$ 15203 $1.323$ 10401 $1.225$ 5213 $1.222$ 10321 $1.222$ 10321 $1.222$ 10321 $1.222$ 10321 $1.222$ 10321 $1.222$ 10321 $1.222$ 10321 $1.66$ 54	2.299	20	0	0	2	39.16
$2.088$ $15$ $2$ $1$ $0$ $43.29$ $1.901$ $25$ $2$ $1$ $1$ $47.80$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.842$ $10$ $3$ $0$ $49.45$ $1.767$ $10$ $2$ $0$ $2$ $51.69$ $1.710$ $1$ $3$ $0$ $1$ $595$ $15$ $2$ $2$ $0$ $1.595$ $15$ $2$ $2$ $0$ $1.546$ $10$ $2^{\circ}$ $1$ $2$ $59.78$ $1.532$ $1$ $3$ $10$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $2$ $64.82$ $1.381$ $1$ $4$ $0$ $1.340$ $15$ $2$ $0$ $3$ $2$ $64.82$ $1.340$ $15$ $2$ $0$ $3$ $2$ $72.01$ $1.323$ $10$ $4$ $1.225$ $5$ $2$ $1.310$ $15$ $2$ $2$ $2$ $1.222$ $10$ $3$ $2$ $1.222$ $10$ $3$ $2$ $1.222$ $10$ $3$ $2$ $1.222$ $10$ $1.222$ $10$ $1.222$ $10$ $1.222$ $10$ $1.222$ $10$ $1.222$ $10$ $1.222$ $10$ $1.222$ $10$ $1.222$ $10$ $1.222$ $10$ $1.22$	2.122	5	1	0	2	42.57
$1.901$ $25$ $2$ $1$ $1$ $47.80$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.865$ $20$ $1$ $1$ $2$ $48.79$ $1.767$ $10$ $2$ $0$ $2$ $51.69$ $1.710$ $1$ $3$ $0$ $1$ $53.56$ $1.595$ $15$ $2$ $2$ $0$ $57.76$ $1.546$ $10$ $2^{\circ}$ $1$ $2$ $59.78$ $1.477$ $5$ $1$ $0$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $1.437$ $5$ $3$ $0$ $2$ $1.437$ $5$ $3$ $0$ $2$ $1.361$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $1.340$ $15$ $2$ $0$ $3$ $1.340$ $15$ $2$ $2$ $72.01$ $1.323$ $10$ $4$ $0$ $1$ $1.275$ $1$ $3$ $1$ $1.235$ $5$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.064$ $5$ $3$ $1$ $3$ $1.064$ <td>2.088</td> <td>15</td> <td>2</td> <td>1</td> <td>0</td> <td>43.29</td>	2.088	15	2	1	0	43.29
1.8805 $20$ $1$ $1$ $2$ $48.79$ $1.842$ $10$ $3$ $0$ $49.45$ $1.767$ $10$ $2$ $0$ $2$ $51.69$ $1.710$ $1$ $3$ $0$ $1$ $595$ $15$ $2$ $2$ $0$ $57.76$ $1.546$ $10$ $2.1$ $2$ $59.78$ $1.532$ $1$ $3$ $1$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $0$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $0$ $64.82$ $1.381$ $1$ $4$ $0$ $1.381$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $70.18$ $1.323$ $10$ $4$ $1.323$ $10$ $4$ $1.275$ $1$ $3$ $1.235$ $5$ $2$ $1.325$ $5$ $2$ $1$ $3$ $7.715$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1.684$ $5$ $1$ $1$ $2$ $4$ $1.064$ $5$ $1$ $3$ $0$ $68.39$ $1.063$ $1$ $3$ $0$ $2.84$ $1.063$ $1$ $3$ $0$ $2.84$ $1.063$ $1$ $2.94$ $93.10$ $1.026$	1.901	25	2	1	1	47.80
1.842 $10$ $3$ $0$ $49.45$ $1.767$ $10$ $2$ $0$ $2$ $51.69$ $1.710$ $1$ $3$ $0$ $1$ $53.56$ $1.595$ $15$ $2$ $2$ $0$ $57.76$ $1.546$ $10$ $2.1$ $2$ $59.78$ $1.532$ $1$ $3$ $1$ $0$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $62.89$ $1.454$ $15$ $3$ $1$ $63.99$ $1.454$ $15$ $3$ $0$ $2$ $1.381$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $1.323$ $10$ $4$ $0$ $1$ $1.275$ $1$ $3$ $1$ $2$ $1.235$ $5$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.225$ $5$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.225$ $5$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ <t< td=""><td>1.805</td><td>20</td><td>1</td><td></td><td>2</td><td>48.79</td></t<>	1.805	20	1		2	48.79
$1.062$ $1.0$ $2$ $0$ $2$ $51.69$ $1.710$ $1$ $3$ $0$ $1$ $53.56$ $1.595$ $15$ $2$ $2$ $0$ $57.76$ $1.546$ $10$ $2 \cdot 1$ $2$ $59.78$ $1.532$ $1$ $3$ $1$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $1.437$ $5$ $3$ $0$ $2$ $1.381$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $1.323$ $10$ $4$ $0$ $1$ $1.275$ $1$ $3$ $1$ $1.222$ $10$ $3$ $2$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $74.33$ $1.222$ $10$ $3$ $2$ $74.33$ $1.222$ $10$ $3$ $2$ $74.33$ $1.222$ $10$ $3$ $2$ $1$ $1.449$ $1$ $0$ $4$ $1.49$ $1$ $0$ $4$ $1.149$ $1$ $0$ $4$ $1.064$ $5$ $3$ $1$ $1.068$ $5$ $4$ $1$ $2$ $2.35$ $1063$ $1.063$ $1$ $3$ $3$ $1.064$ $1$ $2$ $4$ $93.10$ $1.044$ $4$ $1.066$ $5$ $4$ $0$ $1.018$ $10$ $4$ $2$ $1.026$ $5$ $4$ $0$ <tr< td=""><td>1.842</td><td>10</td><td>3</td><td>0</td><td>0</td><td>49.45</td></tr<>	1.842	10	3	0	0	49.45
1.710 $1$ $3$ $0$ $1$ $53.56$ $1.595$ $15$ $2$ $2$ $0$ $57.76$ $1.546$ $10$ $2.1$ $2$ $59.78$ $1.532$ $1$ $3$ $10$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $1.437$ $5$ $3$ $0$ $2$ $1.381$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $1.323$ $10$ $4$ $0$ $71.22$ $1.310$ $15$ $2$ $2$ $72.01$ $1.275$ $1$ $3$ $1$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $78.16$ $1.206$ $5$ $4$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $1.084$ $5$ $3$ $1$ $3$ $0$ $68.39$ $1.064$ $5$ $4$ $2$ $1.063$ $1$ $3$ $0$ $1.063$ $1$ $3$ $0$ $1.064$ $5$ $4$ $2$ $1.063$ $1$ $3$ $1.064$ $1$ $2$ $4$ $93.10$ $1.044$ $4$ $2$ $1.018$ $10$ $4$ $2$ $1.026$ $5$ $4$ $0$ $1.026$ $5$ $4$ $0$ $1.026$ $5$ $4$ $0$ $1.026$ $5$ $4$ $0$ $1.007$ $1$ <t< td=""><td>1.767</td><td>10</td><td>2</td><td>ő</td><td>2</td><td>51.69</td></t<>	1.767	10	2	ő	2	51.69
$1.595$ $15$ $2$ $2$ $0$ $57.76$ $1.546$ $10$ $2^{\circ}$ $1$ $2$ $59.78$ $1.532$ $1$ $3$ $10$ $60.35$ $1.477$ $5$ $1$ $0$ $3$ $1.477$ $5$ $1$ $0$ $3$ $1.477$ $5$ $1$ $0$ $3$ $1.437$ $5$ $3$ $0$ $2$ $1.381$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $1.323$ $10$ $4$ $0$ $71.22$ $1.310$ $15$ $2$ $2$ $72.01$ $1.275$ $1$ $3$ $1$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $78.16$ $1.206$ $5$ $4$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $79.42$ $1.184$ $5$ $3$ $1$ $3$ $1.084$ $5$ $3$ $1$ $3$ $1.084$ $5$ $3$ $1$ $3$ $1.063$ $1$ $3$ $3$ $92.84$ $1.063$ $1$ $3$ $3$ $92.84$ $1.061$ $1$ $2$ $4$ $93.10$ $1.026$ $5$ $4$ $0$ $3$ $1.018$ $10$ $4$ $2$ $1$ $98.31$ $10$ $4$ $2$ $1$	1.710	1	3	ō	1	53.56
$1.546$ $10$ $2 \cdot 1$ $2$ $59.78$ $1.532$ $1$ $3$ $10$ $60.35$ $1.477$ $5$ $10$ $3$ $62.89$ $1.454$ $15$ $3$ $1$ $63.99$ $1.437$ $5$ $3$ $02$ $64.82$ $1.381$ $1$ $4$ $0$ $67.79$ $1.340$ $15$ $2$ $03$ $70.18$ $1.323$ $10$ $4$ $01$ $71.22$ $1.310$ $15$ $2$ $22$ $72.01$ $1.275$ $1$ $31$ $2$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.266$ $5$ $4$ $0$ $1.484$ $5$ $4$ $02$ $1.184$ $5$ $4$ $02$ $1.084$ $5$ $3$ $1$ $3$ $90.62$ $1.063$ $1$ $3$ $0$ $68.39$ $1.064$ $5$ $4$ $1.063$ $1$ $3$ $0$ $92.35$ $1.063$ $1$ $3$ $0$ $92.84$	1.595	15	2	2	0	57.76
1.5321 $3$ 1 $0$ $60.35$ $1.477$ 510 $3$ $62.89$ $1.454$ 15 $3$ 11 $63.99$ $1.437$ 5 $3$ $0$ $2$ $64.82$ $1.381$ 1 $4$ $0$ $0$ $67.79$ $1.340$ 15 $2$ $0$ $3$ $70.18$ $1.323$ $10$ $4$ $0$ $1$ $71.22$ $1.310$ $15$ $2$ $2$ $72.01$ $1.275$ $1$ $3$ $1$ $2$ $1.235$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $1$ $1.225$ $5$ $2$ $1$ $3$ $1.222$ $10$ $3$ $2$ $1$ $1.222$ $10$ $3$ $2$ $1$ $1.444$ $5$ $4$ $0$ $1.184$ $5$ $4$ $0$ $1.184$ $5$ $1$ $1$ $1.084$ $5$ $3$ $1$ $3$ $0$ $68.39$ $1.068$ $5$ $4$ $1$ $2$ $2$ $4$ $93.10$ $1.068$ $5$ $4$ $1$ $2$ $2$ $1.063$ $1$ $3$ $3$ $0$ $92.84$ $1.061$ $1$ $2$ $0$ $1.026$ $5$ $4$ $0$ $3$ $97.32$ $1.018$ $10$ $4$ $2$ $1$ $2$ $1$ $4$ $2$ $98.31$ </td <td>1.546</td> <td>10</td> <td>2.</td> <td>1</td> <td>2</td> <td>59.78</td>	1.546	10	2.	1	2	59.78
1.5321310 $60.35$ $1.477$ 5103 $62.89$ $1.454$ 15311 $63.99$ $1.437$ 5302 $64.62$ $1.381$ 1400 $67.79$ $1.340$ 15203 $70.18$ $1.323$ 10401 $71.22$ $1.310$ 15222 $72.01$ $1.275$ 1312 $74.33$ $1.235$ 5213 $77.15$ $1.222$ 10321 $78.16$ $1.206$ 5410 $79.42$ $1.184$ 5402 $1.084$ 5313 $90.62$ 104 $1.061$ 541 $1.063$ 130 $92.84$ $1.064$ 542 $95.07$ 12 $1.063$ 13 $97.32$ $1.018$ 1041 $98.31$						
1.477 $5$ $1$ $0$ $3$ $62.89$ $1.454$ $15$ $3$ $1$ $1$ $63.99$ $1.437$ $5$ $3$ $0$ $2$ $64.62$ $1.381$ $1$ $4$ $0$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $70.18$ $1.323$ $10$ $4$ $0$ $1$ $71.22$ $1.310$ $15$ $2$ $2$ $72.01$ $1.275$ $1$ $3$ $1$ $2$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $77.15$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.206$ $5$ $4$ $1$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $1.184$ $5$ $4$ $0$ $88.39$ $1.064$ $5$ $3$ $1$ $3$ $90.62$ $1.063$ $1$ $3$ $90.62$ $1.064$ $5$ $4$ $1$ $2$ $92.35$ $1.063$ $1$ $3$ $92.64$ $1.063$ $1$ $3$ $3$ $92.64$ $1.064$ $1$ $4$ $2$ $95.07$ $1.026$ $5$ $4$ $0$ $3$ $1.018$ $10$ $4$ $2$ $1$ $98.31$ $1.007$ $1$ $2$ $1$	1.532	1	З	1	0	60.35
1.454 $15$ $3$ $1$ $1$ $63.99$ $1.437$ $5$ $3$ $0$ $2$ $64.82$ $1.381$ $1$ $4$ $0$ $0$ $67.79$ $1.340$ $15$ $2$ $0$ $3$ $70.18$ $1.323$ $10$ $4$ $0$ $1$ $71.22$ $1.310$ $15$ $2$ $2$ $72.01$ $1.275$ $1$ $3$ $1$ $2$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $77.15$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.206$ $5$ $4$ $1$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $1.184$ $5$ $4$ $0$ $88.39$ $1.064$ $5$ $3$ $1$ $3$ $90.62$ $1.064$ $5$ $4$ $1$ $2$ $92.35$ $1.063$ $1$ $3$ $3$ $92.64$ $1.064$ $1$ $4$ $2$ $95.07$ $1.026$ $5$ $4$ $0$ $3$ $1.064$ $1$ $4$ $2$ $95.07$ $1.026$ $5$ $4$ $0$ $3$ $1.018$ $10$ $4$ $2$ $1$ $98.31$ $1$ $2$ $1$ $4$	1.477	5	1	0	3	62.89
1.437 $5$ $3$ $0$ $2$ $64.82$ $1.381$ $1$ $4$ $0$ $0$ $67.79$ $1.381$ $1$ $4$ $0$ $1$ $71.22$ $1.323$ $10$ $4$ $0$ $1$ $71.22$ $1.310$ $15$ $2$ $2$ $72.01$ $1.275$ $1$ $3$ $1$ $2$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $77.15$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.149$ $1$ $0$ $4$ $84.17$ $11.05$ $1.064$ $5$ $1$ </td <td>1.454</td> <td>15</td> <td>З</td> <td>1</td> <td>1</td> <td>63.99</td>	1.454	15	З	1	1	63.99
1.3811400 $67.79$ $1.340$ 15203 $70.18$ $1.323$ 10401 $71.22$ $1.310$ 15222 $72.01$ $1.275$ 1312 $74.33$ $1.235$ 5213 $77.15$ $1.222$ 10321 $78.16$ $1.206$ 5410 $79.42$ $1.184$ 5402 $1.184$ 5402 $1.105$ 150 $88.39$ $1.064$ 5313 $90.62$ $1.064$ 5412 $92.35$ $1.063$ 133 $92.64$ $1.064$ 120 $493.10$ $1.044$ 142 $95.07$ $1.026$ 540 $397.32$ $1.018$ 1042 $98.31$	1.437	5	3	0	2	64.82
1.340 $15$ $2$ $0$ $3$ $70.18$ $1.323$ $10$ $4$ $0$ $1$ $71.22$ $1.310$ $15$ $2$ $2$ $72.01$ $1.275$ $1$ $3$ $1$ $2$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $77.15$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.206$ $5$ $4$ $1$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $1.184$ $5$ $4$ $0$ $88.39$ $1.084$ $5$ $3$ $1$ $3$ $90.62$ $1.084$ $5$ $1$ $1$ $1.064$ $5$ $4$ $1$ $2$ $92.35$ $1.063$ $1$ $3$ $1.063$ $1$ $3$ $3$ $92.84$ $1.061$ $1$ $2$ $4$ $93.10$ $1.044$ $1$ $4$ $1.026$ $5$ $4$ $0$ $3$ $97.32$ $1.018$ $10$ $4$ $2$ $1$ $2$ $1$ $98.31$	1.381	1	4	0	0	67.79
1.323 $10$ $4$ $0$ $1$ $71.22$ $1.310$ $15$ $2$ $2$ $2$ $72.01$ $1.275$ $1$ $3$ $1$ $2$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $77.15$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.206$ $5$ $4$ $1$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $81.18$ $1.149$ $1$ $0$ $4$ $84.17$ $1.105$ $1$ $5$ $0$ $88.39$ $1.084$ $5$ $3$ $1$ $3$ $90.62$ $1.061$ $5$ $4$ $1$ $1.063$ $1$ $3$ $0$ $92.84$ $1.063$ $1$ $3$ $3$ $92.84$ $1.061$ $1$ $2$ $4$ $93.10$ $1.026$ $5$ $4$ $0$ $3$ $97.32$ $1.018$ $10$ $4$ $2$ $1.007$ $1$ $2$ $1$ $98.31$	1.340	15	2	0	3	70.18
1.310 $15$ $2$ $2$ $2$ $72.01$ $1.275$ $1$ $3$ $1$ $2$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $77.15$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.206$ $5$ $4$ $1$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $1.184$ $5$ $4$ $0$ $2$ $1.184$ $5$ $4$ $0$ $2$ $1.184$ $5$ $4$ $0$ $88.39$ $1.05$ $1$ $5$ $0$ $88.39$ $1.064$ $5$ $3$ $1$ $3$ $90.62$ $1.063$ $1$ $1$ $1.066$ $5$ $4$ $1$ $2.92.35$ $1.063$ $1$ $3$ $1.063$ $1$ $3$ $0$ $92.64$ $1.064$ $1$ $4$ $2$ $95.07$ $1.026$ $5$ $4$ $1.026$ $5$ $4$ $0$ $3.97.32$ $1.018$ $10$ $4$ $1.007$ $1$ $2$ $1$	1.323	10	4	0	1	71.22
1.275 $1$ $3$ $1$ $2$ $74.33$ $1.235$ $5$ $2$ $1$ $3$ $77.15$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.206$ $5$ $4$ $1$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $81.18$ $1.149$ $1$ $0$ $4$ $84.17$ $1.105$ $1$ $5$ $0$ $88.39$ $1.084$ $5$ $3$ $1$ $3$ $90.62$ $1.084$ $5$ $1$ $1$ $4$ $90.87$ $1.074$ $1$ $5$ $1$ $91.60$ $1.063$ $1$ $3$ $0$ $92.84$ $1.063$ $1$ $3$ $3$ $92.84$ $1.063$ $1$ $2$ $4$ $93.10$ $1.044$ $1$ $4$ $2$ $98.31$ $1.018$ $10$ $4$ $2$ $1$ $98.31$	1.310	15	2	2	2	72.01
1.235 $5$ $2$ $1$ $3$ $77.15$ $1.222$ $10$ $3$ $2$ $1$ $78.16$ $1.206$ $5$ $4$ $1$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $81.18$ $1.149$ $1$ $0$ $0$ $4$ $84.17$ $1.105$ $1$ $5$ $0$ $88.39$ $1.084$ $5$ $3$ $1$ $3$ $90.62$ $1.081$ $5$ $1$ $1$ $4$ $90.87$ $1.074$ $1$ $5$ $0$ $91.60$ $1.063$ $1$ $3$ $3$ $92.84$ $1.063$ $1$ $3$ $3$ $92.84$ $1.061$ $1$ $2$ $4$ $93.10$ $1.026$ $5$ $4$ $0$ $3$ $1.018$ $10$ $4$ $2$ $98.31$ $1.007$ $1$ $2$ $1$ $4$	1.275	1	З	1	2	74.33
1.222 $10$ $3$ $2$ $1$ $78.16$ $1.206$ $5$ $4$ $1$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $81.18$ $1.149$ $1$ $0$ $0$ $4$ $84.17$ $1.105$ $1$ $5$ $0$ $88.39$ $1.084$ $5$ $3$ $1$ $3$ $90.62$ $1.081$ $5$ $1$ $1$ $4$ $90.87$ $1.074$ $1$ $5$ $0$ $91.60$ $1.068$ $5$ $4$ $2$ $92.35$ $1.063$ $1$ $3$ $3$ $92.84$ $1.063$ $1$ $2$ $4$ $93.10$ $1.044$ $1$ $4$ $2$ $95.07$ $1.026$ $5$ $4$ $0$ $3$ $1.018$ $10$ $4$ $2$ $1$ $1.007$ $1$ $2$ $1$ $4$	1.235	5	2	1	З	77.15
1.206 $5$ $4$ $1$ $0$ $79.42$ $1.184$ $5$ $4$ $0$ $2$ $81.18$ $1.149$ $1$ $0$ $0$ $4$ $84.17$ $1.105$ $1$ $5$ $0$ $86.39$ $1.084$ $5$ $3$ $1$ $3$ $90.62$ $1.084$ $5$ $1$ $1$ $4$ $90.87$ $1.074$ $1$ $5$ $0$ $1$ $91.60$ $1.068$ $5$ $4$ $1$ $2$ $92.35$ $1.063$ $1$ $3$ $3$ $92.84$ $1.061$ $1$ $2$ $0$ $4$ $93.10$ $1.026$ $5$ $4$ $0$ $3$ $97.32$ $1.018$ $10$ $4$ $2$ $1$ $98.31$	1.222	10	з	2	1	78.16
1.1845402 $81.18$ $1.149$ 1004 $84.17$ $1.105$ 1500 $88.39$ $1.084$ 5313 $90.62$ $1.081$ 5114 $90.87$ $1.074$ 1501 $91.60$ $1.068$ 5412 $92.35$ $1.063$ 1330 $92.84$ $1.061$ 1204 $93.10$ $1.026$ 5403 $97.32$ $1.018$ 10421 $98.31$ $1.007$ 121 $4$ $92.82$	1.206	5	4	1	0	79.42
$1 \cdot 149$ $1$ $0$ $0$ $4$ $84 \cdot 17$ $1 \cdot 105$ $1$ $5$ $0$ $0$ $88 \cdot 39$ $1 \cdot 05$ $1$ $5$ $0$ $0$ $88 \cdot 39$ $1 \cdot 064$ $5$ $3$ $1$ $3$ $90 \cdot 62$ $1 \cdot 081$ $5$ $1$ $1$ $4$ $90 \cdot 87$ $1 \cdot 074$ $1$ $5$ $0$ $1$ $91 \cdot 60$ $1 \cdot 068$ $5$ $4$ $1$ $2$ $92 \cdot 35$ $1 \cdot 063$ $1$ $3$ $3$ $92 \cdot 84$ $1 \cdot 063$ $1$ $2$ $0$ $4$ $93 \cdot 10$ $1 \cdot 063$ $1$ $2$ $0$ $95 \cdot 07$ $1 \cdot 026$ $5$ $4$ $0$ $3$ $97 \cdot 32$ $1 \cdot 018$ $10$ $4$ $2$ $1$ $98 \cdot 31$ $1$ $90 \cdot 32$	1.184	5	4	0	2	81.18
1.10515088.39 $1.084$ 531390.62 $1.081$ 511490.87 $1.074$ 150191.60 $1.068$ 541292.35 $1.063$ 133092.84 $1.061$ 120493.10 $1.044$ 142095.07 $1.026$ 540397.32 $1.018$ 1042198.31 $1.007$ 121492.82	1.149	1	0	0	4	84.17
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1.105	1	5	0	0	88.39
1.081       5 $1$ $1$ $4$ $90.87$ $1.074$ $1$ $5$ $0$ $91.60$ $1.068$ $5$ $4$ $1$ $2$ $92.35$ $1.063$ $1$ $3$ $3$ $92.84$ $1.061$ $1$ $2$ $4$ $93.10$ $1.044$ $1$ $4$ $2$ $95.07$ $1.026$ $5$ $4$ $0$ $3$ $97.32$ $1.018$ $10$ $4$ $2$ $1$ $98.31$	1.084	5	з	1	з	90.62
$1 \cdot 074$ 1501 $91 \cdot 60$ $1 \cdot 068$ 5412 $92 \cdot 35$ $1 \cdot 063$ 1330 $92 \cdot 84$ $1 \cdot 061$ 1204 $93 \cdot 10$ $1 \cdot 044$ 1420 $95 \cdot 07$ $1 \cdot 026$ 5403 $97 \cdot 32$ $1 \cdot 018$ 10421 $98 \cdot 31$ $1 \cdot 007$ 1214 $92 \cdot 82$	1.081	5	1	1	4	90.87
1.0685412 $92.35$ $1.063$ 1330 $92.84$ $1.061$ 1204 $93.10$ $1.044$ 1420 $95.07$ $1.026$ 5403 $97.32$ $1.018$ 10421 $98.31$ $1.007$ 1214 $92.82$	1.074	1	5	0	1	91.60
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1.068	5	4	1	2	92.35
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1.063	1	3	3	0	92.84
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1.061	1	2	0	4	93.10
1.026     5     4     0     3     97.32       1.018     10     4     2     1     98.31       1.007     1     2     1     4	1.044	1	4	2	0	95.07
	1.026	5	4	0	З	97.32
1.007 1 2 1 4 00.02	1.018	10	4	2	1	98.31
1	1.007	1	2	1	4	99.82
.996 1 5 0 2 101.33	.006	1	5	0	2	101.33
•992 1 5 1 0 101.83	.992	1	5	1	0	101.83
.977 5 3 2 3 104.12	.977	5	3	2	з	104.12
•975 1 3 0 4 104 <b>•</b> 38	.975	1	3	0	4	104.38
•970 5 5 1 1 105•14	.970	5	5	1	1	105.14
.965 5 3 3 2 105-91	-965	5	3	3	2	105-91
•951 1 4 2 2 108-24	.951	1	4	2	2	108-24
.932 5 2 2 4 111.41	.932	5	2	2	4	111.41
.921 1 6 0 0 113.54	.921	1	6	0	0	113.54
•919 1 3 1 4 113•82	•919	1	З	1	4	113.82

d (Å)	I	hkl		20(°) $\lambda = 1.540598A$
•911	1	5 1	2	115.45
•908	1	4 3	0	116.00
•907	1	1 0	5	116.28
•896	1	50	З	118.50
•891	5	4 3	1	119.63

Aluminum Technetium, Al<sub>6</sub>Tc

Г

Orthorhombia Comm(62) 7 = 4 isostructural with	Cal	culated Pa	ttern	(Pea	k hei	ghts)
Al <sub>6</sub> Mn. The structure was determined by Wilkinson $[1967]$ .	d (A)	I		hkl	λ	20(°) = 1.540598A
Atom positions						
4(c) 4 technetium	4.98	100	1	1	0	17.78
8(e) 8 aluminum (1), y = 0.3257	4.50	45	0	0	2	19.72
8(f) 8 aluminum (2), $x_2 = .1338$ , $z_2 = .1030$	4.36	21	1	1	1	20.34
$8(q)$ 8 aluminum (3), $x_3 = .2880$ , $y_3 = .3180$ ,	3.81	30	0	2	0	23.32
$z_3 = .25$	3.341	63	1	1	2	26.66
[Wilkinson, 1978, private communication]						
	3.297	21	2	0	0	27.02
Lattice constants	3.095	9	2	0	1	28.82
a = 6.5948(9) Å	2.910	24	0	2	2	30.70
b = 7.629(9)	2.572	5	1	1	3	34.86
c = 9.0016(11)	2.494	14	2	2	0	35.98
(published values: a = 6.5944(9)A, b = 7.629(9),	2.372	1	1	З	0	37.90
c = 9.0011(11) [Wilkinson, 1967]).	2.294	35	1	3	1	39.24
	2.250	21	0	0	4	40.04
CD cell: $a = 7.629(9); b = 9.0016(11);$	2.219	25	2	0	3	40.62
c = 6.5948(9); a/b = 0.8475; c/b = 0.7326; sp. gp.	2.181	62	2	2	ę	41.36
. (20) anund	2.112	32	з	1	0	42.78
Volume	2.099	75	1	3	2	43.06
452 89 p <sup>3</sup>	2.051	66	- ī	1		44.12
452.05 A	1.918	14	2	2	-	47.36
Density	1.913	12		1	2	47.48
(calculated) 3.826 g/cm <sup>3</sup>	11515		5	•	-	47840
	1.907	11	0	. 4	0	47.64
Thermal parameters	1.859	9	2	0	4+	48.96
Isotropic: aluminum $B = 1.0$ , technetium $B = 0.5$	1.756	6	0	4	2	52.04
	1.727	5	3	1	З	52.98
Scattering factors	1.671	9	2	2	4	54.90
Al <sup>0</sup> , Tc <sup>0</sup> [Cromer and Mann, 1968]						
	1.651	3	2	4	0	55.64
Scale factors (integrated intensities)	1.649	3	4	0	0	55.70
$\gamma = 0.330 \times 10^{-3}$	1.633	9	1	3	4+	56.30
I/I (calculated) 1.97	1.622	2	4	0	1	56.72
corundum	1.580	З	2	0	5	58.36
References	1.560	5	3	3	2	59.18
logr D24 221	1.550	10	2		2	59.60
1091. A24, 321.	1.540		7	1		60.02
WIIKINSON, C. (1967). Acta Crystallogr. <u>22</u> , 924.	1.513	1	Ă	2	0	61.20
	1.500	4	ō	ō	6	61.78
	1 407			~		<i>co</i> 14
	1.493	11	4	2	1	62.14
	1.489		1	5	0	62.32
	1.460	1	. 2	2	5	63.70
	1.440	0	2	4	3	64.36
	1.434	6	1	3	5+	64.96
	1.412	2	1	5	2	66.14
	1.396	5	0	2	6	66.98
	1.370	4	3	1	5	68.42
	1.351	5	4	2	3	69.52
	1.337	1	3	3	4	70.34
	1.330	8	4	0	4+	70.78
	1.286	9	2	2	6+	73.62
	1.271	6	0	6	0	74.58
	1.268	9	1	3	6	74.80
	1.253	6	3	5	0	75.84

Aluminum Technetium,	Al <sub>6</sub> Tc	-	(continued)
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d (Å)	I		hkl		20(°)
				λ	= 1.540598A
1.245	2	1	1	7	76.44
1.240	10	1	5	4+	76.78
1.236	5	4	4	1	77.14
1.223	4	3	1	6+	78.06
1.217	1	2	4	5+	78.56
1.207	1	3	5	2	79.28
1.202	2	4	4	2	79.72
1.186	5	2	1	3	80.99
1.179	3	0	4	6	81.58
1.176	2	2	6	1	81.82
1.161	3	5	3	1	83.12
1.158	5	4	2	5	83.36
1.157	. 3	3	5	3	83.52
1.152	2	4	4	3	83.94
Cal	culated Pa	attern	(Int	egrate	ed)
d(A)	I		hkl	2	20(°)
					- 1.9409900
4.99	100	1	1	0	17.76
4.50	45	Ō	0	2	19.71
4.36	21	1	1	1	20.33
3.81	32	0	2	0	23.30
3.342	68	1	1	2	26.65
3.297	21	2	0	0	27.02
3.096	10	2	0	1	28.81
2.910	27	0	2	2	30.70
2.571	5	1	1	3	34.86
2.495	16	2	2	0	35.97
2.373	1	1	3	0	37.89
2.294	41	1	3	1	39.23
2.250	25	0	0	4	40.03
2.182	29	2	2	3	40.62
20102	15	2	-	-	
2.112	34	3	1	0	42.77
2.099	88	1	3	2	43.06
2.056	34	3	1	1	44.00
2.051	59	1	1	4	44+11
1.918	17	2	2	3	4/+35
1.912	5	3	1	2	47.51
1.861	3	1	+	3	48.00
1.850	3	1	0	4	48.94
1.756	8	0	4	2	52.04
1.727	6	3	1	3	52.97
1.671	11	2	2	4	54.90
1.651	3	2	4	0	55.62
1.649	2	4	0	0	55.71
1.635	4	3	3	1	56.20

d (Å)	I	hkl	λ	20(°) ° = 1.540598A
1.633	10	1 3	4	56.30
1.622	2	4 0	1	56.72
1.580	4	2 0	5	58.35
1.560	6	3 3	2	59.18
1.550	13	2 4	2	59.60
1.540	5	3 1	4	60.02
1.513	2	4 2	0	61 • 19
1.500	5	0 0	6	61.79
1.492	14	4 2	1	62.15
1.487	4	1 5	0	62.42
1.460	2	2 2	5	63.69
1.446	8	2 4	3	64.35
1.43/	1	1 1	6	64.84
1.434	4	4 2	2	64.96
1 •4 34	4	1 3	5	64.97
1.412	3	1 5	2	66 • 15
1.396	7	0 2	6	66.97
1.370	5	3 1	5	68.41
1.351	7	4 2	3	69.51
1.337	2	33	4	70.33
1.332	1	1 5	3	70.66
1.331	4	2 4	4	70.71
1.330	8	4 0	4	70.79
1.286	2	5 1	1	73.57
1.286	11	2 2	6	73.62
1.272	8	0 6	0	74.58
1.268	9	1 3	6	74+81
1.253	7	3 5	0	75.84
1.245	1	1 1	7	76.43
1.241	7	35	1	76.70
1.240	11	1 5	4	76.78
1.235	5	4 4	1	77.14
1.224	1	0 6	2	78.03
1.223	3	3 1	6	78.07
1.217	1	2 4	5	18.55
1.208	1	35	2	79.28
1.202	2	4 4	2	79.71
1.193	7	5 1	3	80.47
1.186	2	26	0	80.98
1.179	4	0 4	6	81.57
1.176	1	2 6	1	81.83
1.161	3	5 3	1	83.13
1.158	5	4 2	5	83.36
1.157	2	3 5	3	83.52
1.152	3	4 4	3	03.42

Aluminum Terbium, Al<sub>2</sub>Tb

r and a second
<pre>Structure Cubic, Fd3m(227), Z = 8, a Laves phase, iso- structural with Cu<sub>2</sub>Mg [Harris et al., 1965].</pre>
Atom positions 8(a) 8 terbium 16(d) 16 aluminum
origin at 43m [ibid.]
Lattice constant a = 7.8658  Å
(published value: 7.8495 kX [ibid.])
Volume . 486.66 Å <sup>3</sup>
Density (calculated) 5.811 g/cm <sup>3</sup>
Thermal parameters Isotropic: aluminum B = 1.0; terbium B = 0.5.
Scattering factors Al <sup>0</sup> [Cromer and Mann, 1968] Tb <sup>0</sup> [International Tables, 1974]
Scale factor (integrated intensities) $\gamma = 0.892 \times 10^{-3}$
References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321. Harris, I. R., Mansey, R. C. and Raynor, G. V. (1965). J. Less-Common Metals <u>9</u> , 270. International <u>Tables for X-ray Crystallography</u> , <u>IV</u> (1974). (The Kynoch Press, Birmingham,
Eng.) p. 101.
Calculated Pattern (Peak heights)

С	alculated	Pattern	(Pea	ak he	eights)
d (Å)	I		hkl		$2\Theta(^{\circ})$ ° $\lambda = 1.540598 \text{\AA}$
4.539 2.7811 2.3708 2.2707 1.9666 1.8045 1.6056 1.5137 1.3905 1.3294	70 100 95 5 10 15 30 25 15 10	1 2 3 2 4 3 4 5 4 5	1 2 1 2 0 3 2 1 4 3	1 0 1 2 0 1 2 1+ 0 1	19.54 32.16 37.92 39.66 46.12 50.54 57.34 61.18 67.28 70.82
1.2437	10 10	6 5	2 3	0 3	76.54 79.90
1.1858 1.1352 1.1013	1 1 5	6 4 7	2 4 1	2 4 1+	81.02 85.46 88.76
1.0510 1.0241 .9832 .9610 .9270	15 15 1 1	6 7 8 7 8	4 3 0 3 2	2 1+ 0 3 2+	94.26 97.56 103.16 106.56 112.40

						-
d (Å)	I		hkl	λ	20(°) = 1.5405982	° A
•9082	10	7	5	1+	116.02	
.8795	5	8	4	ō	122.30	
.8634	5	7	5	3+	126.30	
.8385	5	6	6	4	133.46	
•8246	5	9	3	1	138.20	
	10				147 28	
•8028	10	•	4	4	14/020	
•7905	5	7	5	5+	154.02	

	Calculated	Pattern	(Int	egr	ated)
d (Å)	I		hkl		$20(^{\circ})$ , $\lambda = 1.540598A$
4.541	65	1	1	1	19.53
2.781	0 100	2	2	0	32.16
2.371	6 95	3	1	1	37.91
2.270	7 5	2	2	2	39.66
1.966	5 10	4	0	0	46.12
1.804	5 15	З	З	1	50.54
1.605	6 35	4	2	2	57.34
1.513	8 20	5	1	1	61.18
1.513	8 5	3	З	З	61.18
1.390	5 20	4	4	0	67.28
1.329	6 10	5	з	1	70.81
1.243	7 15	6	2	0	76.54
1.199	5 10	5	3	3	79.91
1.185	8 1	6	2	2	81.02
1.135	3 1	4	4	4	85.45
11100	-				
1.101	4 5	5	5	1	88.75
1.101	4 5	7	1	1	88.75
1.051	1 20	6	4	2	94.25
1.024	0 10	7	З	1	97.57
1.024	0 5	5	5	3	97.57
•983	2 5	8	0	0	103.15
.961	0 5	7	З	З	106.57
.927	0 10	8	2	2	112.40
.927	0 5	6	6	0	112.40
•908	3 10	7	5	1	116.01
.908	3 1	5	5	5	116.01
.879	4 5	8	4	0	122.31
.863	4 5	7	5	3	126.30
.863	4 5	9	1	1	126.30
.838	5 10	6	6	4	133.46
.824	6 15	9	з	1	138.20
.802	8 20	8	4	4	147.28
.790	5 5	7	7	1	154.01
.790	5 5	9	З	З	154.01
.790	5 5	7	5	5	154.01

95

Structure Tetragonal, $P4_2nm$ (102), $Z = 4$ , isostructural	Calculated Pattern (Peak heights)					
with $Al_2Gd_3$ , from powder data [Buschow, 1965]. Baenziger and Hegenbarth [1964] determined the structure for $Al_2Gd_3$ .	d (Ă)	I		hkl	λ	20(°) ° = 1.540598A
Atom positions	5.832	10	1	1	0	15.18
4(c) 4 aluminum(l)	5.576	5	1	0	1	15.88
4(c) 4 aluminum(2)	4.619	5	1	1	1	19.20
4(c) 4 terbium(1)	3.783	5	0	0	2	23.50
4(c) 4 terbium(2)	3.690	55	2	1	0	24.10
4(b) 4 terbium(3)						
	3.175	50	1	1	2	28.08
Information on atomic position parameters was not	2.917	40	2	2	0	30.62
available. From considerations of atomic size.	2.790	100	2	0	2	32.06
the parameters for AlaGda were used instead.	2.723	10	2	2	1	32.86
	2.642	75	2	1	2	33.90
Lattice constants	2.611	45	7		•	74 72
a = 8.255 A	2.011	65	3	1		34.32
c = 7.568 [Buschow, 1965]	2.408	25	3	1	1	30.38
	2.413	5	1		3	37.24
c/a = 0.9168	2.310	5	1	1	3	38.80
Valuma	2.511	, 5	2	٤	٤	30.94
FIE 7 $\pi/cm^3$	2.290	1	3	2	0	39.32
515.7 g/cm	2.191	1	3	2	i	41.16
Donaitu	2.148	ī	3	1	2	42.02
$(a_1)(a_2) \in \mathbb{R}^{3}$	2.002	15	4	1	0	45.26
(carculated) 6.856 g/cm	1.946	1	3	3	0.	46.64
Thormal parameters		-			- •	
Tectropice aluminum $B = 1.97$ terbium(1) $B = 1.55$	1.936	5	4	1	1	46.90
$f_{1,2,2} = 1$ (2) $B = 1$ (5, $f_{1,2,2} = 1$ (2) $B = 1$ (2) $B = 1$ (2)	1.908	1	2	2	3	47.62
(eibium(2) B = 1.03; ceibium(3) B = 1.73	1.892	10	Ō	0	4	48.06
Controling factors	1.860	1	3	Ō	3	48.94
Al <sup>0</sup> [International mables 1962]	1.846	5	4	2	0	49.34
mb <sup>0</sup> [International Tables, 1902]						
ID <sup>2</sup> (International Tables, 1974)	1.812	10	4	0	2+	50.32
Carla factor (intermetal intermities)	1.800	1	1	1	4	50.68
scale factor (integrated intensities) $x = 0.426 \times 10^{-3}$	1.770	15	4	1	2	51.60
$\gamma = 0.436 \text{ x} 10^{-1}$	1.731	20	З	3	2	52.86
Defenses	1.695	1	3	2	3	54.06
References						
Baenziger, N.C. and Regendarin, J. J., Jr. (1904)	1.683	10	2	1	4	54.46
Acta Crystallogr. 17, 620.	1.659	5	4	2	2	55.34
Buschow, K. H. J. (1965). J. Less-Common Metals	1.619	5	5	1	0	56.84
0, 209. International Mahlag fam V you Crustallagyanhu	1.613	10	4	3	1+	57.04
<u>III</u> (1962). (The Kynoch Press, Birmingham, Eng.)	1.587	10	2	2	4	58.06
p. 202.	1.583	10	5	1	1	58.22
International Tables for X-ray Crystallography,	1.568	5	4	1	3	58.84
10 (19/4). (The Kynoch Press, Birmingham, Eng.)	1.541	1	з	3	3	60.00
p. 101.	1.532	15	З	1	4	60.38
	1.513	1	4	3	2	61.20
	1 500	-	=	2		61.70
	1.400	5	5	2	-	62 34
	1.488	10	5	1	2	67 44
	1.450	I E	L	1	5	63 70
	10423	5	*	*	U	03072

Aluminum Terbium,  $Al_2Tb_3$  - (continued)

	Calculated	Pattern	(Int	egra	ted)	
d (Å)	I		hkl	;	$2\Theta(^{\circ})$ A = 1.5405	• 598A
5.837 5.578 4.622	10 5 2 5	1 1 1	1 0 1	0 1 1	15.17 15.87 19.19	,
3.784 3.692	5 50	0 2	0 1	2 0	23.49 24.09	•
3.175 2.919 2.789	45 40 100	1 2 2	1 2 0	2 0 2	28.08 30.61 32.06	8   
2.723 2.642	10 75	2	2 1	1 2	32.86 33.90	5
2.610 2.586 2.468	60 1 25	3 3 3	1 0 1	0 1 1 3	34.32 34.66 36.38	2
2.316	5	1	1	3	38.94	5
2.290 2.191 2.149		3 3 3	2 2 1	0 1 2	39.32 41.16 42.01	,
2.002	15	4 3	1 3	0 0	45.26	5
1.936 1.909 1.892	5 1 15	4 2 0	1 2 0	1 3 4	46.90 47.61 48.05	5
1.859	5	4	2	3	48.94	
1.812 1.800 1.770	5 5 1 15	4	0 1 1	2 4 2	50.23 50.32 50.68 51.61	
1.730 1.720	25 1	3	3 0	2 4	52.87 53.21	,
1.695 1.684 1.659	1 10 10	3 2 4	2 1 2	3 4 2	54.05 54.45 55.33	5
1.619	5	5	1 0	0 1	56.82 57.05	
1.588	10 5	* 2 5	2	4	58.05 58.23	
1.568 1.541 1.533	5 1 1	4 3 5	1 3 2	3 3 0	58.84 60.00 60.33	
1•532 1•513	15 1	3	1 3	42	60.37 61.20	
1.502 1.488 1.465 1.459	5 10 1 5	5 5 1 4	2 1 1 4	1 2 5 0	61.69 62.33 63.44 63.72	

Structure	Ca	lculated Pa	attern	(Pe	ak h	eights)
Hexagonal, $Pb_3/mmc(194)$ , $Z = 1$ , isostructural with Al <sub>2</sub> Th and Ni <sub>2</sub> Sn, from powder data [van	(Å) b	т		hk 0		2
Vucht, 1966].				100%		$\lambda = 1.$
Atom positions	5.54		_			
2(c) 1 thorium and 1 uranium	5.50	35	1	0	0	15
6(h) $6$ aluminum with $x = 0.957$	3.55	100	1	0	1	25
O(n) = O(n) +	3.21	50	1	1	0	27
From geometric considerations, the atomic	2.78	20	2	0	0	32
by Murray [1956], slightly modified.	2.38	65	2	0	1	37
	2.30	15	0	0	2	39
Lattice constants	2.13	5	1	0	2	42
a = 6.43 Å	2.10	10	2	1	0	42
c = 4.61 [van Vucht, 1966]	1.91	25	2	1	1	47
(	1.87	20	1	1	2	48
c/a = 0.11/0	1 96	1.0	_	_	_	
Volume	1.00	10	3	0	0	49
	1.78	10	2	0	2	51
103.1 A	1.61	10	2	2	0	57
	1.55	5	2	1	2	59
(calculated) 6.36 g/cm <sup>3</sup>	1.54	1	З	1	0	59
(,,,,,	1.48	5	1	0	з	62
Thermal parameters	1.46	15	3	1	1	63
Isotropic: aluminum B = 1.0; thorium, uranium	1.45	5	3	ō	2	64
B = 0.75	1.39	1	4	ō	0	67
	1.35	10	2	0	З	69
Scattering factors	1 77	-				
MI / MI / O (INCOINCEIONAI TADICS, 1902)	1.33	5	4	0	1	70
Scale factor (integrated intensities)	1.00	10	2	2	2	71
$x = 1.042 \times 10^{-3}$	1.20	1	3	1	2	73
γ - 1.043 X 10	1.24	5	2	1	3	76
References	1.623	5	3	2	1	77
International Tables for X-ray Crystallography	1.22	5	4	1	0	78
III (1962). (The Kynoch Press, Birmingham,	1.19	1	4	0	2	80
Eng.) pp. 202, 212.	1.15	1	0	õ	4	83
Murray, J.R. (1956). J. Inst. Metals 84, 1663.	1.11	1	5	ō	0	87
van Vucht, J. H. N. (1966). J. Less-Common	1.09	5	3	1	3	90
Metals <u>11</u> , 308).	1 0.9	-				
	1.00	5	-	1	4	90
	1.07	5	5		1	90
	1.07	5		-	2	91
	1.06	1	2	0	4	91
	1.05	1	4	2	0	94
	1.03	5	4	0	3	96
	1.03	5	4	2	1	97
	1.01	1	2	1	4	99
	1.00	1	5	0	2	100
	1.00	1	5	1	0	100
	•982	5	З	2	З	103
	•979	5	З	0	4	103
	•977	5	5	1	1	104
	•972	1	З	З	2	104
	.957	1	4	2	2	107
	.937	5	2	2	4	110
		-	_	-	-	110

l (A)	I		hkl		20(°)
					λ = 1.540598A
5.56	35	1	0	0	15.92
8.55	100	1	Ō	1	25.06
.21	50	1	1	0	27.74
•78	20	2	0	0	32.12
2.38	65	2	0	1	37.72
2.30	15	0	0	2	39.06
•13	5	1	0	2	42.42
2.10	10	2	1	0	42.94
•91	25	2	1	1	47.46
.87	20	1	1	2	48.56
.86	10	З	0	0	49.04
•78	10	2	0	2	51.42
•61	10	2	2	0	57.26
•55	5	2	1	2	59.42
•54	1	3	1	0	59.84
.48	5	1	0	з	62.66
•46	15	З	1	1	63.48
•45	5	З	0	2	64.40
•39	1	4	0	0	67.20
.35	10	2	0	З	69.86
•33	5	4	0	1	70.62
•32	10	2	2	2	71.50
•28	1	З	1	2	73.80
•24	5	2	1	3	76.74
•23	5	3	2	1	77.46
•22	5	4	1	0	78.68
•19	1	4	0	2	80.54
•15	1	0	0	4	83.88
•11	1	5	0	0	87.52
•09	5	3	1	3	90.00
•08	5	1	1	4	90.48
•08	5	5	0	1	90.74
•07	5	4	1	2	91.56
•07	5	3	З	0	91.86
•06	1	2	0	4	92.66
•05	1	4	2	0	94 • 10
•03	5	4	0	З	96.60
•03	5	4	2	1	97.32
•01	1	2	1	4	99.28
•00	1	5	0	2	100.38
•00	1	5	1	0	100.74
.982	5	3	2	3	103.28
•979	5	3	0	4	103.76
•9// 072	5	5	1	1	104.02
2	*	3	3	2	104.88
957	1	4	2	2	107.16
.937	5	2	2	4	110.66
928	1	6	0	0	112.20
019	1	3	1	4	113.02
910	1	5	1	2	114.18

Aluminum Thorium Uranium, Al<sub>6</sub>ThU - (continued)

d (Å)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
.915	1	4	З	0	114.60
.910	1	1	0	5	115.74
.902	1	5	0	З	117.34
.898	1	4	З	1	118.16
.892	1	5	2	0	119.50
.888	1	4	0	4	120.38
.875	5	2	0	5	123.30
.868	5	4	2	З	125.04
.861	1	6	0	2	126.94
.851	1	4	З	2	129.74

d (Å)	I	1	hkl		$2\Theta(^{\circ})$ , $\lambda = 1.540598A$
1.22	5	4	1	0	78.68
1.19	1	4	0	2	80.54
1.15	1	0	0	4	83.88
1.13	1	1	0	4	86.08
1.12	1	3	2	2	87.16
1 • 1 1	1	5	0	0	87.52
1.09	5	3	1	З	90.00
1.08	5	1	1	4	90.47
1.08	1	5	0	1	90.72
1.07	5	4	1	2	91.55
1.07	1	З	3	0	91.91
1.06	1	2	0	4	92.67
1.05	1	4	2	0	94.10
1.03	5	4	0	3	96.60
1.03	5	4	2	1	97.32
1.01	1	2	1	4	99.28
1.00	1	5	0	2	100.38
1.00	1	5	1	0	100.74
•982	5	3	2	3	103.28
•979	5	3	0	4	103.76
.977	5	5	1	1	104.02
.972	5	З	З	2	104.87
.957	1	4	2	2	107.15
.937	5	2	2	4	110.65
•928	1	6	0	0	112.19
.924	1	з	1	4	113.01
.917	1	5	1	2	114 • 19
•915	1	4	З	0	114.58
.910	1	1	0	5	115.74
.902	1	5	0	3	117.34
•898	5	4	з	1	118.15
.892	5	5	2	0	119.51
.888	1	4	0	4	120.38
.875	5	2	0	5	123.30
.868	5	4	2	3	125.04
.861	5	6	0	2	126.95
.851	5	4	3	2	129.75
	Ŭ	•		-	

	Calculated	Pattern	(Int	egr	ated)
å (A)	I		hkl		$20(^{\circ})$ $\lambda = 1.540598 ^{\circ}$
5.57	35	1	0	0	15.90
3.55	100	1	0	1	25.06
3.22	50	1	1	0	27.73
2.78	20	2	0	0	32.12
2.38	75	2	0	1	37.71
2.31	15	0	0	2	39.05
2.13	5	1	0	2	42.41
2.10	10	2	1	0	42.94
1.91	30	2	1	1	47.45
1.87	20	1	1	2	48.56
1.86	10	3	0	0	49.04
1.78	10	2	0	2	51.42
1.61	15	2	2	0	57.27
1.55	10	2	1	2	59.42
1.54	5	3	1	0	59.84
1.48	5	1	0	з	62.67
1.46	15	3	1	1	63.47
1.45	10	3	0	2	64.39
1.39	1	4	0	0	67 • 19
1.35	10	2	0	3	69.86
1.33	10	4	0	1	70.62
1.32	10	2	2	2	71.49
1.28	5	3	1	2	73.79
1.24	5	2,	1	З	76.73
1.23	10	3	2	1	77.47

Structure Heyagonal $P6_{2}(173)$ $T = 2$ probably isostructural	Calculated Pattern (Peak heights)				
with MoAl <sub>5</sub> ; the structure was determined by Adam and Rich [1955]. Previous work [Clark, 1940] had indicated a formula $Al_9W_2$ .	d (Å)	I	h	<b>c</b> l	20(°) 。 λ = 1.540598A
Atom positions	4.427	33	0	0 3	20.04
2(b) 2 tungsten	4 247	22			20.04
2(b) 2 aluminum(1)	4+243	22	1	0 0	20.92
2(a) 2 aluminum(2)	3.8276	100	1	0 1	23.22
6(c) 6 aluminum(3) [ibid]	3.0641	18	1	0 2	2 29.12
	2.4507	30	1	1 (	30+04
Lattice constants	2.4238	28	1	0 3	37.06
a = 4.9023(3) A	2.3624		;	1 1	39.06
c = 8.8576(5)	2.2140	10	â		40.72
	2.1446	76	1	1 2	40.12
c/a = 1.8068	2.1234	5	2	0 0	42.54
(a)			-		
(published values: $a = 4.9020(3)$ A, $c = 8.8570(5)$	2.0643	16	2	0 1	43.82
[Adam and Rich, 1955]).	1.9634	5	1	0 4	46.20
	1.9141	4	2	0 2	47.46
Volume	1.8857	3	1	1 3	48.22
184.35 A <sup>3</sup>	1.7233	9	2	0 3	53.10
Densitu			-		
(a a b a b a b a b) = 742 a (a a 3)	1.6429	15	1	1 4	55.92
(calculated) 5.742 g/cm <sup>2</sup> (maximum d) 5.5 $\pi$ (m <sup>3</sup> [ldem and Disk 1055]	1.6349	9	1	0 9	5 56.22
(measured) 5.5 g/cm <sup>3</sup> [Adam and Rich, 1955]	1.6046	2	2	1 0	+ 57.38
	1.5789	13	1	2 1	+ 58.40
Thermal parameters	1.5323	2	2	0 4	60.36
Isotropic: aluminum $B = 1.0$ ; tungsten $B = 0.5$			_	-	
Scattering factors	1.5088	4	2	1 2	2+ 61.40
Al <sup>0</sup> W <sup>0</sup> [International Tables 1962]	1.4764	1	0	0 6	62.90
AL, W [International Tables, 1902]	1.4356	1	1	1 5	64.90
	1.4151	11	3	0 (	65.96
Scale factors (integrated intensities) $\gamma = 1.129 \times 10^{-3}$	1.4102	10	1	2 3	66.22
I/I (calculated) 8.47	1.3945	1	1	0 6	67.06
	1.3600	4	2	0 5	5 69.00
References	1.3480	5	3	0 2	69.70
Adam, J. and Rich, J. B. (1955). Acta Crystallogr.	1.2993	2	2	1 4	+ 72.72
<u>8</u> , 349. Clark, W. D. (1940). J. Inst. Metals <u>66</u> , 271.	1.2645	10	1	1 6	75.06
International Tables for X-ray Crystallography,	1.2256	з	2	2 (	77.88
III (1962). (The Kynoch Press, Birmingham, Eng.)	1.2126	3	1	0 7	78.88
pp. 202, 212.	1,1924	11	• ٦	0	80.48
	1,1895	10	1	2 6	5+ 80.72
	1.1813	8	2	2 2	2 81.40
	1.1671	4	3	1 1	+ 82.60
	1.1380	1	1	3 2	2+ 85.20
	1.1073	1	0	0 8	88.16
	1.0938	4	3	1 3	89.54
	1.0867	3	2	0 7	7+ 90.28
				_	
	1.0723	3	2	2 4	91.84
	1.0338	2	3 4	2 4	95.94
	1.0396	1	ε.	5 4	95.62
	1.0216	2	23	0 6	97.88
	1.0090	3	٤	1 5	99.54
	.9989	1	4	0 3	3 100.92
	•9936	3	, 1	2 7	+ 101.66
	.9806	3	3	1 9	5+ 103.54
	•9681	3	2	3 1	+ 105.44
	.9587	1	1	0 9	106.92
Aluminum	Tungsten,	Al <sub>5</sub> W,	δ-phase	-	(continued)
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Cal	culated Pa	ttern	(Int	egr	ated)
d(A)	I	]	hkl		20(°) 。
					$\lambda = 1.540598A$
4.420	71	0	0	2	20.03
4.246	21	1	õ	2	20.91
3.8285	100	1	õ	1	23.21
3.0648	19	- 1	ō	2	29.11
2.4512	33	1	1	0	36.63
2.4240	30	1	0	з	37.06
2.3624	7	1	1	1	38.06
2.2144	21	0	0	4	40.71
2.1446	87	1	1	2	42.10
2.1228	3	2	0	0	42.55
2.0643	19	2	0	1	43.82
1.9634	5	1	0	4	46.20
1.9142	5	2	0	2	47.46
1.8859	3	1	1	3	48.21
1.7235	11	2	0	3	53.09
1.6432	18	1	1	4	55.91
1.6349	9	1	0	5	56.22
1.6047	1	2	1	0	57.38
1.6047	1	1	2	0	57.38
1.5790	8	2	1	1	58.40
1.5790	8	1	2	1	58.40
1.5324	2	2	0	4	60.35
1.5087	2	2	1	2	61.40
1.5087	2	1	2	2	61.40
1.4763	1	0	0	6	62.90
1.4358	1	1	1	5	64.89
1.4152	13	3	0	0	65.96
1.4099	5	2	1	З	66.23
1.4099	5	1	2	3	66.23
1.3944	2	1	0	6	67.07
1.3601	5	2	0	5	68.99
1.3480	6	3	0	2	69.70
1.2994	1	2	1	4	72.72
1.2994	1	1	2	4	72.72
1.2646	14	1	1	0	/5.05
1.2256	3	2	2	0	77.88
1.2127	3	1	0	7	78.87
1.2120	1	2	0	6	78.92
1.1925	14	3	0	4	80.48
1.1893	3	2	T	5	80.74
1.1893	3	1	2	5	80.74
1.1812	11	2	2	2	81.41
1.1672	3	3	1 7	1	82.59
1.1380	1	3	1	2	85.21
1 1 7 6 6			-	-	
1.1070	1	1	3	2	85.21
1.0037	2	0	1	7	80.54
1.0937	2	1	3	7	89.54
1.0869	2	2	Q	7	90.26
	-	-			20020

d (Å)	I	ł	nkl		20(°) $\lambda = 1.540598 \text{\AA}$
1.0864	1	2	1	6	90.31
1.0864	1	1	2	6	90.31
1.0723	4	2	2	4	91.84
1.0714	1	1	0	8	91.94
1.0538	2	4	0	1	93.93
1.0397	1	3	1	4	95.62
1.0397	1	1	3	4	95.62
1.0322	1	4	0	2	96.54
1.0216	3	3	0	6	97.88
1.0090	4	1	1	8	99.53
•9988	2	4	0	з	100.93
•9936	2	1	2	7	101.66
•9936	2	2	1	7	101.66
.9806	2	3	1	5	103.54
•9806	2	1	З	5	103.54
•9682	2	з	2	1	105.43
•9682	2	2	З	1	105.43
.9588	2	1	0	9	106.92

Aluminum Vanadium, Al<sub>10</sub>V

(Peak heights)

20(°)

 $\lambda = 1.540598A$ 

10.58

17.30

20.32

21.22

24.56

26.80

30.20

32.08

35.00

36.66

37.20

39.28

40.80

41.30

43.22

44.62

46.88

51.58

53.62

54.82

55.20

56.78

57.92

58.30

62.76

63.86

65.64

67.06

69.50

69.84

71.22

73.92

74.94

75.26

76.60

77.60

79.26

80.24

81.88

84.48

85.46

85.78

87.08

88.06

88.38

89.68

90.64

95.84

97.46

98.44

0

hkl

1 1

2 0

1 1

2 2

0 0

З

2

1 1

4 0

3 1

4 2

2 0

з з

2 2

4 4

1

4 2

3 3

2

5 5+

6 2

4 0

5

4 2

4

З

2 0

2

5 3

6 4

4

8 0

5 5+

4 4

6 6

3 3

8

7

2

4

9 1

4 2

8 2

5 5+

6 6

4 4 3 1+

5

8 6+

5

1+

3+

1+

2+

3+

4

3+

2+

2

4+ 7+

2+

0

.

1

Structure	Calc	culated Pa	ttern
Cubic, Fd3m(227), $Z = 16$ , isostructural with Mg <sub>3</sub> Cr <sub>2</sub> Al <sub>18</sub> [Brown, 1957]. The phase exists over a range of composition from Al <sub>10</sub> V to Al <sub>10,25</sub> V [Ray and Smith, 1957].	d (Å)	I	
Atom positions	8.355	100	1
Atom positions $06(\alpha) = 06(\alpha)$	5.122	12	2
90(g) 90 aluminum 49(f) 49 aluminum	4.367	4	з
48(1) 46 aluminum	4.184	9	2
l6(c) l6 vanadium [Brown, 1957]	3.622	12	4
Lattice constant	3.324	12	з
a = 14.493(4) Å	2.957	'9	4
a 11.195(1) fr	2.788	1	5
(published value: 14.492(4) A (Ray and Smith.	2.562	13	4
1957])	2.449	31	5
Volume	2.415	15	4
3044-2 A <sup>3</sup>	2.292	19	6
	2.210	62	5
Density	2.184	99	6
(calculated) 2.799 g/cm <sup>3</sup>	2.092	37	4
$(measured)$ 2.79(5) $q/cm^3$ [Brown, 1957]			
	2.029	55	7
Thermal parameters	1.936	5	6
Isotropic: aluminum B = 1.0; vanadium B = 0.5.	1.771	2	7
	1.708	9	8
Scattering factors	1.673	3	5
Al', V' [International Tables, 1962]	1.663	1	6
Scale factor (integrated intensities)	1.620	7	8
$v = 0.352 \times 10^{-3}$	1.591	7	7
1 0.002 0 10	1.581	2	8
References	1.479	З	8
Brown, P. J. (1957). Acta Crystallogr. <u>10</u> , 133.	1 450		~
International Tables for X-ray Crystallography,	1.421	4	10
III (1962). (The Kynoch Press, Birmingham,	1.3045	10	10
Eng.) pp. 202, 204.	1.3514	2	Q
Ray, A. E. and Smith, J. F. (1957). Acta Crys- tallogr. 10, 604.	1.3457	1	8
· <u> </u>	1.3229	6	10
	1.2811	26	8
	1.2662	5	9
	1.2616	5	10
	1.2429	2	8
	1.2293	11	11
	1.2077	2	8
	1.1954	5	7
	1.1755	2	12
	1.1459	2	12
	1.1352	1	9
	1.1318	1	12
	1.1182	2	10
	1.1083	З	11
	1.1051	7	10
	1.0924	7	12
	1.0833	5	13
	1.0378	1	13
	1.0249	2	10
	1.0173	2	13

Aluminum Vanadium,  $Al_{10}V$  - (continued)

	Calculated	Pattern	(Int	egr	ated)
d (Å)	I		hkl		20(°) 。
					$\lambda = 1.540598A$
8.368	79	1	1	1	10.56
5.124	10	2	2	ō	17.29
4.370	3	3	1	1	20.31
4.184	8	2	2	2	21.22
3.623	10	4	0	0	24.55
7 7 05		7	-		06 70
3.325	11	3	3	1	26.79
2.700		4	2	2	30.19
2.562	13	4	4	Â	34.00
2.450	30	5	3	1	36.65
2.416	14	4	4	2	37.19
2.292	19	6	2	0	39.28
2.210	60	5	3	3	40.79
2.185	100	6	2	2	41.29
2.092	37	4	4	4	43+21
2.029	35	7	1	1	44.61
2.029	22	5	5	1	44.61
1.937	5	6	4	2	46.87
1.771	2	7	З	З	51.58
1.708	4	6	6	0	53.61
1.708	5	8	2	2	53.61
1.674	1	7	5	1	54.81
1.674	2	5	5	5	54.81
1.662	1	6	6	2	55.21
1.620	8	8	4	0	56.77
1.591	1	9	1	1	57.92
1.591	7	7	5	З	57.92
1.581	2	8	4	2	58.30
1.479	З	8	4	4	62.77
1.457	4	9	3	3	63.85
1.457	1	7	5	5	63.85
1.421	2	10	2	0	65.64
1.394	6 15	10	2	2	67.06
1.394	6 7	6	6	6	67.06
1.351	5 2	9	5	3	69.50
1.345	6 1	8	6	4	69.84
1.323	0 7	10	4	2	71.21
1.281	0 31	8	8	0	73.93
1.266	32	11	З	1	74.94
1.266	3 1	9	7	1	74.94
1.266	3 3	9	5	5	74.94
1.261	5 5	10	4	4	75.27
1.242	8 2	8	6	6	76.61
1.229	3 13	11	З	з	77.60
1.224	9 1	10	6	2	77.93
1.207	8 2	8	8	4	79.26
1.195	4 1	11	5	1	80.24
1.195	4 4	7	7	7	80.24
1.175	5 2	12	2	2	81.88
1.145	8 3	12	4	0	84.49

d (Å)	I	1	nkl		$2\theta (°)$ $\lambda = 1.540598A$
					05.44
1.1352	1	9	9	1	85.40
1.1317	1	12	4	2	85.79
1.1182	2	10	8	2	87.09
1.1083	3	11	5	5	88.06
1.1051	7	10	6	6	88.38
1.0925	8	12	4	4	89.68
1.0833	4	13	З	1	90.65
1.0833	З	9	7	7	90.65
1.0684	1	12	6	2	92.27
1.0379	1	13	5	1	95.84
1.0248	1	14	2	0	97.47
1.0248	1	10	8	6	97.47
1.0172	1	13	5	З	98.45
1.0172	1	11	9	1	98.45
1.0147	1	10	10	2	98.78

Aluminum Vanadium, Al

З

6

5

13

12

13

1+

2

1+

20(°)

 $\lambda = 1.540598A$ 

10.56

17.28

20.28

21.20

24.52

26.76

30.14

34.94

36.60

37.14

39.22

40.72

41.22

43.14

44.54 46.80

51.48

51.90

53.52

54.72

56.66

57.82

58.20

59.70

60.82

62.66

63.74

65.52

66.94

69.36

69.70

71.08

73.78

74.80

75.12

76.46

77.46

79.10

80.08 81.72

84.32

85.30 85.60

86.90

87.88

88.20

89.48

90.46

92.08

95.62

0

Structure	Cal	culated Pa	attern	(Pea	k hei	ghts)
Cubic, $Fd3m(227)$ , Z = 16. The phase exists over the range from $Al_{10}V$ to $Al_{10.25}V$ [Ray and Smith, 1957; Brown, 1957].	å (Å)	I		hkl	λ	2 = 1.
Atom positions						
96(q) 96 aluminum	8.371	68	1	1	1	10
48(f) 48 aluminum	5.128	4	2	2	0	17
16(d) 16 aluminum	4.375	9	3	1	1	20
8(b) 4 aluminum	4.188	9	2	2	2	21
16(c) 16 vanadium	3.628	6	4	0	0	24
The R(h) site is 50% occupied (Pay and Smith	3.329	8	з	3	1	26
Ine 8(b) Site is 50% occupied [Ray and Smith,	2.963	5	4	2	2	30
1957].	2.566	16	4	4	0	34
	2.453	37	5	-	1	36
Lattice constant	2.410	10	5	~	2	37
a = 14.517 A	2.419	14	*	4	2	51
(published value: 14.516 A [Ray and Smith, 1957])	2.295	24	6	2	0	39
	2.214	68	5	3	3	40
Volume	2.188	100	6	2	2	41
3059.4 A <sup>3</sup>	2.095	34	4	4	4	43
	2.033	50	7	1	1+	44
Density (calculated) 2 844 g/cm <sup>3</sup>	1.940	з	6	4	2	46
(caroaracca, brown g, cm	1.774	з	7	З	3	51
Thermal naramaters	1.760	1	6	4	4	51
Isotropic. [Pay and Smith 1957]	1.711	11	8	2	2+	53
isotiopic. (May and Smith, 1957].	1.676	З	5	5	5	54
Scattering factors	1.623	6	А	4	0	56
Al°, V° [International Tables, 1962]	1.503	6	7	5	34	57
	1.584	2	8	4	2	54
Scale factors (integrated intensities)	1.548	1	6	6	<u>د</u>	50
$\gamma = 0.360 \times 10^{-3}$ I/I (calculated) = 1.74	1.522	1	9	3	1	60
	1.481	з	8	4	4	62
Additional pattern	1.459	6	q	3	3+	63
1. PDF card /-281 [Carlson, et al., 1955].	1.424	. 3	10	2	0+	65
It appears to be this phase but is labelled	1.397	19	10	2	2+	66
ALIIV.	1.354	2	9	5	3	69
References	1.348	,	R	6	٨	60
Brown, P. J. (1957). Acta Crystallogr. <u>10</u> , 133.	1.325	6	10	۵	2	71
Carlson, O. N. Kenny, D. J. and Wilhelm, H. A.	1.283	30		A	0	73
(1955). Trans. Amer. Soc. Metals <u>47</u> , 520.	1.268	6	ő	5	5+	74
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham,	1.264	5	10	4	4	75
Eng.) pp. 202, 204.	1.245	2	8	6	6	76
Ray, A. E. and Smith, J. F. (1957). Acta Crys-	1.231	14	11	З	з	77
tallogi. <u>10</u> , 604.	1.210	1	8	8	4+	79
	1.1974	5	7	7	7+	80
	1.1774	1	12	2	2+	81
	1.1476	3	12	4	0	84
	1.1369	1	9	9	1	85
	1.1337	1	12	4	2	85
	1.1201	2	10	8	2	86
	1.1101	5	11	5	5+	87
	1.1069	8	10	6	6	85
	1.0943	7	12	4	4	89

1.0850

1.0701

1.0396

6

1

Aluminum Vanadium,	A1 <sub>10,25</sub> V	-	(continued)	
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	Calculated	Pattern	(Int	egr	ated	)
d (Å)	I		hkl		λ =	20(°) 1.540598Å
8.381	54	1	1	1		10.55
5.133	4	2	2	0		17.26
4.377	8	3	1	1		20.27
4.191	8	2	2	2		21.18
3.629	) 6	4	0	0		24.51
3.330	8	З	з	1		26.75
2.963	5	4	2	2		30.13
2.566	16	4	4	0		34.93
2.454	30	5	3	-		30.59
2.419	9 14	4	4	2		37.13
2.295	24	6	2	0		39.22
2.190		5	2	2		40.12
2.005		4	<u>د</u>	2		41.22
2.033	19	5	5	1		44.54
2.033	32	7	1.	1		44.54
1.940	3	6	4	2		46.79
1.774	3	7	з	З		51.49
1.760	1	6	4	4		51.90
1.711	6	6	6	0		53.52
1.711	7	8	2	2		53.52
1.676	3	5	5	5		54.71
1.623	5 7	. 8	4	0		56.67
1.593	5 1	9	1	1		57.82
1.593	6	7	5	3		57.82
1.584	2	8	4	2		58.20
1.548	1	6	6	4		59.70
1.522	2 2	9	ک	1		60.82
1.482	2 4 \ E	8	4	4		67 74
1.409	. 5	9	3	3		03.14
1.459		7	5	5		63.74
1.424	- 15	10	2	0		65.52
1 307	10	10	2	2		66 07
1.354	2	9	5	3		69.36
1.348	3 1	8	6	4		69.71
1.325	5 6	10	4	2		71.08
1.283	3 36	8	8	0		73.79
1.268	3 1	9	7	1		74.79
1.268	3 2	11	3	1		74.79
1.268	3 3	9	5	5		74.79
1.264	5	10	4	4		75.13
1.245	3	8	6	6		76.46
1.231	16	11	З	3		77.45
1.227	1	10	6	2		77.78
1.210	) 1	8	8	4		79.10
1.197	73 1	11	5	1		80.08
1.197	73 5	7	7	7		80.08
1.177	75 1	12	2	2		81.72
1.147	77 3	12	4	0		84.32

å (Å)	I		hkl		$20(^{\circ})$ $\lambda = 1.540598 ^{\circ}$
1.1371	1	9	9	1	85.29
1.1336	1	12	4	2	85.61
1.1200	2	10	8	2	86.91
1.1101	4	11	5	5	87.88
1.1069	8	10	6	6	88.20
1.0943	8	12	4	4	89.49
1.0851	4	13	З	1	90.46
1.0851	з	9	7	7	90.46
1.0702	1	12	6	2	92.07
1.0396	1	13	5	1	95.63

Structure	Cal	culated Pat	ttern	(Pea	k hei	ghts)
Hexagonal, $P6_{3}/mmc(194)$ , $Z = 2$ . The structure was determined by Smith and Ray [1957] and re- fined by Ray and Smith [1960].	d (Å)	I	]	nkl	λ	20(°) ° = 1.540598A
Atom positions	8.515	33	0	0	2	10.38
2(a) 2 vanadium(1)	6.662	7	1	õ	0	13.28
6(h) 6 vanadium(2)	6.197	35	1	0	1	14.28
12(k) 12 aluminum(1)	5.248	23	1	ō	2	16.88
12(k) 12 aluminum(2)	4.321	15	1	0	3	20.54
12(k) 12 aluminum(3)		• •		-	-	
6(h) 6 aluminum(4)	4.259	11	0	0	4	20.84
4(f) 4 aluminum(5) [Ray and Smith, 1960].	3.844	1	1	1	0	23.12
	3.587	3	1	0	4	24.80
Lattice constants	3.504	12	1	1	2	25.40
*a = 7.6933 Å *c = 17.041	3.331	4	2	0	0	26.74
0 1/10/1	7.060	-	~	~	•	07 06
c/a = 2.2150	3.209		2	0	1	27.020
-,	3.034	1	1	0	5	29.42
*published values: $a = 7.6928$ Å, $c = 17.040$	2.873	1	2	0	3	31.10
[Ray and Smith, 1960].	2.024	4	2		1	34.14
	2.518	9	2	T	0	35.62
Volume	2.491	19	2	1	1	36.02
873.48 A <sup>3</sup>	2.415	11	2	1	2	37.20
Lange and the second	2.382	6	2	0	5	37.74
Density	2.302	37	2	1	3	39.10
(calculated) 3.134 g/cm <sup>3</sup>	2.286	48	1	0	7	39.38
Thermal parameters	2.220	19	٦	0	0	40.60
<pre>Isotropic: vanadium(1): B = 0.49; vanadium(2):</pre>	2.202	27	7	ŏ	1	40.96
B = 0.57; aluminum(1): $B = 1.14$ ; aluminum(2):	2.167	100	2	1	Å	41.64
B = 0.82; aluminum(3): $B = 0.87$ ; aluminum(4):	2.162	100	2	â	6	41.74
B = 0.74; aluminum(5): $B = 0.81$ .	2.130	18	0	ŏ	8	42.40
Costtoring factors			_		_	
Al <sup>0</sup> V <sup>0</sup> [International Tables 1962] corrected	2.068	68	3	0	3	43.74
for dispersion [Cromer and Liberman 1970]	2.025	33	2	1	5	44.72
for dispersion [eromer and discriman, 1970].	1.966	12	2	0	~	40.14
Scale factors (integrated intensitions)	1.923	17	2	2	0	47.22
$\gamma = 0.410 \times 10^{-3}$	1.863	2	1	T	8+	40.04
$I/I_{corundum}$ (calculated) = 2.42	1.837	2	З	1	1	49.58
corunaum	1.806	1	З	1	2	50.50
Additional pattern	1.795	9	2	0	8	50.84
1. PDF card 7-359 [Carlson et al., 1955]. It	1.757	1	З	1	3	52.00
is called $Al_6V$ , $\beta$ -phase, and is the phase described above	1.750	2	3	0	6+	52.24
	1.704	2	0	0	10	53.74
References	1.696	1	3	1	4	54.04
Carlson, O. N., Kenny, D.J., and Wilhelm, H. A.	1.665	1	4	0	0	55.10
(1955). Trans. Amer. Soc. Metals 47, 520.	1.651	3	1	0	10	55.62
International Tables for X-ray Crystallography,	1.641	3	З	0	7	56.00
Eng.) pp. 202. 204.	1.626	7	2	1	8	56.54
Ray, A. E. and Smith. J. F. (1960). Acta Crys-	1.509	1	4	0	3	57-62
tallogr. 13. 876.	1.559		1	1	10	59.26
Smith, J. F. and Rav. A. E. (1957). Acta Crys-	1.555	0	4	ò	4	59.56
tallogr. <u>10</u> , 169.	1.549	10	3	1	6	59.64
	1 476		-	2	7	62.92
	1.470	4	3	2	0	63-98
	1.454	2	4	1	1	64 . 18
	1 430	1	4		64	64.84
	1 437	2	4	1	2	65-02
	1.433	2	-	•	-	00.02

Aluminum Vanadium,  $Al_{23}V_4$  - (continued)

d (Å)	I	hkl 20( $\lambda = 1.54$	°) 0598Å
1.427	4	2 2 8 65.3	2
1•420	1	0 0 12 65.7	0
1.408	4	4 1 3 66.3	32
1.395	2	3 2 5+ 67.0	4
1.352	5	3 0 1 0 69.4	6
1.346	2	3 2 6 69.6	2
1.328	3	5 0 1 70.8	8
1.319	3	2 1 11 71.4	4
1.317	3	5 0 2 71.6	2
1.306	3	2 0 12 72.2	6
1.297	7	5 0 3 72.8	6
1.294	22	3 2 7 73.0	4
1.282	22	3 3 0 73.8	4
1.271	30	3 0 11+ 74.6	4
1.256	1	4 2 1 75.6	8

C	Calculated	Pattern	(Int	egr	ated)
d (Å)	I		hkl		$2\Theta(\circ)$ $\lambda = 1.540598A$
0.500					
0.520	28	0	0	2	10.37
0.003	6	1	0	0	13.28
5.205	30	1	0	-	14.20
5.249	21	1	0	2	10.68
4+323	14	1	0	3	20.53
4.260	10	0	0	4	20.83
3.847	1	1	1	0	23.10
3.589	2	1	0	4	24.79
3.506	12	1	1	2	25.38
3.331	4	2	0	0	26.74
3.269	7	2	0	1	27.25
3.034	1	1	0	5	29.41
2.874	1	2	0	З	31.10
2.624	4	2	0	4	34 . 14
2.613	1	1	0	6	34.29
2.518	9	2	1	0	35.62
2.491	19	2	1	1	36.02
2.415	11	2	1	2	37.20
2.382	5	2	0	5	37.73
2.302	36	2	1	3	39.10
2.287	48	1	0	7	39.37
2.285	1	1	1	6	39.40
2.221	18	3	0	0	40.59
2.202	27	з	0	1	40.95
2.168	100	2	1	4	41.63
2.161	41	2	0	6	41.76
2.149	11	3	0	2	42.01
2.130	18	0	ő	8	42.40
2.068	74	3	ō	3	43.73
2.029	9	1	ō	8	44.62

d (Å)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
2.025	71	2	1	5	44.71
1 040	31	2	â	4	44.05
1.909	13	3	0	-	40.05
1.023	13	2	2	6	40.13
1.923	19	2	2	0	4/022
1.603	2	•	•	0	40.03
1.861	1	3	0	5	48.91
1.837	2	3	1	1	49.58
1.806	1	З	1	2	50.50
1.795	10	2	0	8	50.84
1.757	1	3	1	3	52.00
1.750	2	з	0	6	52.25
1.704	2	0	0	10	53.75
1.695	1	З	1	4	54.05
1.666	1	4	0	0	55.09
1.651	3	1	0	10	55.62
1.641	з	3	0	7	56.00
1.626	3	2	1	8	56.54
1.598	1	4	0	3	57.62
1.558	2	1	1	10	59.26
1.551	8	4	0	4	59.54
1.549	8	З	1	6	59.65
1.476	5	З	2	3	62.92
1.472	1	3	1	7	63.11
1.454	2	4	1	0	63.99
1.449	1	4	1	1	64.25
1 .4 37	1	4	0	6	64.84
1.433	1	4	1	2	65.02
1.428	5	2	2	8	65.31
1.420	1	0	0	12	65.70
1.411	1	2	1	10	66.16
1.408	4	4	1	3	66.31
1.396	1	3	1	8	66.99
1.395	2	З	2	5	67.05
1.352	6	3	0	10	69.47
1.346	2	3	2	6	69.82
1.328	3	5	0	1	70.88
1.319	З	2	1	11	71.43
1.317	2	5	0	2	71.62
1.306	4	2	0	12	72.27
1.297	5	5	0	3	72.85
1.294	24	з	2	7	73.03
1.282	27	З	З	0	73.85
1.272	14	5	0	4	74.56
1.271	31	З	0	11	74.64
1.268	1	З	3	2	74.82

Monoclini	.c, $C2/m$ (12), $Z = 2$ . The structure was	Cal	culated P	attern	(Pea	ak hei	ights)
determine	ed by Brown [1959].		т				20(0)
Atom positi	ons	U(A)	1		117.2	λ	= 1.540598A
2(a)	2 vanadium(0)						
2(d)	2 aluminum(0)						
4(i)	4 vanadium(1)	10.59	33	-2	0	1	8.34
4(i)	4 each of aluminum(3), $(4)$ , $(5)$	9.95	8	2	0	0	8.88
0(-1)	(6), (7), (8), (9), and (10)	8.61	2	0	0	1	10.26
8()	8 each of aluminum(11), $(12)$ , $(13)$	6.79	2	- 1	1	0	12.44
	[ibid]	0.30	19	-+	v	+	13.00
		6.21	70	-1	1	1	14.24
Lattice con	stants 。	5.37	1	-2	0	2	16.50
a = 25.6	605(14) A	5.30	2	-4	0	2	16.72
b = 7.6	5218 (18)	5.12	15	2	0	1	17.32
c = 11.0 $\beta = 128.9$	982 (12) 92 (3) °	4.968	8	1	1	1	17.84
p - 120.9	0	4.480	1	-3	1	2	19.80
(publishe	d values: a=25.604(14)A, b=7.6213(18),	4.308	11	0	0	2	20.60
c=11.081(	12), β=128° 55(2)' [Brown, 1959]).	4.188	23	-6	0	2+	21.20
	0	4.118	2	-1	1	2	21.56
CD cell: c = 11.08	a = 20.540(14)A, b = 7.6218(18), 32(12), $\beta$ = 104.10(3)°, sp. gp. I2/m;	4.074	2	-6	0	1	21.80
a/b = 2.6	949, c/b = 1.4540.	3.684	4	-4	0	З	24.14
		3.645	1	3	1	1	24.40
Volume	3	3.584	4	-2	2	1	24.82
1682.0 AS		3.559	2	2	2	0	25.00
Density		3.531	3	5	1	U	23.20
(calculat	(ed) $3.100 \text{ g/cm}^3$	3.469	2	4	0	1	25.66
(measured	l) 3.10(3) g/cm <sup>3</sup> [Brown, 1959]	3.383	3	-2	0	З	26.32
		3.368	4	1	1	2	26.44
Thermal par	ameters	3.307	5	6	0	0+	26.94
Isotropic	: aluminum B = 1.0; vanadium B = 0.5	3.274	2	-4	2	1	27.22
Scattering	factors	3.241	1	-3	1	з	27.50
A1 <sup>0</sup> , V <sup>0</sup> [	Cromer and Mann, 1968]	3.108	3	-2	2	2+	28.70
		3.040	5	-7	1	З	29.36
Scale facto	ors (integrated intensities)	2.932	1	-8	0	1	30.46
$\gamma = 0.078$	$16 \times 10^{-3}$	2.901	2	-1	1	3	30.80
I/I corund	(calculated) 0.45	2.873		0	0	٦	31.10
Peferences		2.820	3	-6	2	2	31.70
Brown, P.	J. (1959). Acta Crystallogr, 12, 995.	2.771	3	5	1	1	32.28
Cromer, D	T. and Mann, J.B. (1968). Acta Crystal-	2.695	11	3	1	2	33.22
logr. A	.24, 321.	2.650	5	-8	0	4+	33.80
		2.627	8	-9	1	З	34.10
		2.590	6	-6	2	3+	34.60
		2.566	5	4	2	1	34.94
		2.531	3	-2	2	3	35.44
		2.520	3	1	3	0	35.60
		2.504	14	-10	0	2+	35.84
		2.490	10	8	0	0	36.04
		2.485	8	2	2	2	36.12
		2.473	20	-1	З	1	36.30
		2.448	13	-2	0	4+	36.68
		2.390	23	2	0	3+	37.60
		2.368	13	1	3	1	37.96
		2.324	2	-8	2	1	38.72
		2.309	8	-3	3	2	38.98
		2.294	15	0	2	3	39.24

Aluminum Vanadium,  $Al_{45}V_7$ ,  $\alpha$ '-phase - (continued)

34.10

34.59

34.61

34.94

35.44

З

З

1 2 3

2 1 2

1 4

-9

-6

-5

4

-2

d (Å)	I		hkl		$2\Theta(^{\circ})$	Calc	culated Pa	ttern	(Int	egra	ted)
					- 1.540598A	d (Å)	I		hkl	;	2Θ(°) 。 λ = 1.540598A
2.281	10	-10	0	1	39.48				· · · · · · · · · · · · · · · · · · ·		
2.254	15	-1	З	2	39.96	10.60		- 2	~		0 77
2.244	40	-5	З	2	40.16	0.06	10	-2	0		0.33
2.226	54	-11	1	З	40.50	9.90	10	2	0		10.25
2.207	61	7	1	1+	40.86	7.12	2	1	1	0	12.42
						6.30	23	-4	•	ĭ	13.85
2.196	51	-4	2	4+	41.06	0.39	25	-+	Ŭ		13.05
2.175	37	-8	2	4	41.48	6.22	07	-1	1	1	14.23
2.167	52	3	З	1	41.64	5.37	1	-1	ò	2	16.48
2.155	29	0	0	4	41.88	5.30	• ٦	-4	õ	2	16.71
2.142	22	5	3	0	42.16	5.12	21		0	1	17.31
						5.01	5		ĩ	â	17.70
2.120	18	-10	0	5	42.62	5.01	5	5	*	v	1/6/0
2.099	40	-12	0	4+	43.06	4.080			0	0	17.90
2.092	58	-10	2	2	43.20	4.969	8	- T	,	ĭ	17.84
2.085	92	8	2	. 0+	43.36	4.481	2	-3	1	2	19.80
2.072	100	-3	3	3+	43.64	4.711	16	-5	ò	5	20.50
						4.198	21	-6	õ	2	21.15
2.070	98	<del>~</del> 5	1	5	43.70	40190	21	-0	v	٤.	21015
2.037	12	-12	0	2+	44.44	4.185	1.9	-5		1	21.21
2.025	23	2	2	3+	44.72	4.100	2	-5	-	•	21.55
2.004	3	4	0	З	45.22	4.077	2	-1		2	21.90
1.992	2	10	0	0	45.50	4.073	2	-0	0	-	21.00
						3.000	0		1	3	24.12
1.945	1	1	1	4	46.66	3.044	2	5			24040
1.932	2	5	З	1	47.00	7 5 96	e		~		24 01
1.906	9	0	4	0	47.68	3.500	6	-2	2	1	24.81
. 895	7	7	З	0	47.96	3.559	1	2	2	0	25.00
1.876	2	0	2	4+	48.48	3.531	3	5			25.20
						3.470	3	- 0	0	-	25.05
1.861	З	-12	0	1+	48.90	3.305	4	-2	0	3	20.30
1.853	З	-10	2	5	49.14	7 760	•			2	26.66
1.834	3	-10	0	6+	49.66	3.300	* =	1		2	20.44
1.824	2	9	1	1	49.96	3.320	5			-	20.03
1.814	1	-13	1	5	50.26	3.305	5	-5		3	20.90
						3.295	1	- /	-	2	27.04
1.806	3	-9	З	1+	50.50	3.273	٤		۲		21023
1.802	3	-14	0	З	50.60	7 242				-	27 40
1.796	3	-12	2	2+	50.80	3.242	1	-3		3	21.49
1.792	3	-6	0	6+	50.92	3.117	2	-7	-	-	20.02
1.780	1	4	4	0	51.28	3.109	4	-2	2	2	28.69
						3.05/	2	2	2	1	29.19
1.773	1	-14	0	5+	51.50	3.041		- /		3	29.35
1.766	1	10	2	0	51.72		_		~	•	
1.758	1	-11	1	6	51.98	3.027	3	4	2	0	29.49
1.743	З	-12	2	5	52.46	2.934	1	-8	0	1	30.45
1.725	1	0	0	5+	53.06	2.901	4	-1	1	3	30.80
						2.874	1	0	0	3	31.09
1.708	2	-14	0	2	53.62	2.822	5	-6	2	2	31.68
1.703	2	5	З	2	53.78		_		-		
.683	2	2	2	4+	54.46	2.783	3	-6	2	1	32.14
1.670	2	-7	З	5+	54.94	2.771	4	5	1	1	32.28
						2.696	18	3	1	2	33.20
						2.650	6	-8	0	4	33.80
						2.649	1	-4	2	3	33.80

2.627

2.591

2.589

2.566

2.531

12

5

4

6

З

Aluminum Vanadium,  $A1_{45}V_7$ ,  $\alpha'$ -phase - (continued)

0			11.0	-	20 (0)		т		hk0		20(0)
d (A)	I		nĸl		$\lambda = 1.540598A$	a (A)	I		117.2		$\lambda = 1.540598 \text{\AA}$
2.520	2	1	3	0	35.59	2.071	2	8	0	1	43.68
2.504	15	-10	0	2	35.83	2.069	66	-5	1	5	43.72
2.503	6	6	2	0	35.84	2.060	6	-2	2	4	43.92
2.490	10	8	0	0	36.04	2.039	7	-7	3	1	44.40
2.484	1	2	2	2	36.12	2.037	9	-12	0	2	44.45
2.470	,	1	1	٦	36.21		_				
2.472	31	-1	-	-	36.31	2.027	9	-10	2	4	44.68
2.440	11	-2	0	4	36.67	2.025	30	2	2	3	44.72
2.008	8	- 2	2	2	36.68	2.017	5	-7	3	3	44.91
2.445	1	-7	1	4	36.73	2.003	3	4	0	3	45.23
20000	•		•	1	30113	1.992	2	10	0	0	45.50
2.432	1	-3	з	1	36.94	1.045	1	1	1	4	46.65
2.403	7	-9	1	4	37.40	1.032		5	-	1	47.00
2.393	15	-10	0	4	37.55	1 013		-2	0	5	47.49
2.390	24	2	0	3	37.60	1.011	1	-8	2	5	47.54
2.386	1	-8	2	3	37.67	1.906	2	7	7	2	47.68
						1.900	2	5		-	
2.373	2	3	3	0	37.89	1.905	13	0	4	0	47.69
2.369	18	1	3	1	37.95	1.895	9	7	3	0	47.96
2.325	2	-8	2	1	38.70	1 • 877	1	2	0	4	48.46
2.309	12	-3	3	2	38.97	1.876	2	0	2	4	48.48
2.295	22	0	2	3	39.23	1.862	2	-12	0	1	48.88
2.281	13	-10	0	1	39.48	1.861	2	-7	3	4	48.91
2.266	4	-5	3	1	39.75	1.853	Δ	-10	2	5	49.14
2.255	16	-1	3	2	39.94	1.830	2	-12	2	4	49.54
2.244	56	-5	з	2	40.15	1.835	1	7	1	2	49.63
2.240	8	-6	2	4	40.22	1.834	3	-10	Ō	6	49.67
2.226	86	-11	1	3	40.49	1 9 2 7	,	-14	0	۵	49.86
2.209	29	-8	0	5	40.82	1.824	1	-14	1	1	49.96
2.207	68	7	1	1	40.86	1.024	2	-13	1	5	50.25
2.205	1	-1	1	4	40.90	1.806	2	-15	-	1	50.50
2.197	10	5	1	2	41.05	1.803	2	-14	o	3	50.59
0.000	50		•		44.07						
2.196	52	-4	2	4	41.07	1.796	2	-12	2	2	50.79
2.195		-6	0	5	41.09	1.796	1	-2	4	2	50.80
2.170	50	-8	2	4	41.47	1.793	1	5	1	3	50.88
2.107	70	3	3	1	41.00	1.791	1	-6	0	6	50.94
20150	32	Ŭ	v	4	41.00	1.780	1	4	4	0	51.30
2.154	1	-11	1	4	41.90	1.773	1	-14	0	5	51.50
2.147	4	6	2	1	42.05	1.765	1	10	2	0	51.74
2.142	27	5	3	0	42.15	1.758	2	-11	1	6	51.97
2.126	1	9	1	0	42.49	1.743	5	-12	2	5	52.45
2.120	25	-10	0	5	42.61	1.743	1	0	4	2	52.46
2.104	13	1	3	2	42.95	1 775	,	8	•	2	52.71
2.100	1	3	1	3	43.04	1.720	2	0	ŏ	5	53.06
2.099	40	-12	0	4	43.06	1.700	2	-14	õ	2	53.62
2.093	54	-10	2	2	43.20	1.703	1	5	3	2	53.79
2.089	3	-5	З	3	43.29	1.684	2	2	2	4	54.45
2.026	E 1	_ 7	7	~	A7 74					-	<b>FA</b> 45
2.005	51	-/	2	2	43.34	1.684	1	-11	3	2	54.45
2.085	17	8	2	5	43.30	1.683	1	-11	3	4	54.49
2.075	13	-4	0	0	43.50	1.674	1	-13	1	6	54.78
2.073	100	- 7	7	2	43.59	1.673	1	-12	2	1	54.84
2.0012	100	-3	3	5	73004	1.670	1	4	4	1	54.93
L											

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# Aluminum Ytterbium, $Al_2Yb$

Structure			d (A)	I	1	hkl	,	2⊖ (°)
Cubic, Fd3m(227), Cu <sub>2</sub> Mg [Havinga et a	Z = 8, isosti al., 1973].	ructural with						1.540598A
			.909	10	7	5	1+	115.80
Atom positions			.880	5	8	4	0	122.06
16(d) 16 aluminur	n		.864	5	7	5	3+	126.04
8(a) 8 ytterbi	m		.839	5	6	6	4	133.16
			•826	5	9	3	1	137.84
Lattice constants								
a = 7.875 A [ibid]	•]		•804	5	8	4	4	146.82
			•791	5	7	5	5+	153.44
Volume								
488.4 A3			L					
			0-1	and the design of the	1. I	(7		h a J )
Density	, 3		Cal	culated Pa	ttern	(Int	egra	
(calculated) 6.175	g/cm <sup>o</sup>					- 		20 ( 9 )
				1	1	ΠKL	,	
Thermal parameters							/	( = 1.540598A
Isotropic: alumin	$\operatorname{um} B = 1.0; \text{ ytte}$	erbium B = 0.5						
			4.547	65	1	1	1	19.51
Scattering factors			2.784	100	2	2	0	32.12
Al <sup>0</sup> [Cromer and Mar	nn, 1968]		2.374	95	3	1	1	37.86
Yb <sup>0</sup> [International	Tables, 1974]		2.273	5	2	2	2	39.61
			1.969	10	4	0	0	45.07
Scale factor (integra	ated intensities	5)	1.909		-	•	Č	40001
$\gamma = 1.770 \times 10^{-3}$			1.807	20	ч	٦	1	50.47
			1.007	20		2	-	57 27
References			1.007	35	+	2	2	51.21
Cromer, D. T. and	Mann, J. B.	(1968). Acta	1.510	20	5	1	-	61.10
Crystallogr, A24	. 321.		1.516	5	3	3	3	61.10
Havinga, E. E. B	ischow, K.H.J.	and van Daal.	1.392	20	4	4	0	67.19
н.т (1973)	Solid State Com	nun 13 621						
International Table	of for V-ray Cri	vstallography	1.331	10	5	3	1	70.72
	es tor A-ray cry	Birmingham	1.245	15	6	2	0	76.43
$\frac{1}{1}$ (1974). (11	ne kynoch Press,	, Birmingham,	1.201	10	5	З	3	79.80
Eng.) p. 101.			1.187	1	6	2	2	80.91
			1.137	1	4	4	4	85.33
Calculated 1	Pattern (Peak he	eights)	1.103	5	5	5	1	88.62
0			1.103	5	7	1	1	88.62
d(A) I	hkl	20(0)	1.052	20	6	4	2	94.11
		$\lambda = 1.540598A$	1.025	10	7	3	1	97.41
			1.025	5	5	5	3	97.41
				Ĩ	-	-	•	
4.544 75	1 1 1	19.52	.984	5	8	0	0	102.98
2.784 100	2 2 0	32.12	.962	5	7	3	Ř	106.39
2.374 90	3 1 1	37.86	0.20	10		2	2	112.20
2.273 5	222	39.62	.920	10	6	5	2	112.20
1.969 10	4 0 0	46.06	.928	5	7	5	1	115 00
			.909	10		5	+	112.00
1.806 15	3 3 1	50.48			-	_	_	
1.608 35	4 2 2	57.26	.909	1	5	5	5	115.80
1.515 25	5 1 1+	61.10	•880	5	8	4	0	122.06
1.392 15	4 4 0	67.20	•864	5	7	5	3	126.03
1.331 10	5 3 1	70.72	•864	5	9	1	1	126.03
			•839	10	6	6	4	133.15
1.245 10	620	76.44						
1.201 10	5 3 3	79.80	.826	15	9	3	1	137.85
1,187 1	6 2 3	80.90	.804	20	8	4	4	146.83
1,177 1		85.32	•791	5	9	З	З	153.44
1 1 1 0 7		00.52	•791	5	7	7	1	153.44
1.103 5	7 1 1+	00.02	.791	5	7	5	5	153.44
		04 40						
1.052 15	6 4 2	94.10	L					
1.025 15	7 3 1+	97.42						
•984 1	800	102.98						
•962 1	7 3 3	106.38						
•928 10	8 2 2+	112.20						

Aluminum Yttrium, Al,Y

hkl

0 0

1 0

0

1

0

1

2

0

0

З

2

0

2

2

З

1

0

4

0

4

З

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0

1

0

4

З

1

0 0 5

2 0

2 0

2 1

2 1

1 1

3 0

2 0 2

3 0 1

2 2 0

2 1 2

3 1

1 0

30

4 0

2 2

2 1

3 2

1

4 0 2

0 0

5 0

1 1

3 1

2 0

3 3

4 2 0

4

4 2

2 1 4

5 0 2

5 1

3 0

3 2

5 1

3 3 2

4 2 2

2 2 4

6 0

1

4 1 2

0 3

2 0 З

4 0 1

3

4 1

3 1 1

1

1 0 1

1

0 0 2

1 0 2 20(°)

16.30

25.42

28.42

32.94

38.48

39.30

42.80

44.04

48.52

49.20

50.32

52.18

54.42

58.80

60.48

61.46

63.18

65.08

65.64

69.06

70.70

72.50

73.04

75.42

77.88

79.62

81.00

82.46

84.52

90.24

91.42

91.76

93.74

94.00

94.86

97.18

98.72

100.44

100.78

103.32

104.20

105.42

105.78

107.56

108.10

110.54

112.74

116.50

116.96

 $\lambda = 1.540598A$ 

```
Structure
                                                              Calculated Pattern (Peak heights)
  Hexagonal, P6_3/mmc (194), Z = 2, isostructural
  with Ni<sub>3</sub>Sn. The structure refinement was based
                                                        d (A)
                                                                      Ι
  on two-dimensional data [Bailey, 1967].
Atom positions
                                                        5.434
                                                                     10
  2(c)
       2 yttrium
                                                        3.501
                                                                     65
  6(h)
          6 aluminum, x = 0.8534
                                                        3.138
                                                                     30
                                                        2.717
                                                                     25
  These are a transformation of positions from
                                                                    100
                                                        2.338
  those given by Bailey [1967], to show more
  clearly the relation to the isostructural com-
                                                        2.291
                                                                     25
  pounds.
                                                        2.111
                                                                      1
                                                        2.055
                                                                     10
Polymorphism
                                                        1.875
                                                                     10
  This form occurs in small quantities in the resi-
                                                        1.850
                                                                     10
  dues of preparations of the high temperature
  rhombohedral polymorph [ibid.]. A third form
                                                        1.812
                                                                      5
  with cubic cell a = 4.323 was found by Dagerhamn
                                                        1.752
                                                                     10
  [1967].
                                                        1.685
                                                                      1
                                                        1.569
                                                                     15
Lattice constants
                                                        1.530
                                                                      5
  a = 6.276(2) Å
  c = 4.582(1) [ibid.]
                                                        1.507
                                                                      1
                                                                      5
                                                        1.470
  c/a = 0.7301
                                                        1.432
                                                                     10
                                                                      5
                                                        1.421
Volume
                                                        1.359
                                                                      1
  156.3 A<sup>3</sup>
                                                        1.331
                                                                     10
Density
                                                        1.303
                                                                     10
  (calculated) 3.609 g/cm<sup>3</sup>
                                                        1.294
                                                                     15
                                                        1.259
                                                                       1
Thermal parameters
                                                        1.226
                                                                       5
  Isotropic: aluminum B = 1.38; yttrium B = 0.16
              [ibid.]
                                                                      5
                                                        1.203
                                                                       5
                                                        1.186
Scattering factors
                                                        1.169
                                                                      1
  Al<sup>0</sup>, Y<sup>0</sup> [International Tables, 1962]
                                                        1.145
                                                                      1
                                                        1.0871
                                                                       1
Scale factor (integrated intensities)
  \gamma = 0.986 \times 10^{-3}
                                                        1.0761
                                                                       1
                                                        1.0730
                                                                       5
References
                                                        1.0555
                                                                       1
  Bailey, D. M. (1967). Acta Crystallogr. 23, 729.
                                                        1.0533
                                                                       5
  Dagerhamn, T. (1967). Ark. Kemi 27, 363.
                                                                       1
  International Tables for X-ray Crystallography,
                                                        1.0460
                  (The Kynoch Press, Birmingham,
    III (1962).
                                                        1.0271
                                                                       1
    Eng.) pp. 202, 211.
                                                        1.0151
                                                                       5
                                                                       5
                                                        1.0023
                                                          .9999
                                                                       5
                                                          .9821
                                                                       1
                                                          .9762
                                                                       1
                                                                       1
                                                          .9682
                                                                       5
                                                          .9659
                                                          .9548
                                                                       5
                                                          .9515
                                                                       5
                                                          .9373
                                                                       1
                                                          .9251
                                                                       5
                                                          .9059
                                                                       1
```

.9036

Aluminum	Yttrium,	A1_Y -	(continued)
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	Calculated	Pattern	(In	tegr	rated)
d(Å)	I		hkl		20(°) 。
					$\lambda = 1.540598A$
5.435	10	1	0	0	16.30
3.503	60	1	0	1	25.40
3.138	25	1	1	0	28.42
2.718	25	2	0	0	32.93
2.337	100	2	0	1	38.48
2.291	20	o	0	2	39.29
2.111	1	1	0	2	42.80
2.054	10	2	1	0	44.04
1.875	10	2	1	1	48.53
1.850	10	1	1	2	49.20
1.812	5	З	0	0	50.32
1.752	15	2	0	2	52.18
1.685	1	3	0	1	54.41
1.569	15	2	2	0	58.81
1.529	5	2	1	2	60.48
1.507	1	З	1	0	61.46
1.470	5	1	0	З	63.19
1.432	10	3	1	1	65.09
1.421	5	З	0	2	65.65
1.359	1	4	0	0	69.07
1.331	15	2	0	з	70.70
1.303	10	4	0	1	72.50
1.295	15	2	2	2	73.03
1.259	1	3	1	2	75.42
1.226	5	2	1	3	77.87
1.203	5	З	2	1	79.62
1.186	5	4	1	0	81.00
1.169	5	4	0	2	82.46
1.145	1	0	0	4	84.51
1.087	0 1	5	0	0	90.25
1.076	0 1	1	1	4	91.43
1.072	9 5	3	1	З	91.77
1.055	5 1	2	0	4	93.73
1.053	35	4	1	2	94.00
1.046	0 1	3	3	0	94.86
1.027	2 1	4	2	0	97.17
1.015	2 5	4	0	З	98.71
1.002	3 10	4	2	1	100.45
1.000	5 1	2	1	4	100.70
•982	1 1	5	0	2	103.32
.976	2 1	5	1	0	104.20
.968		3	0	4	105.42
.965	y 5	3	2	3	103.78
.954	5 5	3	3	2	108.10
.037	3 1	۸	2	2	110.54
-937		* 2	2	4	112.73
.912	1 1	2	1	4	115-25
-905	9 1	6	ò	o	116.50
.903	6 1	1 -	ō	5	116.96

Synonyms	Cal	culated Pa	ttern	(Peal	k hei	ghts)
5-Ethyl-5-isoamylbarbituric acid Amytal	d (Å)	I		hkl	λ	20(°) = 1.5405987
Structure						
Monoclinic, $C2/c$ (15), $Z = 8$ . The structure was	10.64	34	2	0	0	8.30
determined by Craven and Vizzini [1969].	10.18	100	1	1	0	8.68
	7.46	32	- 1	1	1	11.86
Atom positions	7.03	79	1	1	1	12.58
Seven hydrogen positions were not located in the structure determination. All other atoms were in	6.05	6	3	1	0	14.62
general positions 8(f). The data for H(112) appar-	5.79	2	0	2	0	15.28
ently had errors and was omitted from the powder	5.47	22	-3	1	1	16.18
data calculations here.	5.32	16	4	0	0	16.64
	5.15	6	0	0	2	17.22
Polymorphism A polymorph called form II is also monoclinic	5.09	4	2	2	0	17.40
with similar cell volume and space group P21/c	4.996	2	Э	1	1	17.74
(14). The two forms crystallize simultaneously	4.870	21	- 2	0	2	18.20
from the same aqueous ethanol solution by slow	4.672	12	-2	2	1	18.98
evaporation at room temperature [Craven and	4.458	10	2	2	1	19.90
Vizzini, 1969].	4.423	10	2	0	2	20.06
Lattice constants	4.141	1	-3	1	2	21.44
a = 21.481(10) Å	4.001	7	5	1	0	22.20
b = 11.591(6)	3.802	35	1	з	0	23.38
c = 10.371(6)	3.733	10	з	1	2+	23.82
$\beta = 97.07(3)^{\circ}$	3.590	5	5	1	1	24.78
a/b = 1.8532	3.542	4	6	0	0+	25.12
c/b = 0.8947	3.517	4	2	2	2	25.30
	3.394	1	з	з	0	26.24
(published values: $a = 21.480(10)A$ , $b = 11.590(6)$ ,	3.351	4	-5	1	2	26.58
$c = 10.370(6), \beta = 97^{\circ} 4(2)$ [Craven and Vizzini, 1969]).	3.264	1	-4	2	2	27.30
1,00,00	3.193	6	1	1	з	27.92
Volume	3.108	з	-6	° 0	2	28.70
2562.6 A <sup>3</sup>	3.026	2	1	з	2	29.50
	2.992	4	-6	2	1+	29.84
Density	2.951	5	0	2	З	30.26
(calculated) 1.173 g/cm <sup>3</sup>	0.005	•	-		• •	
(measured) 1.167 (7) g/cm <sup>3</sup> [Craven and Vizzini,	2.925	2	- /	1	1+	30.54
1969]	2.897		U	4		30.84
	2.819	1	0	2	1+	31.72
Thermal parameters	2.796	6	2	4	0	31.98
Overall isotropic B = 5.0 for hydrogen atoms. Anisotropic, for all others, as given [Craven	2.709	2	2	2	3+	32.30
and Vizzini, 1969].	2.698	5	-7	1	2	33.18
	2.676	3	2	4	1	33.46
Scattering factors	2.595	3	-5	3	2	34.54
$C^0$ , $H^0$ , $N^0$ , $O^0$ [International Tables, 1962]	2.573	5	0	0	4	34.84
Scale factors (integrated intensities)	2.546	1	4	4	0	35.22
$\gamma = 2.742 \times 10^{-3}$	2.529	1	- 1	1	4	35.46
I/I (calculated) 1.08	2.494	2	-8	0	2+	35.98
corundum (called a contraction)	2.474	1	4	2	з	36.28
Additional patterns	2.468	1	5	1	з	36.38
1. Williams [1959]	2.438	1	-4	0	4+	36.84
PDF card 27-1596 is labelled form I but is either	2.418	1	-8	2	1+	37.16
form II or a mixture of the two forms	2.399	1	-6	2	З	37.46
TOTA II OF A MIXCULE OF CHE LWO TOTAS.	2.379	1	-7	1	з	37.78
Deferences	2.336	1	-4	4	2	38.50
References	2.282	1	7	з	1+	39.46
Crystallogr. <u>B25</u> , 1993. <u>International</u> <u>Tables for X-ray</u> <u>Crystallography</u> , <u>III</u> (1962). (The Kynoch Press, Birmingham, Eng.)	1					
p. 202. Williams, P. P. (1959). Anal. Chem. <u>31</u> , 140.						

Amobarbital, form I,  $C_{11}H_{18}N_2O_3$  - (continued)

_						
	d(Å)	I		hkl		$2\Theta(^{\circ})$ , $\lambda = 1.540598A$
	0.053	1	7		24	70.00
	2.253	1	-/	3	2+	39.98
	2.243	2	1	5	1+	40.18
	2.213	1	0	4	3+	40.74
	2.208	1	3	5	0+	40.84
	2.172	1	⇒3	5	1	41.54
	2.159	1	6	4	1+	41.80
	2.153	1	-1	3	4	41.92
	2.120	1	-6	4	2	42.62
	2.092	1	7	3	2+	43.20
	2.059	1	5	1	4+	43.94
	2.040	1	- 1	1	5	44.36
	2.037	1	5	5	õ	44.44
	2.015	1	-3	1	5	44.96
	2.000	1	10	2	5	44.50
	2.009	1	-10	2	1	45.10
	1.995	1	1	1	5+	45.42
	1.971	1	6	0	4	46.00
	1.950	1	-9	3	2+	46.54
	1.932	1	0	6	0	47.00
	1.924	1	0	4	4+	47.20
	1.901	1	1	5	3+	47.80
	1.901	•	•	5	2.	4/000
	1.890	1	10	0	2+	48.10
	1.881	1	8	2	з	48.34
	1.863	1	2	4	4+	48.86
	1.837	1	-9	1	4+	49.58
	1.823	1	9	1	3+	50.00
	C	1 1 at ad . Day		17-4		
_		alculated Pat	ttern	(Int	egra	ited)
	d (A)	I		hkl		20(°)
						$\lambda = 1.540598A$
_				_		
	10.66	32	2	0	0	8.29
	10.18	100	1	1	0	8.68
	7.46	32	-1	1	1	11.85
	7.03	81	1	1	1	12.57
	6.06	6	3	1	0	14.61
	0000					
	5.80	2	0	2	0	15.28
	5.48	23	-3	1	1	16.17
	5.33	17	4	0	0	16.62
	5.15	6	0	0	2	17.22
	5.09	3	2	2	0	17.40
	5005					
	5.05	1	0	2	1	17.55
	4.997	1	З	1	1	17.74

-2 0 2 -1 1 2 -2 2 1

23

1

13

1

 4.461
 10

 4.426
 10

 4.142
 1

 4.001
 8

4.875

4.706

4.674

4.488

d(Å)	I	hkl	$2\Theta(^{\circ})$ $\lambda = 1.540598A$
3.884	1	=5 1	1 22.88
3.734	7	1 J 7 1	2 23.91
3.731	4	-2 2	2 23.83
3.592	5	5 1	1 24.77
3.553	2	6 0	0 25.04
3.517	2	1 3	1 25.13
3.493	5	2 2	2 25.30
3.394	1	3 3	0 26.23
3.352	4	=5 1	2 26.57
3.266	1	-4 2	2 27.29
3.195	-	1 1	3 27.90
3.109	1	3 3	1 28.14
3.100	3	-6 0	2 20.70
3.026	1	=1 3 1 7	2 28.87
2.992	4	-6 2	1 29.94
2.992	1	4 2	2 29.84
2.952	6	0 2	3 30.25
2.945	1	7 1	0 30.32
2.926	1	-2 2	3 30.53
2.925	1	-7 1	1 30.53
2.898	8	04	0 30.83
2.827	1	62	1 31.63
2.819	1	=5 3	1 31.72
2.796	7	2 4	0 31.98
2.789	1	0 4	1 32.06
2.769	1	6 0	3 32.28 2 32.31
2.701	1	53	1 33.14
2.699	6	-7 1	2 33.17
2.677	З	2 4	1 33.45
2.665	1	8 0	0 33.61
2.595	3	-5 3	2 34.54
2.575	1	=1 3	3 34.81
2.546	6	0 0	4 34.84
2.530	1	-1 1	0 35.23
2.520	1	1 3	3 35.60
2.495	2	-8 0	2 35.97
2.491	1	⇔2 4	2 36.03
2.487	1	-33	3 36.08
2.474	1	4 2	3 36.29
2.407	1	5 1	3 36,38
2.418	1	-8 2	1 37.16
2.379	1	-7 1	3 37.046
2.337	1	-4 4	2 38.40
2.288	1	-5 1	4 39.35
2.282	1	7 3	1 39.46
2.255	1	-1 5	1 39.94
2.246	1	-7 3 2	2 39.97
2.243	2	1 5	40.12
	-		40.10

18.18

18.84

18.97

19.77

19.89 20.05 21.43 22.20

Amobarbital,	form	Ι,	С,	,H,	N203	-	(continued)
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d (Å)	I	ł	ıkl		$20(°)$ ° $\lambda = 1.540598A$
2.218	1	=6	0	4	40.65
2.214	1	0	4	з	40.73
2.207	1	9	1	1	40.85
2.204	1	З	5	0	40.92
2.172	1	-3	5	1	41.54
2.159	1	6	4	1	41.80
2.153	1	-1	З	4	41.93
2.119	1	-6	4	2	42.62
2.093	1	. 7	З	2	43.19
2.093	1	1	5	2	43.19
2.059	1	5	1	4	43.95
2.041	1	-1	1	5	44.35
2.037	1	5	5	0	44.45
2.014	1	-3	1	5	44.96
2.008	1	-10	2	1	45.12
1.998	1	з	5	2	45.34
1.995	1	1	1	5	45.43
1.972	1	6	0	4	45.99
1.951	1	-9	з	2	46.52
1.949	1	-2	2	5	46.57
1.932	1	о	6	0	47.00
1.891	1	-8	4	2	48.08
1.889	1	10	0	2	48.13
1.881	1	8	2	З	48.34
1.837	1	-9	1	4	49.58
1.823	1	9	1	з	49.99

Synonyms

5-Ethyl-5-isoamyl barbituric acid Amytal

### Structure

Monoclinic,  $P2_1/c$  (14), Z = 8. The structure was determined by Craven and Vizzini [1969].

### Atom positions

Fourteen hydrogen atoms were not located in the structure determination. All other atoms were in general positions 4(e). Data for H(112), molecule B, appeared to be in error and was omitted from the powder data calculations here.

#### Polymorphism

A polymorph, form I, is also monoclinic with similar cell volume and space group C2/c (15). The two forms crystallize simultaneously from the same aqueous ethanol solution by slow evaporation at room temperature [Craven and Vizzini, 1969].

Lattice constants.

a = 10.282(6) A b = 22.602(10) c = 11.680(6)

 $\beta = 109.1(3)^{\circ}$ 

(published values: a = 10.281(6)A, b = 22.601(10), c = 11.679(6),  $\beta = 109^{\circ} 6(2)^{\circ}$  [Craven and Vizzini, 1969])

CD cell: a = 11.680(6)Å, b = 22.602(10), c = 10.282(6),  $\beta = 109.1(3)$ °; sp. gp. P2<sub>1</sub>/a; a/b = 0.5167; c/b = 0.4549.

Volume °3 2564.9 Å<sup>3</sup>

```
Density
```

```
(calculated) 1.172 g/cm<sup>3</sup>
(measured) 1.185(7) g/cm<sup>3</sup> [Craven and Vizzini,
1969]
```

Thermal parameters Overall B = 5.0 for hydrogen atoms Anisotropic for all others, as given [Craven and Vizzini, 1969].

Scattering factors C<sup>0</sup>, H<sup>0</sup>, N<sup>0</sup>, O<sup>0</sup> [International Tables, 1962]

- Scale factor (integrated intensities)  $\gamma = 2.847 \times 10^{-3}$ I/I corundum (calculated) 1.12
- Additional patterns
- PDF card 23-1682 [Eli Lilly and Co., Indianapolis, Ind.]
   PDF card 27-1596 [Cleverly and Williams,
- 1959]. The card is labelled "Amobarbital I," but is apparently form II given here.

## References

Cleverly, B., and Williams, P. P. (1959). Tetrahedron 7, 277.

Craven, B. M. and Vizzini, E. A. (1969). Acta Crystallogr. B25, 1993. International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

	carcuraced	raccern	(Pec	ix ne.	rgiics)
d(Ă)	I		hkl	;	20(°) \ = 1.540598
11.30	100	0	2	0	7.82
9.91	53	0	1	1	8.92
8.93	12	1	1	0	9.90
7.36	1	1	2	0	12.02
6.98	58	- 1	2	1	12.68
6.21	1	0	З	1	14.24
5.95	16	1	3	0	14.88
5.65	4	0	4	0	15.68
5.52	40	1	2	1+	16.04
5.36	5	0	1	2	16.54
5.05	2	-1	2	2	17.54
4.962	7	0	2	2+	17.86
4.855	22	2	0	0	18.26
4.762	10	-1	4	1	18.62
4.521	6	-1	3	2	19.62
4.436	11	-2	0	2	20.00
4.354	1	-2	1	2	20.38
4.180	12	0	5	1	21.24
4.130	2	-2	2	2	21.50
3.767	22	0	6	0	23.60
3.675	7	-1	2	3+	24.20
3.630	5	0	1	з	24.50
3.565	1	0	6	1	24.96
3.490	6	-2	4	2+	25.50
3.269	5	-3	1	2	27.26
3.204	2	-2	З	3+	27.82
3.166	3	2	0	2	28.16
3.097	13	0	7	1	28.80
3.050	ç	2	2	2	29.26
3.026	6	-3	З	2	29.50
2.992	2	2	5	1	29.84
2.929	2	-3	4	1+	30.50
2.872	2	-2	6	2+	31.12
2.826	5	0	8	0	31.64
2.786	1	U	~	2+	32.10
2.759	1	0	0	4	32.42
2.730	2	1	4	З	32.78
2.679	1	0	2	4	33.42
2.668	2	⇒3	5	2	33.56
2.552	6	-4	0	2	35.14
2.546	5	2	1	З	35.22
2.510	1	2	7	1	35.74
2.448	1	0	9	1+	30.68
2.425	2	2	6	2+	37.04
2.295	1	-1	9	2	39.22
2.223	1	- 4	5	1+	40.54
2.128	1	1	10	1+	42.44
2.109	1	2	8	2+	42.84
2.004	1	2	7	3+	45.20
1.999	1	⇒5	2	1+	45.34

Amobarbital, form II,  $C_{11}H_{18}N_2O_3$  - (continued)

d(Å)	I	hkl	λ	20(°) = 1.540598A
1.981	2	-4 1	5+	45.76
1.883	1	0 12	0+	48.30
1.774	1	33	4	51.46

	Calculated	Pattern	(Int	egr	ated)
0			<u> </u>		
d(A)	I		hkl		20(°)
					$\lambda = 1.540598A$
11.30	100	0	2	0	7.82
9.92	53	0	1	1	8.91
8.93	12	1	1	ō	9.90
7.37	1	1	2	0	12.00
6.98	60	-1	2	1	12.67
6.22	1	0	З	1	14.22
5.95	16	1	З	0	14.87
5.65	3	0	4	0	15.67
5.53	25	1	2	1	16.02
5.52	19	0	0	2	16.05
5.36	5	0	1	2	16.52
5.06	1	-1	2	2	17.51
4.970	a 3	-2	1	1	17.80
4.959	5	0	2	2	17.87
4.858	3 24	2	0	0	18.25
4.766	5 10	- 1	4	1	18.60
4.525	5 б	-1	З	2	19.60
4.463	3 2	2	2	0	19.88
4.452	2 1	0	3	2	19.93
4.437	11	-2	0	2	20.00
4 35		-		~	0.0.70
4.354		-2	1	2	20.38
4.193	/ J	1	4	1	21.00
4.130		-2	2	2	21.50
3.767	25	0	6	0	23.60
		•	Ĩ	-	
3.684	4 З	2	4	0	24.14
3.670	5 5	-1	2	З	24.19
3.631	. 5	0	1	З	24.49
3.565	5 1	0	6	1	24.96
3.501	1 2	-2	1	3	25.42
7 400		- 2		2	25 50
3.270		-2	1	2	23.30
3.207	7 1	-2	- -	2 7	27.80
3.168	3 3	2	õ	2	28.14
3.099	14	0	7	1	28.79
3.092	2 2	1	5	2	28.85
3.064	• 3	1	7	0	29.12
3.05	9	2	2	2	29.25
3.026	6	-3	3	2	29.49
3.00	1	1	2	3	29.69
2.99	2 2	2	5	1	29.84
2.920	2	-3	4	1	30.49
2.92	1	2	3	2	30.59
2.872	2 2	=2	6	2	31.12
2.82	5 6	0	8	0	31.64

d (Å)	I	h	kl	λ	20(°) = 1.540598A
2.787	1	0	7	2	32.09
2.759	1	0	0	4	32.42
2.731	2	1	4	з	32.77
2.681	1	0	2	4	33.40
2.668	1	-3	5	2	33.56
2.552	7	-4	0	2	35.13
2.541	4	2	1	з	35.29
2.510	1	2	7	1	35.74
2.425	1	2	6	2	37.05
2.341	1	З	З	2	38.42
2 205			~	•	
2.295	1	=1	9	2	39.21
2.224	1	-4	5	1	40.53
2.005	1	2	7	3	45.19
1.999	1	-5	2	1	45.34
1.982	1	-4	1	5	45.75
1.830	1	=3	з	6	49.79
1.775	1	з	З	4	51.45

Amphetamine Sulfate, d-,  $C_{18}H_{28}N_2O_4S$ 

Synonyms	Cal	culated	Pattern	(Pe	ak he	eights)
(+)-Methylphenethylamine sulfate	(A)	т		hkl		20(°)
Dexedrine sulfate						$\lambda = 1.540598 \text{\AA}$
d-l-Phenyl-2-aminopropane sulfate						
Ctructuro	15.60	100	0	0	2	5.66
Monoclinic, P2, $(4)$ , $7 = 4$ . The structure was	6.215	Э	0	1	4	14.24
determined by Bergin and Carlström [1971].	5.878	7	ő	1	2	15.06
	5.420	18	0	1	3+	16.34
Atom positions						
25 atoms in general positions 2(a). The hydrogen	5.298	4	1	1	1	16.72
atom positions were not determined [ibid.].	5.199	26	=1	1	2+	17.04
Lattice constants	5.058	33	-2	1	2 +	17.52
a = 10.509(2) Å	4.908	14	-1	1	3+	18.06
b = 6.350(1)						
c = 31.338(5)	4.844	7	-2	0	3+	18.30
$\beta = 94.99(6)^{\circ}$	4.726	18	1	1	З	18.76
	4.535	8	-2	0	4+	19.56
(published values: a=10.508(2) A, D=0.350(1),	4.363	4	1	1	5	19.94
(-51.558(5), p-94.99(6)) [Bergin and Caristion, 19711].	4.303	40	1		-	20.34
15,11,.	4.191	23	-2	0	5	21.18
CD cell: a=31.338(5) A, b=6.350(1), c=10.509(2),	4.037	7	2	1	0+	22.00
β=94.99(6)°; sp. gp. P2 <sub>1</sub> ; a/b=4.9351; c/b=1.6550.	4.008	5	1	1	5	22.16
	3.973	4	2	1	1+	22.36
Volume	3.897	2	0	0	8	22.80
2083.3 A	3.844	16	= 1	1	6+	23,12
Density	3.675	3	1	1	6	24.20
(calculated) 1.175 g/cm <sup>3</sup>	3.548	6	-2	0	7	25.08
(measured) 1.172(2) g/cm <sup>3</sup> [Bergin and Carlström,	3.498	2	З	0	0+	25.44
1971]	3.435	1	3	0	1	25.92
Thermal parameters	3.371	3	1	1	7	26.42
Isotropic B., estimated from $\beta_{11}$ , $\beta_{22}$ , $\beta_{33}$ for	3.293	1	-3	0	4+	27.06
each atom.	3.257	1	2	0	7+	27.36
	3.239	2	=1	1	8	27.52
Scattering factors	3.173	3	0	2	0	28.10
C', N', O', S' [International Tables, 1962]	3.110	10	0	2	2	28.68
Scale factors (integrated intensities)	3.064	5	⇒3	1	1	29.12
$\gamma = 1.318 \times 10^{-3}$	3.019	e	З	1	1+	29.56
I/I (calculated) 1.16	2.996	6	-3	1	З	29.80
corundan	2.940	7	0	2	4	30.38
Additional pattern	2.975				7	71 09
1. Folen [1975]	2.833	4	- 3	1	5+	31.56
References	2.759	1	-1	1	10+	32.42
Bergin, R. and Carlström, D. (1971). Acta Crys-	2.714	2	2	2	0+	32.98
tallogr. <u>B27</u> , 2146.	2.695	1	-2	2	2+	33.22
Folen, V. A. (1975). J. Forens. Sci. 20, 348.						
International Tables for X-ray Crystallography,	2.656	2	-2	2	3+	33.72
III (1962). (The Kynoch Press, Birmingham,	2.589	2	- 3	0	1+	34.62
Eng.) p. 202.	2.529	1	2	2	4	35.46
	2.4702	1	1	1	11	36.34
	2.3053	1	1	1	12	39.04
	2.2587	2	-2	ō	13+	39.88
	2.1822	1	-2	2	9+	41.34
	2.0953	1	2	2	9+	43.14
	2.0607	1	-1	3	2+	43.90
	I .					

Amphetamine Sulfate, d-,  $C_{18}H_{28}N_2O_4S$  - (continued)

_								
	d (Å)	I	-	hkl		λ	=	20(°) 1.540598A
	2.0519	1	1	3	2			44.10
	2.0078	1	-2	2	11+			45.12
	1•9886 1•9157	1 1	-4 1	2 3	4+ 6+			45.58 47.42
	1.8850	1	4	2	5+			48.24

	Calculated	Pattern	(In	tegi	rated)
d (Å)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
15.61	100	0	0	2	5.66
7.80	9	0	0	4	11.33
7.72	1	-1	0	З	11.45
6.223	3	0	1	1	14.22
5.882	7	0	1	2	15.05
5.429	9	1	1	0	16.31
5.421	10	0	1	З	16.34
5.390	1	-1	1	1	16.43
5.309	2	1	1	1	16.69
5.237	2	-2	0	1	16.92
5.235	5	2	0	0	16.92
5.203	10	0	0	6	17.03
5.201	14	-1	1	2	17.03
5.098	24	=2	0	2	17.38
5.091	(	2	0	1	17•41
5.058	26	1	1	2	17.52
4.926	7	0	1	4	17.99
4.905	10	-1	1	3	18.07
4.849	4	-2	0	3	18.28
4.838	2	2	0	2	18.32
4.727	20	1	1	3	18.76
4.554	4	-1	1	4	19.48
4.534	6	-2	0	4	19.57
4.452	2	0	1	5	19.93
4.366	51	1	1	4	20.33
4.195	22	=2	0	5	21.16
4.182	5	2	0	4	21.23
4.040	3	-2	1	1	21.98
4.039	4	2	1	0	21.99
4.008	4	1	1	5	22.16
3.976	1	= 2	1	2	22.34
3.972	2	2	1	1	22.36
3.902	2	0	0	8	22.77
3.862	4	-2	0	6	23.01
3.854	1	-2	1	3	23.06
3.850	4	2	0	5	23.08
3.848	1	2	1	2	23.09
3.844	11	-1	1	6	23.12
3.675	4	1	1	6	24.20
3.551	6	-2	0	7	25.06

d (Å)	I	ł	ıkl		$20(^{\circ})$ $\lambda = 1.540598A$
3.540	1	2	0	6	25.14
3.525	2	-1	1	7	25.24
3.502	1	-3	0	1	25.41
3.490	1	3	0	0	25.50
3.435	1	3	0	1	25.92
3.372	4	1	1	7	26.41
3.239	2	-1	1	8	27.52
3.175	4	0	2	0	28.08
3.159	1	0	2	1	28.23
3.122	2	O	0 1	0	28.57
3.111	10	0	2	2	28.67
3.103	1	1	1	8	28.75
3.067	4	-3	1	1	29.10
3.058	1	3	1	0	29.18
3.045	1	⇒3	1	2	29.30
3.038	1	1	2	0	29.37
3.037	1	0	2	3	29.39
3.031	1	-1	2	1	29.44
3.021	5	3	1	1	29.54
3.015	2	-2	0	9	29.61
2.997	6	-3	1	3	29.79
2.941	8	0	2	4	30.37
2.876	5	З	1	3	31.08
2.865	1	1	1	9	31.19
2.833	1	-3	1	5	31.55
2.761	1	-1	1 1	0	32.40
2.715	2	2	2	0	32.97
2.695	1	-2	2	2	33.21
2.656	1	-2	2	3	33.72
2.589	1	4	0	1	34.61
2.529	1	2	2	4	35.47
2.4699	1	1	1 1	1	36.34
2.4526	1	=2	2	6	36.61
2.3060	1	1	1 1	2	39.03
2.2585	2	-2	0 1	3	39.88
2.1862	1	⇒2	2	9	41.26
2.0612	1	-1	3	2	43.89
2.0520	1	1	3	2	44.10
2.0137	1	-1	З	4	44.98
1.8849	1	4	2	5	48.24

Structure Hexagonal, P63/mmc(194), isostructural with NiAs, from powder data [Fürst and Halla, 1938]. Atom positions 2(c) 2 antimony 2 cobalt 2(a) Lattice constants a = 3.880 Åc = 5.185 [Rosenqvist, 1953] c/a = 1.3363Volume . 67.6 Å<sup>3</sup> Density (calculated) 8.876 g/cm<sup>3</sup> • Thermal parameters Isotropic: cobalt B = 1.0; antimony B = 0.75 Scattering factors Co<sup>0</sup>, Sb<sup>0</sup> [Cromer and Mann, 1968] Scale factor (integrated intensities)  $\gamma = 0.638 \times 10^{-3}$ References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321. Fürst, U. and Halla, F. (1938). Z. Phys. Chem.

Rosenqvist, T. (1953). Acta Met. 1, 761.

Abt. <u>B40</u>, 285.

	Calculated	Pattern	(Pea	ak h	eights)
d (A)	I		hkl		$2\Theta(^{\circ})$ , $\lambda = 1.540598A$
2.819	9 100	1	ο	1	31.72
2.592 2.053	2 5 5 50	0 1	0	2 2	34.58 44.08
1.940	<b>45</b>	1	1	0	46.80
1.55	. 5	-	-	2	59.46
1.537	10	1	0	3	60.16
1.410	b 10 b 5	2	0	2 4	66•24 72•92
1.234	10	2	1	1	77.28
1.205	5 5	2	0	3	79.50
1.120	) 5	3	ō	0	86.90
1.078	3 <b>10</b> 3 <b>1</b>	1 3	1	4	91.24 97.04
1.02	3 5	2	1	з	97.64
.991	1	1	0	5	102.04
.970	) 5	2	2	0	105.14
•917	7 5	3	1	1	114.24
•909	9 1	2	2	2	115.96

d(Å)	I	h	hkℓ		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
.882 .877 .848 .837 .829	1 5 5 1	2 3 3 1 4	0 1 0 0 0	5 2 4 6	121.60 122.88 130.70 133.96 136.54		
•820 •803 •799 •789	5 5 1 1	3 2 4 1	1 1 0 1	3 5 2 6	139.78 147.06 149.12 154.74		

	Calculated	Pattern	(Int	egr	ated)
d (Å)	I		hkl		$2\Theta(°)$ $\lambda = 1.540598A$
2.820	) 100	1	0	1	31.71
2.593	3 5	0	0	2	34.57
2.053	3 50	1	0	2	44.08
1.940	50	1	1	0	46.79
1.598	B 15	2	0	1	57.63
1.553	3 5	1	1	2	59.46
1.537	7 15	1	0	З	60.16
1.410	) 15	2	0	2	66.23
1.296	5 5	0	0	4	72.92
1.23	4 10	2	1	1	77.28
1.205	5 5	2	0	з	79.50
1.14	10	2	1	2	84.97
1.120	) 5	3	0	0	86.90
1.07	в 10	1	1	4	91.24
1.028	3 1	3	0	2	97.04
1.02	3 5	2	1	З	97.64
.991	1 5	1	0	5	102.04
•97	0 5	2	2	0	105.14
•91	7 5	3	1	1	114.24
•90	в 1	2	2	2	115.97
.88	2 5	2	0	5	121.60
.87	7 5	3	1	2	122.88
.84	в 10	3	0	4	130.71
.83	7 5	1	0	6	133.96
.82	9 5	4	0	1	136.54
.82	0 10	3	1	з	139.79
.80	3 10	2	1	5	147.06
.79	9 5	4	0	2	149.12
•78	9 5	1	1	6	154.75

Antimony Cobalt, CoSb<sub>2</sub>

Structure	Calculated Pattern (Peak heights)					
Monoclinic, $P2_1/c$ (14), $Z = 4$ , isostructural with CoAs <sub>2</sub> and FeAsS. The structure was determined by Zhdanov and Kuz'min [1962], and confirmed by Kiekshus [1971]. Previously, the structure was	d (Å)	I		hkl		20(°) $\lambda = 1.540598\lambda$
assumed to be orthorhombic.	5.764	1	1	0	0	15.36
	4.203	1	-1	1	1	21.12
Atom positions	2.986	20	1	1	1	29.90
All atoms were in general positions.	2.897	25	ō	ō	2	30.84
	2.882	30	2	õ	0	31.00
Lattice constants, a = 6.5081(3)A	2.773	100	-1	2	1	32.26
b = 6.3883(4)	2.638	55	•	1	2	33.96
c = 6.5434(3)	2.627	55	2	1	2	34.10
$\beta = 117.660(4)^{\circ}$	2.557	20	-2	1	2	35-06
	2.210	5	1	0	2	40.80
CD cell: $a = 6.5434(3)$ , $b = 6.3883(4)$ , $c = 6.5081(3)$ , $\beta = 117.660(4)^\circ$ ;	2 146		-	Š	-	40.00
Sp.Gp. $P2_1/a(14)$ ; $a/b = 1.0243$ .	2.140	1	0	2	2	42.08
c/b = 1.0188	2.140	5	2	2	0	42.20
,	2.102	10	-2	2	2	43.00
(Published values: $a = 6.5077(3)$ , $b = 6.3879(4)$ ,	2.089	1	1	1	2	43.20
$c = 6.5430(3), \beta = 117.660(4)$ [Kjekshus, 1971].)	2.045	25	-1	1	3	44.20
Volumo	2.033	25	-3	1	1	44.52
240 96 Å <sup>3</sup>	2.016	5	-2	1	З	44.92
240.90 A	1.989	10	-1	З	1	45.56
Density	1.849	1	0	1	3	49.24
(calculated) 8 337 $\alpha/cm^3$	1.801	35	1	З	1	50.64
(measured) 8.30 [Kjekshus, 1971]			_			
	1.787	25	-3	1	3+	51.06
Thermal parameters	1.782	20	-3	2	1	51.22
Tsotropic: overall $B = 0.16$	1.710	5	0	3	2	53.30
	1.690	10	2	3	0	53.40
Scattering factors	1.089	15	2	U	2	54.28
$Co^0$ , $Sb^0$ [Cromer and Mann, 1968]	1.653	1	0	2	7	55.56
	1.634	5	-2	0	4	56.24
Scale factor (integrated intensities)	1.626	5	-4	ñ	2	56.56
$\gamma = 0.329 \times 10^{-3}$	1.608	5	-3	2	3	57.24
	1.5969	5	0	4	ñ	57.68
Additional pattern		5	Ŭ	•	Ŭ	0.000
<ol> <li>PDF card 4-0890 [Fürst and Halla, 1938].</li> </ol>	1.5834	5	-2	1	4	58.22
	1.5755	5	-4	1	2	58.54
References	1.5355	1	-1	4	1+	60.22
Cromer, D. T. and Mann, J. B. (1968). Acta	1.5318	1	2	з	1	60.38
Crystallogr. <u>A24</u> , 321.	1.5159	5	-1	3	3	61.08
Fürst, U. and Halla, F. (1938). Z. Phys. Chem.						
Abt. B, <u>40</u> , 285.	1.5115	5	-3	З	1+	61.28
Kjekshus, A. (1971). Acta Chem. Scand. <u>25</u> , 411.	1.4548	1	-2	2	4	63.94
Zhdanov, G. S. and Kuz'min, R. N. (1961). Sov.	1.4488	5	-4	2	2+	64.24
Phys. Crystallogr. <u>6</u> , 704.	1.4443	10	1	2	з	64.46
	1.4404	15	3	2	1+	64.66
	1.4128	1	0	1	4	66.08
	1.4057	5	4	1	0	66.46
	1.4015	5	-3	3	3	66.68
	1.3960	1	-4	0	4	66.98
	1.3861	10	-2	4	2	67.52
	1.3638	5	-4	1	4	68.78
	1.3403	1	З	0	2	70.16
	1.3194	1	0	2	4	71.44
	1.3137	1	4	2	0	71.80
	1.2889	1	1	З	3	73.40
	1.2859	5	з	з	1	73.60
	1.2791	1	-2	1	5+	74.06

# Antimony Cobalt, $CoSb_2$ - continued

	Calculated	Pattern	(In	tegr	ated)
đ	(Å) I	ł	nkl		20 ( <sup>0</sup> )
					$\lambda = 1.540598 \text{\AA}$
5.764	4 1	1	0	0	15.36
2.986	+ I 5 20	-1	1	1	21 • 12
2.910	) 1	-1	1	2	30.70
2.898	3 20	0	0	2	30.83
2.007	25	~	•	•	71.00
2.792	25	-2	0	2	31.00
2.773	3 100	-2	2	1	32.26
2.639	50	0	1	2	33.94
2.627	50	2	1	0	34.10
2.558	3 20	-2	1	2	35.05
2.210	5	1	ò	2	40.80
2.146	5 <b>1</b>	0	2	2	42.07
2.140	) 1	2	2	0	42.20
2.102	2 10	-2	2	2	42.99
2.085	. 1	1	1	2	43.29
2.045	25	-1	1	3	44.26
2.034	25	-3	1	1	44.51
2.016	1	-2	1	3	44.93
1.990	15	-1	З	1	45.55
1.849	1	0	1	7	49.24
1.801	40	ĩ	3	1	50.63
1.788	10	-1	2	3	51.03
1.787	20	3	1	3	51.07
1.781	10	-3	2	1	51.25
1.716	5	0	з	2	53.35
1.713	5	2	З	0	53.46
1.693	1	-2	З	2	54.12
1.689	15	2	0	2	54.27
1.653	1	0	2	3	55.55
1.634	5	-2	0	4	56.24
1.626	5	-4	0	2	56.56
1.608	5	-3	2	З	57.24
1.597	1 5	0	4	0	57.67
1.583	3 5	-2	1	4	58.22
1.575	7 5	-4	1	2	58.53
1.535	5 1	-1	4	1	60.22
1.531	6 1	2	3	1	60.39
1.515	9 5	-1	з	3	61.08
1.511	4 5	-3	3	1	61.28
1.510	6 1	-3	1	4	61.32
1.454	9 1	-2	2	4	63.94
1.449	0 1	-4	2	2	64.23
1.448	9 1	0	0	4	64.23
1.444	2 10	1	2	3	64.47
1.441	1 1	4	0	0	64.62
1.440	4 10	3	2	1	64.66
1.413	0 1	0	1	4	66.07
1.405	8 5	4	1	0	66.45
1.401	4 5	-3	3	3	66.69

a (Å)	I	h	kl		$2\Theta(^{\circ})$ $\lambda = 1.540598(^{\circ}A)$
1.3959	1	-4	0	4	66.99
1.3863 1.3637	10	-2	4	2 4 2	67.51 68.78 70.16
1.3403	1	3	2	4	71.43
1.3136	1	4	2	0	71.81
1.2889	1 5	1 3	3	3	73.40

Cubic, F43m (216), Z=4, isostructural with AgAsMg
[Webster and Ziebeck, 1973], from x-ray and neutron powder data.
Atom positions
4(a) 4 cobalt
4(c) 4 titanium
4(d) 4 antimony

Lattice constant a = 5.884 Å [ibid.]

Volume 203.71 Å<sup>3</sup>

Structure

Density (calculated) 7.454 g/cm<sup>3</sup>

Thermal parameters Isotropic: overall B = 1.0

Scattering factors Co<sup>0</sup>, Sb<sup>0</sup>, Ti<sup>0</sup> [Cromer and Mann, 1968]

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Scale factor (integrated intensities)

\gamma = 0.660 \times 10^{-3}
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References

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Cromer, D.T. and Mann, J.B. (1968). Acta Crystal-
logr. <u>A24</u>, 321.
Webster, P. J. and Ziebeck, K. R. A. (1973). J.
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Phys. Chem. Solids <u>34</u>, 1647.
```

Calculated Pattern (Peak heights)						
d (A)	I		hkl	λ	20(°) = 1.540598A	
7 70						
3.39	0 55	1	1	1	26.22	
2.94	2 35	2	0	0	30.36	
2.08	1 100	2	2	0	43.46	
1.11	4 20	3	1	1	51.48	
1.69	8 5	2	2	2	53.94	
1.47	1 15	4	0	0	63.16	
1.35	0 5	3	3	1	69.60	
1.31	6 5	4	2	0	71.68	
1.20	1 20	4	2	2	79.78	
1.13	24 5	5	1	1+	85.72	
1.04	01 5	4	4	0	95.56	
.99	46 5	5	3	1	101.52	
•98	06 5	4	4	2+	103.54	
.93	04 10	6	2	0	111.78	
•89	73 1	5	3	3	118.28	
			_			
•88	71 1	6	2	2	120.54	
•84	93 5	4	4	4	130.18	
•82	39 5	7	1	1+	138.42	
.81	60 1	6	4	0	141.48	
•78	63 15	6	4	2	156.86	

	Calculated	Pattern	(Int	egra	ated)
d (Å)	I		hkl		$2\Theta(\circ)$ $\lambda = 1.540598A$
7.707	50	,			26.21
2 042	30				20.26
2.0942	100	2	2	~	43.47
1.774	20	7	1	ĭ	51.47
1.600		2	2	2	53.04
1.075	, J	-	~	-	55094
1.471	15	4	ο	0	63.16
1.350	) 5	3	З	1	69.59
1.316	5 10	4	2	0	71.67
1.201	25	4	2	2	79.78
1.132	4 5	5	1	1	85.73
1.132	24 1	3	3	З	85.73
1.040	2 5	4	4	0	95.56
•994	6 5	5	3	1	101.52
.980	7 5	4	4	2	103.53
.980	7 1	6	0	0	103.53
•930	3 10	6	2	0	111.78
.897	3 1	5	3	З	118.29
.887	0 5	6	2	2	120.54
.849	3 5	4	4	4	130.19
.823	9 5	5	5	1	138.43
•823	9 5	7	1	1	138.43
.816	0 5	6	4	0	141.48
.786	50	6	4	2	156.86

```
Structure
  Cubic, F43m(216), Z = 4, isostructural with
  AgAsMg, from powder data [Kripyakevich and
  Markiv, 1963].
Atom positions
  4(d) 4 antimony
         4 cobalt
  4(a)
         4 vanadium
  4(c)
Lattice constant
  a = 5.796 Å [ibid.]
Volume
  194.71 A<sup>3</sup>
Density
  (calculated) 7.902 g/cm<sup>3</sup>
Additional pattern
  1. PDF card 26-104 [Terada et al., 1972]
Thermal parameters
  Isotropic: overall B = 1.0
Scattering factors Co^0, Sb^0, V^0 [Cromer and Mann, 1968]
Scale factor (integrated intensities)
  \gamma = 0.652 \times 10^{-3}
References
  Cromer, D. T. and Mann, J. B. (1968).
                                               Acta
    Crystallogr. A24, 321.
  Kripyakevich, P. I. and Markiv, V. Ya. (1963).
    Dopov. Akad. Nauk Ukr. RSR 12, 1606.
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Terada, M., Endo, K., Fujita, Y., and Kimura, R. (1972). J. Phys. Soc. Jap. 32, 91.

d (Å)	I	h	kl	$20(^{\circ})$ $\lambda = 1.5405982$	o A
3.346	50	1	1 1	26.62	
2.897	35	2	0 0	30.84	
2.049	100	2	2 0	44.16	
1.747	20	3	1 1	52.32	
1.673		2	2 2	54.82	
		-		JACL	
1.449	10	۵	0	64.22	
1.330	5	7	3 1	70.80	
1.296	5	4	2 0	72.04	
1.187	20	-	2 0	91 26	
1 115	20	-	~ ~	01+24	
1.115	5	5	1 14	. 87+36	
1 0 05	-				
1.025	5	4	4 0	97.50	
•980	5	5	31	103.68	
•966	5	4	4 21	105.76	
•916	10	6	20	114.40	
.884	1	5	33	121.26	
.874	1	6	2 2	123.66	
.837	5	4	4 4	134.08	
.812	5	7	1 14	143.28	
.804	1	6	4 0	146.82	

Calculated Pattern (Peak heights)

	Calculated	Pattern	(Integrated)				
å (A)	I		hkl	,	$20(^{\circ})$ $\lambda = 1.540598A$		
3.346 2.898 2.049 1.748	45 30 100 20	1 2 2 3	1 0 2 1	1 0 0 1	26.62 30.83 44.16 52.31		
1.673	5	2	2	2	54.82		
1.449 1.330 1.296 1.183 1.115 1.115 1.025 .980	15 5 10 25 5 1 5	4 3 4 5 3 4 5	0 3 2 2 1 3 4 3	0 1 2 1 3 0	64.23 70.80 72.93 81.25 87.35 87.35 97.49 103.67		
•966	5	4	4	2	105.77		
.916 .884 .874 .837 .812	10 1 5 5 5	6 5 6 4 5	23245	0 3 2 4 1	114.40 121.27 123.66 134.08 143.28		
.812	5	6	4	0	145.28 146.82		

Synonyms	(	Calculated	Pattern	(Pe	ak he	eights)
5,5-Diethylbarbituric acid, form I		т		bk0		20(0)
Veronal		T		IIK.		$\lambda = 1.540598A$
Diethylmalonylurea						
	13.46	14	1	1	0	6.56
Structure	7.77	100	З	0	0	11.38
Hexagonal, R3 (148), $Z = 18$ . The structure was	6.72	7	2	2	0	13.16
determined by Craven, Vizzini, and Rodrigues	6.54	8	1	0	1	13.52
[1969].	5.89	5	0	2	1	15.04
Atom positions	5.39	70	1	2	-1+	16.42
All atoms are in general positions 18(f).	5.09	65	1	4	0	17.42
	4.69	25	З	1	-1+	18.90
Polymorphism	4.48	9	3	З	0	19.78
Six forms of barbital have been reported though forms V and VI have not been isolated as single	4.21	8	3	2	1+	21.10
crystals. Form I described here is the most sta-	3.88	6.	6	0	0	22.88
ble. Crystals of forms I, II, and IV were obtained	3.85	7	0	5	1	23.08
from the same ethanol solution by slow evapora-	3.73	7	2	5	0	23.82
tion at room temperature [ibid.].	3.70	5	4	2	-1+	24.02
	3.57	8	5	1	1+	24.94
Lattice constants	7 76	1.4	A	•	0	26 49
a = 26.923(6) A	3.30	14	* *	4	-1-	26.66
C = 0.828(9)	3.28	2	2	ō	2	27.20
c/a = 0.2536	3.18	8	1	2	2	28.02
c/u = 0.2550	3.15	9	6	1	=1+	28.28
(published values: $a = 26.921(6) \stackrel{\circ}{A}$ , $c = 6.828(9)$						
[Craven et al., 1969]).	3.09	23	1	7	0+	28.90
	3.02	10	1	З	-2+	29.58
Volume .	2.994	5	5	З	-1+	29.82
4286.2 A <sup>3</sup>	2.938	4	0	4	2+	30.40
	2.877	3	2	З	2	31.06
Density			~	~	_	70.40
(calculated) 1.284 g/cm <sup>3</sup>	2.754	4	5	0	-14	32.48
(measured) $1.287(7)$ g/cm <sup>3</sup> [Craven et al., 1969]	2.645	2	1	5	2	33.86
Thermal parameters	2.629	11	7	2	= 1	34.08
Isotropic B estimated from Ry, Roo Roo for	2.590	4	. 9	ō	ō	34.60
each atom.						
	2.543	8	2	8	0	35.26
Scattering factors	2.490	2	4	6	1	36.04
$C^0$ , $H^0$ , $N^0$ , $O^0$ [International Tables, 1962]	2.418	1	4	7	0	37.16
	2.301	5	1	9	1+	39.12
Scale factors (integrated intensities) $\gamma = 2.484 \times 10^{-3}$	2.276	2	0	0	٩	39.50
I/I (calculated) 1.02	2.244	4	1	1	3+	40.16
corundum	2.213	3	1	10	0+	40.74
Additional patterns	2.178	1	9	2	1+	41.42
1. PDF card 5-129 [Huang, TY., 1951]	2.155	2	2 7	2	- 24	41.00
2. Williams [1959]. The pattern appears to represent a mixture of forms I and II.	2.019	2	,	5		43.30
	2.024	1	0	11	1	44.74
References	2.002	1	10	2	-1+	43.20
Craven, B.M., Vizzini, E.A., and Rodrigues, M.M.	1.030	2	2 C	<u>ح</u>	-3+	46.82
[1969]. Acta Crystallogr. <u>B25</u> , 1978.	1.923	1	2	11	- 1+	47.22
International Tables for X-ray Crystallography,	10923	•	2			
III (1962). (The Kynoch Press, Birmingham, Eng.)	1.867	1	10	4	0+	48.74
p. 202.	1.851	1	8	4	-2	49.18
Williams, P. P. (1959). Anal. Chem. <u>31</u> , 140.	1.846	1	8	6	-1	49.34
	1.739	2	9	7	27	52.72
		6	<u> </u>			

Barbital, form I,  $C_8H_{12}N_2O_3$  - (continued)

d (Å)	I	hkl $\lambda =$	20(°) = 1.540598Å
1.711	1	3 10 2+	53.52
1.696	1	3 12 0+	54.02
1.658	1	5 9 2+	55.38
1.634	2	1 12 - 2 +	56.26
1.618	1	0 14 1	56.86
1.607	1	2 13 1+	57.30

Calculated Pattern (Integrated)						
d(Å)	I	hkl	$2\Theta(^{\circ})$ , $\lambda = 1.540598A$			
13.46	14	1 1 0	6.56			
7.77	100	300	11.38			
6.73	7	2 2 0	13.14			
6.55	8	1 0 1	13.50			
5.89	5	0 2 1	15.02			
5.40	24	2 1 1	16.41			
5.40	48	1 2 -1	16.41			
5.09	69	1 4 0	17.42			
4.70	9	1 3 1	18.89			
4.70	17	3 1 -1	18.89			
4.49	× 10	330	19.77			
4.21	5	321	21.08			
4.21	4	2 3 -1	21.08			
3.89	7	600	22.87			
3.85	7	0 5 1	23.08			
3.73	6	2 5 0	23.81			
3.70	2	2 4 1	24.02			
3.70	3	4 2 -1	24.02			
3.57	6	5 1 1	24.92			
3.57	2	1 5 = 1	24.92			
3.37	15	4 4 0	26.46			
3.34	З	4 3 1	26.65			
3.34	9	3 4 = 1	26.65			
3.28	2	2 0 2	27.20			
3.18	8	1 2 2	28.01			
3.15	З	1 6 1	28.28			
3.15	6	6 1 -1	28.28			
3.09	8	7 1 0	28.89			
3.09	19	170	28.89			
3.02	4	3 1 2	29.56			
3.02	7	1 3 - 2	29.56			
2.994	2	701	29.82			
2.994	2	5 3 -1	29.82			
2.946	2	0 4 2	30.32			
2.938	2	630	30.40			
2.938	2	360	30.40			
2.922	2	6 2 1	30.57			
2.878	З	2 3 2	31.05			
2.755	4	5 0 2	32.48			
2.735	2	4 5 - 1	32.71			

d (Å)	I	hkl	20(°) = 1.540598A
2.646	3	1 5 2	33.85
2.629	13	7 2 -1	34.08
2.591	5	900	34.60
2.544	9	280	35.25
2.534	1	8 1 1	35.39
2.534	1	1 8 - 1	35.39
2.490	2	4 6 1	36.04
2.418	1	470	37.16
2.301	2	1 9 1	39.11
2.301	2	651	39.11
2.301	1	5 6 - 1	39.11
2.301	1	9 1 -1	39.11
2.276	3	0 0 3	39.56
2.244	1	1 1 - 3	40.15
2.244	2	1 1 3	40.15
2.244	1	6 6 0	40.16
2.217	2	8 0 2	40.67
2.213	2	1 10 0	40.74
2.177	1	921	41.44
2.156	1	223	41.87
2.156	1	2 2 - 3	41.87
2.080	1	7 3 - 2	43.47
2.078	1	4 1 3	43.53
2.053	1	8 5 0	44.08
2.024	1	0 1 1 1	44.73
2.002	1	10 2 -1	45.26
1.943	1	2 5 - 3	46.70
1.939	1	4 9 1	46.83
1.939	1	9 4 -1	46.83
1.851	1	8 4 -2	49.18
1.735	1	8 7 1	52.73
1.711	1	310 2	53.50
1.658	1	592	55.35
1.634	1	1 12 = 2	56.26
1.618	1	0 14 1	56.86

Synonyms	Cal	culated Pa	attern	(Pea	k he	eights)
5,5-Dietnyl barbituric acid	۵ (۳)	т		b1=0		20(8)
Veronal	U(A)	1		nĸĸ		$\lambda = 1.540598\lambda$
Diethylmalonylurea		· · - ·· ·				A 1.5405501
	7.08	4	o	2	o	12.50
Structure	6.36	4	1	1	0	13.92
Monoclinic, $C_2/C$ (15), $Z = 4$ . The structure was determined by Graven Vizzini and Podrigues	5.73	20	0	2	1	15.44
[1969].	5.36	36	1	1	1	16.54
[1505].	5.30	100	- 1	1	1	16.70
Atom positions	4.90	5	0	0	2	18-08
4(e) 4 C(2)	3.90	1	1	1	2	22.76
4(e) 4 C(5)	3.86	2	-1	1	2	23.02
4(e) $4 O(2)$	3.66	5	1	з	1	24.30
All other atoms in general positions 8(1) [ibid.]	3.54	5	0	4	0	25.14
Polymorphism			_			
Six forms of barbital have been reported though	3.33	1	0	4	1	26.76
forms V and VI have not been isolated as single	3.04	4	2	3	2	28.98
crystals. The hexagonal form I is the most stable.	2.968	9	0	2	3	30.08
Form II described here is the 2nd most stable.	2.893	2	-1	1	з	30.88
Crystals of forms I, II, and IV were obtained						
from the same ethanol solution by slow evaporation	2.863	14	-2	0	2	31.22
at room cemperature [ibid.].	2.682	З	2	2	2	33.38
Lattice constants	2.653	5	-2	2	2	33.76
a = 7.120(5) Å	2.543	2	1	5	1	35.26
b = 14.163(10)	2:524	C	1	3	5	35.54
c = 9.810(7)	2.340	1	з	1	0	38.44
$\beta = 89.23(3)^{\circ}$	2.294	1	2	2	3+	39.24
(published values: $a = 7.120(5)A$ , $b = 14.162(10)$ ,	2.278	1	- 1	1	4	39.52
$c = 9.810(7), \beta = 89^{\circ} 14(2)^{\circ}$ [Craven et al.,	2.243	1	2	4	2	40.18
1903]).	2.226	3	-2	4	2	40.50
CD cell: $a = 9.810(7)A$ , $b = 14.163(10)$ ,	1.953	1	2	2	^	46.46
$c = 7.120(5), \beta = 90.77(3)^{\circ}, \text{ sp. gp. } A2/a;$	1.947	1	1	7	0	46.62
a/b = 0.6926; c/b = 0.5027	1.931	1	2	6	1+	47.02
	1.891	2	-3	1	з	48.08
989.2 Å <sup>3</sup>	1.762	1	2	4	4+	51.84
L		·			_	
Density						
(calculated) 1.237 g/cm <sup>3</sup> (Groups at al. 1969)						
(measured) 1.238(7) g/cm <sup>3</sup> [Craven et al., 1969]						
Thermal parameters	Cal	culated Pa	attern	(Int	egra	ated)
Isotropic B. estimated from $\beta_{11}$ , $\beta_{22}$ , $\beta_{33}$ for each		т		bk l		20(0)
atom.	U(A)	-		1112~		$\lambda = 1.540598A$
Scattering factors	7.08	4	0	2	0	12.49
C°, H°, N°, O° [International Tables, 1962]	6.36	4	1	1	0	13.91
Scale factors (integrated intensities)	5.74	20	0	2	1	15.42
$\gamma = 5.144 \times 10^{-3}$	5.37	26	1	1	1	16.51
I/I (calculated) 2.12	5.31	100	- 1	1	1	16.69
Corundam	4.90	5	0	0	2	18.07
Additional patterns	3.91	1	1	1	2	22.74
1. PDF card 14-953 [Huang, 1951]	3.86	2	- 1	1	2	23.01
2. Williams [1959]. The pattern appears to	3.66	6	1	3	1	24.29
represent a mixture of forms i and if	3.54	6	0	4	0	25.13
References	<b>-</b> -		•			06 75
Craven, B. M., Vizzini, E. A., and Rodrigues, M.M.	3.08	1	1	4	2	28.96
(1969). Acta.Crystallogr. <u>B25</u> , 1978.	3.04	10	2	2	1	29.39
Huang, TY. (1951). Acta Pharm. Int. 2, 95.	2.969	10	0	2	з	30.08
International Tables of X-ray Crystallography,	2.894	1	-1	1	З	30.87
p. 202.						1
Williams, P. P. (1959). Anal. Chem. <u>31</u> , 140. 128						

Barbital, form II,  $C_8H_{12}N_2O_3$  - (continued)

d (Å)	I	ł	ıkl		$2\Theta(^{\circ}) \circ \\ \lambda = 1.540598 \text{\AA}$		
2.871	1	0	4	2	31.13		
2.863	16	-2	0	2	31.22		
2.683	3	2	2	2	33.37		
2.654	6	-2	2	2	33 34		
2 545		- 2	~	2	33 • 14		
2.345	2	1	5	1	35.23		
2.524	6	1	З	З	35.54		
2.340	1	З	1	0	38.43		
2.294	1	2	2	з	39.25		
2.279	1	-1	1	4	39.51		
2.243	1	2	4	2	40.17		
	-	-	•	-	40011		
2.226	٦	- 2	^	2	40.40		
1 067		2	7	2	40.49		
1.955	1	2	2	4	46.45		
1.946	1	1	7	0	46.63		
1.891	З	-3	1	З	48.07		
1.763	1	2	4	4	51.83		

Synonyms	Calc	ulated Pat	tern (Pe	ak heig	hts)
5,5-Diethylbarbituric acid Diemal Voropal	d (Å)	I	hkl		20(°) 。
Diethylmalonylurea				A	= 1.540598A
	11.04	77	0	2 0	8.00
Structure	6.49	100	0	1 1	13.64
Monoclinic, $P2_1$ (4), Z = 8. The structure was	5.93	9	1	0 1	14.94
determined by Craven and Vizzini [1971].	5.78	58	0	2 1	15.32
	5.47	69	2	20	16.20
Atom positions		_			
All atoms were in general positions 2(a). Posi-	5.28	3	-1	2 1	16.78
tions for hydrogen (72) (molecule 3) appeared to	5.22	2	1	21	10.90
be in error and were omitted from these calcula-	4.78	13	2	3 0	18.54
CIONS.	4.65	10	-2	0 1+	19.06
Polymorphism			_		
Six forms of barbital have been reported though	4.55	14	-2	1 1	19.50
forms V and VI have not been isolated as single	4.48	15	2	1 1	19.80
crystals. The phase described as form III may not	4.28	2	0	4 1+	20.72
exist [Craven and Vizzini, 1971]. Crystals des-	4.23	1	2	2 1	21.00
cribed here were hand-picked from the mixture of forms I. II. and IV. obtained from the same	4.15	10	2	40	21.40
ethanol solution by slow evaporation at room	4.04	5	1	4 1	21.98
temperature.	3.678	5	0	60	24.18
	3.613	21	2	50	24.62
Lattice constants	3.548	13	-3	1 1+	25.08
a = 12.586(8) Å	3.498	2	3	1 1	25.44
b = 22.084(10)	<b>-</b>	0	7	2 1	26 40
c = 6.788(9)	3.257	4	1	0 2	27.36
$\beta = 90.92(3)^{\circ}$	3.245	4	0	2 2	27.46
a/b = 0.5699	3.175	5	2	6 0	28.08
c/b = 0.3074	3.144	13	4	0 0	28.36
(n) (number of the second s	3.116	6	4	1 0	28.62
(published values: a = 12.565(6)A; b = 22.065(10), a = 6.788(0)	3.081	10	0	3 2	28.96
(19711).	3.004	17	-1	3 2+	29.72
	2.982	11	1	3 2+	29.94
Volume	2.968	10	2	02	30.08
1886.5 A <sup>3</sup>					
	2.940	4	2	1 2	30.38
Density	2.901	10	=2	2 2	30.80
(calculated) 1.297 g/cm <sup>3</sup>	2.824	10	-1	4 2	31.66
(measured) 1.296(7) g/cm <sup>3</sup> [Craven and Vizzini,	2.820	11	-1	7 0+	31.70
1971}	20020	••	-		
Thermal parameters	2.812	5	1	4 2	31.80
Isotropic for hydrogens: anisotropic for all	2.793	8	-1	71	32.02
others [Craven and Vizzini, 1971]	2.784	9	-2	3 2+	32.12
	2.753	6	2	3 2+	32.50
Scattering factors	2.735	2	4	4 0	32.72
$C^0$ , $H^0$ , $N^0$ , $O^0$ [International Tables, 1962]	0.650		-		77 60
	2.009	4	-3	1 2	33.04
Scale factors (integrated intensities)	2.624	6	- 5	5 2	34.14
$\gamma = 1.804 \times 10^{-3}$	2.599	5	3	1 2	34.48
I/I (calculated) 0.743	2.572	1	-3	6 1	34.86
Additional pattern	0.540	_	-	2 2	75 00
1. PDF card 5-0083 [Huang, 1951]	2.548	3	3	8 0	35.49
and the second se	2.502	4	2	8 14	35,86
References	2.466	2	3	3 2	36.40
Craven, B. M. and Vizzini, E. A. (1971). Acta	2.453	1	-1	6 2	36.60
Crystallogr. <u>B27</u> , 1917. Huang, TY. (1951). Acta Pharm. Int. <u>2</u> , 95. International <u>Tables for X-ray</u> <u>Crystallography</u> , III (1962) (The Kynoch Press Birmingham Eng.)		-			
p. 202.					

Barbital, form IV,  $C_8H_{12}N_2O_3$  - (continued)

d (Å)	I	hkl	λ	20(°) 。 = 1.540598A
2.371	1	-3 7	1+	37.92
2.358	2	-5 1	1+	38.14
2.348	2	5 0	1	38.30
2.310	4	C 7	2+	38.96
2.275	2	=4 2	2+	39.58
20210	-			07000
2.258	1	-5 3	1	39.90
2.241	1	4 2	2	40.20
2.217	2	-4 3	2+	40.66
2.185	2	4 3	2+	41.28
2.142	1	08	2	42.16
2.114	1	-1 8	2+	42.74
2.088	2	6 1	0+	43.30
2.073	1	5 5	1+	43.62
2.055	1	-4 5	2+	44.02
2.032	1	2 3	3+	44.56
0.017		6 7		44.00
2.017	1	<b>C</b> 3	0+	44.90
2.003	2	=5 2	2	45.24
1.998	3	5 1	2+	45.36
1.979	2	56	1+	45.82
1.973	2	-3 2	3+	45.96
1.962	2	64	0+	46.24
1.926	2	06	3+	47.14
1.910	2	33	3+	47.56
1.901	2	-2 9	2+	47.80
1.891	1	29	2+	48.08
1.885	1	-3 4	3+	48.24
1.865	1	-4 9	1	48.78
1.856	1	4 9	1	49.04
1.840	1	0 12	0+	49.50
1.825	1	-4 2	3+	49.92
1.803	1	-7 0	2+	50.58
1.798	1	-6 0	24	50.72
1.773	1	2 10	2+	51.54
1.750	1	6 0	2+	51.54
1 744	1		27	52.24
1.140	1	-0 3	2+	52.30
1.728	1	0 11	2+	52.96
1.711	1	-1 11	2+	53.50
1.693	1	5 7	2+	54.14
1.688	1	3 10	2+	54.30
1.639	1	-5 8	2+	56.06
	-		-	
1.589	1	4 12	0	58.00
1.569	1	1 5	4+	58.82

	Calculated	Pattern	(Int	egrat	ced)
d (A)	I		hkl	λ	20(°) = 1.540598A
11.04	74	0	2	0	8.00
6.49	100	0	1	1	13.64
5.93	8	1	0	1	14.92
5.80	9	-1	1	1	15.26
5.78	51	0	2	1	15.31
5.52	22	0	4	0	16.04
5.47	67	2	2	0	16.20
5.28	1	-1	2	1	16.77
5.23	4	1	2	1	16.95
4.99	43	0	3	1	17.76
4.78	13	2	3	0	18.54
4.66	4	-1	3	1	19.04
4.65	5	-2	0	1	19.06
4.62	1	1	3	1	19.20
4.58	4	2	0	1	19.37
4.55	12	■2	1	1	19.49
4.48	15	2	1	1	19.79
4.28	1	0	4	1	20.72
4.23	1	2	2	1	20.99
4.15	1	2	4	0	21.39
4.04 3.681 3.619 3.560 3.557	5 5 23 0 1 7 1	1 0 2 -1 -2	4 6 5 5 4	1 0 1 1	21.97 24.16 24.61 24.99 25.01
3.548 3.524 3.498 3.374 3.354	3     12       4     1       3     1       4     10       4     4	-3 2 3 3 0	1 4 1 2 1	1 1 1 2	25.08 25.25 25.44 26.40 26.55
3.263	3     3       4     1       4     2       7     5       3     2	1	0	2	27.31
3.254		-1	1	2	27.39
3.244		0	2	2	27.47
3.17		2	6	0	28.06
3.153		-1	2	2	28.28
3.140	5 11	4	0	0	28.35
3.130	0 4	1	2	2	28.50
3.120	8 1	1	6	1	28.51
3.119	5 4	4	1	0	28.64
3.082	2 10	0	3	2	28.95
3.020	6 3	4	2	0	29.50
3.007	7 8	-2	0	2	29.68
3.000	4 11	-1	3	2	29.72
2.983	3 6	1	3	2	29.93
2.983	2 2	3	4	1	29.94
2.98 2.96 2.94 2.90 2.89	0 2 7 8 1 3 1 10 3 2	= 2 2 -2 4	1 0 1 2 3	2 2 2 2 0	29.97 30.10 30.37 30.79 30.88

Barbital, form IV,  $C_8H_{12}N_2O_3$  - (continued)

d (Å)	I	hkl	$2\Theta(°)$ $\lambda = 1.540598A$
2.865 2.861 2.848 2.826 2.820	10 1 1 10 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	31.19 31.24 31.38 31.63 31.70
2.814 2.809 2.794 2.784 2.780	1 5 5 5	4 1 1 1 4 2 -1 7 1 -2 3 2 -4 2 1	31.77 31.83 32.01 32.13 32.18
2.761 2.752 2.733 2.659 2.641	2 5 1 4 1	0 8 0 2 3 2 4 4 0 -3 0 2 -2 4 2	32.41 32.51 32.74 33.68 33.92
2.640 2.638 2.625 2.614 2.600	4 1 5 1 5	-3 1 2 -1 5 2 1 5 2 2 4 2 3 1 2	33.93 33.95 34.13 34.28 34.47
2.572 2.547 2.528 2.503 2.467	1 3 4 4 2	-3 6 1 3 2 2 2 8 0 1 8 1 3 3 2	34.86 35.20 35.48 35.85 36.40
2.453 2.371 2.359 2.356 2.348	1 1 1 2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	36.61 37.92 38.12 38.17 38.31
2.311 2.276 2.258 2.241 2.218	4 1 1 1	0 7 2 -4 2 2 -5 3 1 4 2 2 -4 3 2	38.95 39.57 39.89 40.20 40.65
2.186 2.141 2.115 2.088 2.017	1 1 1 1	4 3 2 0 8 2 -1 8 2 6 1 0 6 3 0	41.27 42.16 42.72 43.30 44.90
2.003 1.998 1.979 1.972 1.961	1 2 1 1 1	-5 2 2 5 1 2 5 6 1 -3 2 3 6 4 0	45.22 45.35 45.81 45.97 46.27
1.927 1.910 1.891 1.866 1.856	1 1 1 1	0 6 3 3 3 3 2 9 2 -4 9 1 4 9 1	47.11 47.56 48.08 48.77 49.05

d (Å)	I	hk	cl	λ	20(°) = 1.540598A			
1.803	1	-3	9	2	50+57			
1.746	1	-6	З	2	52.36			
1.722	1	6	З	2	53.13			
1.693	1	5	7	2	54.13			
1.589	1	4	12	0	58.01			

20(°)

 $\lambda = 1.540598A$ 

5+

З 4+

2

-1

-2

З

2

8.26

9.94

11.28

12.50

13.12

14.80

15.24

15.36 16.64

17.08

17.48

18.28 19.80

20.30

20.52

21.18

21.78

22.54

22.86

24.08

24.52 25.12

25.40

26.50

26.76

27.22

27.54

29.56 29.82

30.10

30.78

31.44

31.70

32.34

32.64

32.84

33.30

33.72

34.34 34.64

35.14 35.48

36.06

36.12

36.28

36.76

37.04

37.64

37.86

38.08

0

Companya			-	1-		
Synonyms	Ca.	lculated	Pattern	(Pea	ik hei	.ghts)
5-Hydroxy-N, N-dimethyltryptamine	0					
3-(2-Dimethylaminoethyl)-indol-5-01	d (A)	I		hkl		2
Mappine					λ	= 1.
						·
Structure	10.70	1	0	0	1	ε
Monoclinic, $P_{1/a}$ (14), $Z = 8$ . The structure was	8.89	11	-1	1	1	ç
determined by Falkenburg [1972].	7.84	1	0	1	1	11
	7.08	26	-2	1	1	12
Atom positions	6.74	12	2	0	0	13
All atoms were in general positions 4(e) [ibid.].						
	5.98	40	-2	1	2	14
Lattice constants	5.81	16	2	1	0	15
$a = 17.95(1) \text{ \AA}$	5.76	11	0	2	0	15
b = 11.52(1)	5.32	51	- 1	2	1	16
c = 14.24(2)	5.19	18	-3	1	2	17
$\beta = 131.29(3)^{\circ}$			•	•		
	5.07	21	0	2	1	17
CD cell: $a=14.24(2)A$ , $b=11.52(1)$ , $c=13.70(1)$ .	A 95	67	ő	1	2	1.5
$\beta = 100.07(2)^{\circ}$ ; sp. gp. P21/n; a/b = 1.2361;	4.00	5	- 0	â	2	10
c/b = 1 1891	4 • 4 0	10	-4	2	2	1 -
C/D = 1:1051	4.37	16	-1	2	27	20
Maluma	4.32	19	-3	1	3+	20
				_	_	
2212.5 A°	4.19	46	-4	0	3+	21
	4.08	100	-4	0	1	21
Density	3.94	53	⇔4	1	3	22
(calculated) 1.226 g/cm <sup>3</sup>	3.89	5	1	1	2	22
(measured) 1.205 g/cm <sup>3</sup> [Falkenburg, 1972]	3.69	3	1	3	0+	24
Thermal parameters	3.63	3	-2	2	3	24
For hydrogens: overall $B = 5.0$ ; for other atoms,	3.54	27	3	2	0	25
isotropic $B_i$ estimated from $\beta_{11}$ , $\beta_{22}$ , $\beta_{33}$ for	3.50	15	-4	0	4	25
each atom.	3.36	7	-2	0	4+	26
	3.33	3	-4	2	1	26
Scattering factors						
C <sup>0</sup> , H <sup>0</sup> , N <sup>0</sup> , O <sup>0</sup> [International Tables, 1962]	3.27	17	3	1	1	27
	3.24	19	4	1	0	27
Scale factors (integrated intensities)	3.02	2	-3	2	4	29
$\gamma = 1.845 \times 10^{-3}$	2.994	2	-4	2	4	29
I/I (calculated) 0.602	2.967	1	-3	З	3+	30
corundum		_				
Additional pattern	2.903	12	-6	0	4+	3(
1. PDF card 26-1586 [Physical Data of Indole	2.843	6	2	2	2+	31
and Dihydroindole Alkaloids. Eli Lilly Co.,	2.820	ğ	-6	1	4+	31
edited by N Neussl	2.766	Å	-6	1	24	30
	2.700	7	-0		1	30
References	20141	5	-2	-	•	52
Falkenburg G (1972) Acta Crystallogr B28	0 705	5	-5	1	6	-
$\frac{1}{2210}$	2.725	5	-3		5	32
J219.	2.088	2	-3	1	57	
International Tables for X-ray Crystallography,	2.050	2	-2	4	2+	33
<u>111</u> (1962). (The Kynoch Press, Birmingham, Eng.)	2.609	2	3	1	2+	36
p. 202.	2.587	2	-4	3	4+	34
	0.550	-		~	E .	
	2.552	3	-4	2	5+	35
	2.528	3	-2	3	4+	35
	2.489	2	2	З	2	36
	2.485	2	-5	З	4	36
	2.474	2	-7	1	3	36
	2.443	4	5	2	0	30
	2.425	2	0	2	4+	37
	2.388	1	-7	1	5	37

2.374

2.361

Bufotenine,  $C_{12}H_{16}N_20$  - (continued)

å (A)	I		hkl		20(°)
					- 1. 540590A
2.345	5 3	-6	2	1	38.36
2.252	2 1	0	5	1	40.00
2.239	2	-5	4	3+	40.24
2.212	2 2	-8	0	5+	40.76
2.186	2	-2	4	4+	41.26
2.097	7 2	-8	0	6+	43.10
2.063	3 2	-8	1	€	43.84
2.040	1	-8	0	2	44.38
2.023	3 2	-7	2	1+	44.76
2.019	) 3	-1	3	5+	44.86
2.001	. 1	1	з	4	45.28
1.997	2	-6	З	6+	45.38
1.969	9 1	5	4	0+	46.06
1.933	5 1	-8	0	7+	46.96
1.901	2	7	1	0+	47.82
1.841	. 2	-8	1	1+	49.46
1.836	1	-1	5	4	49.62
1.759	1	-10	1	6+	51.94
1.747	1	-4	з	7+	52.32
1.722	1	7	3	0+	53.16
1.702	2 1	-10	1	7+	53.82
1.665	5 1	-5	2	8+	55.12
1.628	1	-10	0	8+	56.46
1.577	, 1	- 9	2	1+	58.46
	0.1	Detter	17.		
	Calculated	Pattern	(Int	legra	tea)

d (A)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
10.70	1	0	0	1	8.26
8.97	1	-2	0	1	S.85
8.90	10	-1	1	1	9.93
7.84	1	0	1	1	11.28
7.08	24	-2	1	1	12.50
6.74	11	2	0	0	13.12
5.99	38	-2	1	2	14.78
5.82	11	2	1	0	15.21
5.80	з	-1	1	2	15.25
5.76	7	0	2	0	15.37
5.35	11	0	0	2	16.56
5.33	42	-1	2	1	16.63
5.30	4	1	2	0	16.72
5.19	16	-3	1	2	17.06
5.11	3	-3	1	1	17.34
5.07	18	0	2	1	17.47
4.85	60	0	1	2	18.27
4.85	6	-2	2	1	18.29
4.48	4	-4	0	2	19.78
4.45	1	-2	2	2	19.93
	_			-	
4.38	5	2	2	0	20.26
4.37	11	-1	2	2	20.29
4.33	13	-3	1	3	20.49
4.32	5	1	2	1	20.53
4.21	E.	2	1	1	21.11
					1

d(Å)	I	hkl	$2\Theta(^{\circ})$ $\lambda = 1.540598A$
4.19	32	-4 0	3 21.16
4.19	13	31	0 21.20
4.18	2	-4 1	2 21.25
4.09	1	-3 2	2 21.69
4.08	100	-4 0	1 21.77
4.05	1	-3 2	1 21.92
3.95	1	-1 1	3 22.51
3.94	52	-4 1	3 22.54
3.92	1	0 2	2 22.67
3.88	2	1 1	2 22.87
3.70	1	-1 3	1 24.01
3.69	1	1 3	0 24.08
3.63	З	-2 2	3 24.50
3.54	25	32	0 25.11
3.54	2	-4 2	2 25.15
3.53	1	-2 3	1 25.21
3.51	14	-4 0	4 25.39
3.37	2	4 0	0 26.41
3.37	З	-2 3	2 26.44
3.36	3	-2 0	4 26.51
3.35	1	-4 1	4 26.56
3.33	2	-4 2	1 26.76
3.28	16	3 1	1 27.20
3.27	2	2 0	2 27.25
3.24	19	4 1	0 27.54
3.23	1	-2 1	4 27.63
3.02	1	-3 2	4 29.55
2.994	2	-4 2	4 29.81
2.909	9	-6 0	4 30.71
2.902	4	-2 2	4 30.78
2.898	1	1 1	3 30.83
2.894	5	-6 1	3 30.88
2.850	2	-6 0	2 31.36
2.846	2	-4 0	5 31.40
2.844	З	2 2	2 31.43
2.821	3	-1 4	1 31.69
2.820	5	-6 1	4 31.70
2.811	1	1 3	2 31.81
2.796	1	-4 3	1 31.99
2.767	1	-5 2	1 32.32
2.767	3	-6 1	2 32.33
2.763	1	-4 1	5 32.37
2.742	З	-2 4	1 32.63
2.725	5	-5 1	5 32.85
2.690	1	-3 1	5 33.28
2.664	1	-2 4	2 33.61
2.657	1	1 2	3 33.71
2.610	1	3 1	2 34.33
2.589	1	-4 3	4 34.62
2.587	1	-6 1	5 34.65
2.552	2	-4 2	5 35.14
2.529	2	-2 3	4 35.47
2.490	2	2 3	2 36.05
2.484	1	-5 3	4 36.14
2 477	-	-7 1	7 76.20

Bufotenine,  $C_{12}H_{16}N_20$  - (continued)

d (Å)	I	ł	nkl	;	$20(^{\circ})$ $\lambda = 1.540598A$
2.443	5	5	2	0	36.76
2.426	1	0	2	4	37.02
2.423	1	-4	4	2	37.07
2.389	1	-7	1	5	37.62
2.380	1	-1	3	4	37.76
2.374	1	-4	4	з	37.86
2.345	2	-6	2	1	38.36
2.252	1	õ	5	1	40.00
2.212	•	-8	õ	5	40.76
2.187	2	-2	4	4	41.25
	_	-			
2.097	1	-8	0	6	43.09
2.063	2	-8	1	6	43.84
2.039	1	-8	0	2	44.38
2.023	2	-7	2	1	44.75
2.019	1	-4	5	з	44.85
2.016	2	-1	3	5	44.92
2.001	1	1	3	4	45.27
1.901	1	1	6	0	47.81
1.900	1	7	1	0	47.83
1.841	1	-8	1	1	49.46
1.835	1	-1	5	4	49.65
1.702	1	-10	1	7	53.81
1.628	1	-10	0	в	56.47
1.577	1	-9	2	1	58.46

Calcium Borate, CaB<sub>2</sub>0<sub>4</sub>

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Structure	Ca	alculated F	Pattern	(Pea	ak he	eights)
Orthorhombic, $Pnca(60)$ , $Z = 4$ . The structure	0 (7)			440		20 (9)
was determined by Marezio et al. [1963].	d(A)	T		ΠKĩ		$2 \Theta(^{2})$
Atom positions			· · · · · · · · · · · · · · · · · · ·			x 1.540550m
4(c) 4 calcium	5.80	13	0	2	0	15.26
8(d) 8 boron	4.019	1	0	1	1	22.10
8(d) 8 oxygen(1)	3.373	50	1	1	1	26.40
8(d) 8 oxygen(2) [ibid.]	3.106	19	2	0	0	28.72
	3.002	100	2	1	0	29.74
Lattice constants						
a = 6.214(3) Å	2.901	20	0	4	0	30.80
b = 11.605(4)	2.872	16	0	З	1	31.12
c = 4.285(1) [ibid.]	2.738	13	2	2	0	32.68
	2.606	39	1	З	1	34.38
a/b = 0.5355 c/b = 0.3692	2.458	1	2	1	1	36.52
0,5 0,502	2.308	2	2	2	1	39.00
Volume	2.240	12	1	4	i	40.22
$309.0 A^3$	2.143	28	0	0	2	42.14
	2.121	22	2	4	0	42.60
Density	2.040	3	0	5	ĩ	44.36
(calculated) 2.702 g/cm <sup>3</sup>		-	•	-	-	
(	2.025	1	1	0	2	44.72
Thermal parameters	2.010	9	0	2	2	45.08
Anisotropic [Marezio et al., 1963]	1.995	2	1	1	2	45.42
-	1.939	46	1	5	1	46.82
Scattering factors	1.912	6	1	2	2	47.52
Ca <sup>0</sup> , B <sup>0</sup> , O <sup>0</sup> [International Tables, 1962]						
	1.901	7	2	4	1	47.82
Scale factors (integrated intensities)	1.859	2	2	5	0	48.96
$\gamma = 0.289 \times 10^{-3}$	1.841	37	3	1	1	49.46
I/I (calculated) = 1.05	1.763	3	2	0	2	51.80
(hkl = 210  as scale reflection)	1.743	5	2	1	2	52.44
	1.723	з	0	4	2	53.10
Additional patterns	1.696	1	1	6	1	54.04
1. PDF card 18-281 [Stojanovic, Inst. for	1.687	6	2	2	2	54.32
Refractories, Kraljevo, Yugoslaviaj	1.680	9	З	З	1	54.58
2. PDF card 23-407 [Fletcher et al., 1974]	1.661	1	1	4	2	55.26
References	1.642	0	2	6	•	55 06
Fletcher, B. L., Stevenson, J.R. and Whitaker,	1.605	1	2	3	2	57.36
A. (1974). J. Am. Ceram. Soc. <u>53</u> , 95.	1.569	1		4	1	58.82
International Tables for X-ray Crystallography	1.553	ī	4	ò	0	59.46
III (1962). (The Kynoch Press, Birmingham,	1.546	1	0	7	1	59.76
Eng.) pp. 202, 204.		-	-		-	
Marezio, M., Plettinger, H. A., and Zacharia-	1.533	2	2	6	1	60.32
sen, W. H. (1963). Acta Crystallogr. <u>16</u> ,	1.507	8	2	4	2	61.48
390.	1.500	13	4	2	0+	61.78
	1.489	1	3	0	2	62.30
	1.477	1	З	1	2	62.86
	1.454	1	3	5	1	64.00
	1.450	1	4	1	1	64.18
	1.442	2	4	З	0+	64.58
	1.436	1	0	6	2	64.88
	1.417	1	0	1	3+	65.84
	1.404	1	2	5	2	66.54
	1.399	1	1	6	2	66.82
	1.390	1	3	З	2	67.32
	1.382	1	1	1	З	67.74
	1.369	2	4	4	0	68.46

I
Calcium Borate,  $CaB_{2}0_{4}$  - (continued)

d (A)	I	hkl	20(°)
	••••		$\lambda = 1.540598A$
1 767			
1.300	1	1 2 3	69.38
1.325	2	0 3 3	70.18
1.314	1	3 4 2	71.10
1.310	2	280	71.76
1.510	4	1 3 3	72.04
1.303	5	262	72.46
1.290	1	2 1 3	73.34
1.283	1	172	73.80
1.267	1	223	74.92
1.257	1	2 8 1+	75.62
1.255	1	1 4 3	75.74
1.254	1	3 5 2	75.82
1.239	1	3 7 1	76.88
1.236	2	4 5 1	77.10
1.229	3	4 2 2	77.62
1.216	1	0 5 3	78.58
1 201	6	1 9 1+	79.00
1.106	1	0 8 2	79.78
1 104	1	4 3 2	80.20
1.194	2	1 5 3	80.38
1.191	З	290	80.60
1.188	2	5 1 1	80.88
1 •185	3	2 4 3	81.12
1.180	1	1 8 2	81.54
1.170	4	3 1 3+	82.36
1.160	٦	0.10 0	07.10
1.154	2	4 4 2	03.10
1.145	1	3 8 1	84.56
1.141	2	5 3 1	84.96
1.133	1	2 5 3+	85.68
			00.00
1.125	1	3 3 3	86.42
1.120	2	282	86.88
1.102	1	1 10 1	88.66
1.0871	1	2100	90.24
1.0820	1	073	90.78
1.0776	1	263	91.26
1.0712	1	0 0 4	91.96
1.0660	2	173	92.54
1.0604	4	4 8 0+	93.18
1.0543	3	4 6 2	93.88
1.0536	2	0 0 0	
1.0490	1	3 5 3	93.96
1.0471	1	4 1 7	94.50
1.0410	1	2 9 2	94.72
1.0385	1	1 2 4+	95.40
1.0357	1	600	96.10
1.0317	1	610	96.60
1.0217	1	2 7 3	97.86
1.0100	2	0 10 2	98.04
1.0196	2	620	98.14

d(Å)	I	hkl	,	$2\Theta(^{\circ})$ ° = 1.540598Å
1.0127	1	2 0	4	99.04
1.0108	1	1 11	1	99.30
1.0082	1	54	2	99.64
1.0045	1	1 8	3+	100.14
1.0020	1	47	2+	100.48
•9990	1	2 11	0	100.90
•9977	1	22	4	101.08
•9920	1	1 4	4+	101.88
•9854	1	3 10	1	102.84
•9797	1	23	4	103.68
•9754	1	64	0+	104.32
•9687	2	57	1+	105.34
•9671	1	0 12	0+	105.60
•9578	2	4 5	3	107.08
•9562	1	2 4	4	107.34
•9502	2	48	2	108.32
•9459	1	19	3	109.04
•9390	1	32	4	110.24
•9346	1	51	3	111.02
•9325	1	60	2	111.40
•9266	1	16	4	112.46
•9257	1	52	3	112.64
•9234	1	2 12	0+	113.06
•9207	2	62	2	113.58
•9183	4	3 11	1	114.04
•9130	1	66	0+	115.06
•9112	1	53	З	115.42
•9041	1	34	4	116.86
•9020	1	57	2+	117.30
•9004	1	49	2	117.64
.8972	1	26	4	118.32
•8929	1	66	1	119.24
.8922	1	54	3	119.40
•8905	1	1 7	4	119.76

## Calcium Borate, $CaB_2O_4$ - (continued)

20(°)

 $\lambda = 1.540598A$ 

65.83

65.90

66.53

66.83

67.32

67.63

67.74

68.45

68.63

69.37

70.03

70.08

70.18

71.10

71.75

72.04

72.46

73.35

73.80

74.92

75.61

75.72

75.84

76.88

77.09

77.52

77.61

78.58

78.99

79.00

79.77

80.19

80.37

80.60

80.90

81.12

81.56

82.36 82.43

83 . 18

83.76

84.56

84.97

85.61

85.69

86.42

86.87

88.51

88.66

90.23

1 З

2 1

5 2

6 2

з 2

1 з

4 0

З 1

2 З

6 1

3 З

З З

6 2

1 з

7 2

2 З

8 1 4

2 2

5 з

6 0

9 1

3 2

9 0

1 1

4 З

1 З

2 1

4 2

7 0

3 З

4 1

1

1

2

0

з

2

1

1

З

2 8

З

2

0

1

1

З

2

1

0

0

			-47					
hk	I	d (Å)	20(°) = 1.540598A	λ	hkl		I	å (Å)
0 1	1	1.418	15.26	0	2	0	13	5.80
4 2	1	1.416	22.10	1	1	0	1	4.020
2 5	1	1.404	26.39	1	1	1	53	3.375
16	1	1.399	28.71	0	0	2	20	3 • 1 0 7
3 3	1	1.390	29.61	1	2	1	29	3.014
27	1	1.384	29.74	0	1	2	100	3.001
1 1	2	1.382	30.79	0	4	0	21	2.901
4 4	3	1.370	31.12	1	З	0	16	2.871
4 3	1	1.366	32.67	0	2	2	15	2.739
1 2	1	1.354	34.38	1	З	1	44	2.607
з е	1	1.342	36.52	1	1	2	1	2.458
1 8	1	1.342	39.00	1	2	2	2	2.308
0 3	3	1.340	40.21	1	4	1	14	2.241
3 4	1	1.325	42.14	2	0	0	33	2.143
28	2	1.314	42.60	0	4	2	25	2.121
1 3	4	1.310	42.85	1	з	2	2	2.109
2 6	6	1.303	44.35	1	5	0	4	2.041
2 1	1	1.290	44.70	2	0	1	1	2.025
1 7	1	1.283	45.07	2	2	-	11	2.010
2 2	1	1.266	45.42	2	1	1	2	1.995
2 8	1	1.257	46.82	1	5	1	56	1.939
1 4	1	1.255	46.94	0	6	0	1	.934
3 5	1	1.253	47.51	2	2	1	6	.912
3 7	1	1.239	47.82	1	4	2	7	.901
4 5	1	1.236	48.95	ō	5	2	1	•859
2 3	1	1.230	10.14			7		
4 2	- 3	1.229	49.46	1	1	3	46	. 364
0 5	1	1.216	51.79	2		2	4	1.704
4 6	2	1.211	52.43	2	1	2	6	1 707
1 9	5	1.211	54.03	2	6	1	4	1.696
0 1	1	1.201						
4 -	1	1.196	54.32	2	2	2	7	1.688
1 9	3	1.194	54.59	1	3	3	10	.680
2 0	3	1.191	55.27	2	4	1	1	1.661
5 1	2	1.187	55.95	2	6	2	9	1.642
2 4	7	1,185						
1 5	1	1.179	58.82	1	4	3	1	1.569
3 1	5	1.170	59.45	0	0	4	1	1.553
5 3	1	1.169	59.76	1	7	0	1	1.546
0 10	4	1.161	60.32	1	6	2	2	1.526
			00.03	2	5	1	1	1.520
4 4	3	1.154	61.47	2	4	2	10	1.507
5 6	1	1.145	61.77	0	2	4	8	1.501
4	5	1.174	61.78	1	7	1	8	1.500
2 4	1	1.134	62.30	2	0	З	1	1.489
2	•	1.133	62.87	2	1	3	1	1.477
3 3	2	1.125	63.99	1	5	3	1	1.454
2 1	3	1.120	64.23	1	1	4	1	1.449
5 4	1	1.104	64.56	2	2	З	1	.442
1 10	1	1.102	64.60	0	З	4	2	•442
2 1	1	1.0871	64.90	2	6	0	1	. 476

Calcium Borate,  $CaB_2^0_4$  - (continued)

d(A)	I	hk	l	20(°) 。
				$\lambda = 1.540598A$
1.0821	1	07	3	90.77
1.0777	1	26	3	91.25
1.0750	1	5 0	2	91.54
1.0713	1 7	0 0	4	91.95
1.0001	3	1 (	3	92.53
1.0615	2	5 5	1	93.05
1.0606	2	3 9	1	93.15
1.0603	3	4 8	0	93.19
1.0557	1	1 0	4	93.72
1.0544	3	4 6	2	93.87
1.0534	2	0 2	4	93.98
1.0489	1	3 5	3	94.51
1.0472	1	4 1	3	94.72
1.0409	1	29	2	95.46
1.0391	1	3 0	. 2	95+69
1.0386	1	1 2	4	95.74
1.0358	ī	5 3	2	96.09
1.0357	1	6 0	0	96.11
1.0346	1	4 2	3	96.24
1.0316	1	6 1	0	96.62
1.0219	1	27	3	97.84
1.0204	3	0 10	2	98.03
1.0196	2	6 2	0	98 • 14
1.0184	1	1 3	4	98.29
1.0127	1	2 0	4	99.04
1.0108	1	1 1 1	1	99.30
1.0089	1	2 1	4	99.55
1.0081	1	5 4	2	99.66
1.0049	1	0 4	4	100.08
1.0044	1	1 8	3	100.16
1.0029	1	6 1	1	100.36
1.0020	1	4 7	2	100.49
•9990	1	2 11	0	100.90
•9977	1	2 2	4	101.09
.9920	-	1 4	4	101.88
•9853	1	3 10	1	102.85
.9797	1	2 3	4	103-67
.9754	1	6 4	0	104.32
.9695	1	2 10	2	105.23
.9687	з	57	1	105.35
•9672	1	28	З	105.58
.9671	1	0 12	0	105.60
• 9666	1	4 9	1	105.67
.9591	1	3 7	3	106.86
.9310	3	4 5	3	107.08
•9562	1	2 4	4	107-34
.9515	1	3 0	4	108.10
•9511	1	6 4	1	108.18
•9503	3	4 8	2	108.31
•9460	1	1 9	З	109.04

d (Å)	I	hkl		20(°)
			<u> </u>	$\lambda = 1.540598A$
	_			
•9390	1	32	4	110.24
•9345	1	51	3	111.03
•9327	1	1 12	1	111.36
•9324	1	60	2	111.40
.9294	1	61	2	111.95
•9266	1	16	4	112.46
•9256	1	52	3	112.66
•9234	1	2 1 2	0	113.07
.9217	1	58	1	113.38
.9206	3	62	2	113.59
.9182	5	3 11	1	114.04
•9154	1	3 10	2	114.60
.9147	1	29	3	114.73
.9130	1	6 6	0	115.06
.9112	1	5 3	3	115.42
.9041	1	3 4	4	116.85
.9020	1	57	2	117.30
.9003	1	4 9	2	117.65
.8972	2	2 6	4	118.31
.8930	1	6 6	1	119.23
	-		_	
.8921	1	5 4	3	119.41
.8905	1	1 7	4	119.78
	-			

Structure	Ca
phase, isostructural with MgZn <sub>2</sub> , from powder data [Ganglberger et al., 1965].	d (Å)
Atom positions 6(h) 3 chromium(1) and 3 cobalt(1) 2(a) 1 chromium(2) and 1 cobalt(2) 4(f) 4 niobium [Friauf (1927); Faller and Skolnick (1963)] Lattice constants a = 4.849 Å c = 7.907 [Ganglberger et al., 1965] c/a = 1.6306 Volume 161.01 Å <sup>3</sup>	3.708 2.879 2.424 2.232 2.100 2.067 2.029 1.976 1.854 1.789 1.480 1.473
Density (calculated) 8.409 g/cm <sup>3</sup>	1.400 1.360 1.319
Thermal parameters Isotropic: overall $B = 1.0$ Scattering factors Co <sup>0</sup> , Cr <sup>0</sup> , Nb <sup>0</sup> [Cromer and Mann, 1968]	1.263 1.258 1.238 1.212
Scale factor (integrated intensities) $\gamma = 0.320 \times 10^{-3}$	1.120 1.116 1.091 1.065
References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u> , 321. Faller, J. G. and Skolnick, L. P. (1963).	1.050
<ul> <li>Frans. AIME <u>227</u>, 687.</li> <li>Friauf, J. B. (1927). Phys. Rev. <u>29</u>, 34.</li> <li>Ganglberger, E., Nowotny, H., and Benesovsky,</li> <li>F. (1965). Monatsh. Chem. <u>96</u>, 1658.</li> </ul>	1.014 1.003 .962 .938
	.920 .916 .915 .905 .893
	•875 •872 •866

	Calculated	Pattern	(Pea	ak h	eights)
d (7)	τ.		<b>bk</b> 0		20 ( 8 )
u(A)	T		ΠKŁ		$\lambda = 1.540598A$
				_	
3.708	1	1	0	1	23.98
2.879	5	1	0	2	31.04
2.424	50	1	1	0	37.06
2.232	85	- 1	0	3	40.38
2.100	15	2	ō	ō	43.04
2.067	100	1	1	2	43.76
2.029	70	2	0	1	44.62
1.976	10	0	0	4	45.88
1.854	5	2	0	2	49.10
1.789	5	1	0	4	51.02
1.480	5	1	0	5	62.74
1.473	1	2	1	2	63.06
1.400	5	3	0	0	66.78
1.360	25	2	1	3	69.02
1.319	15	3	0	2	71.44
1.263	20	2	0	5	75.16
1.258	5	1	0	6	75.54
1.238	5	2	1	4	76.98
1.212	15	2	2	0	78.90
1.120	5	2	1	5	86.88
1.116	5	2	0	6	87.28
1.091	1	1	0	7	89.86
1.065	10	3	1	З	92.62
1.050	1	4	0	0	94.40
1.041	5	4	0	1	95.50
1.033	5	2	2	4	96.38
1.014	1	2	1	6	98.88
1.003	1	3	1	4	100.28
.962	5	1	0	8	106.38
•938	1	3	1	5	110.44
.920	1	2	1	7	113.66
•916	5	4	1	0	114.40
•915	5	1	1	8	114.62
.905	5	3	2	3	116.70
•893	10	4	1	2+	119.28
.875	5	4	0	5	123.46
.872	5	з	1	6	123.98
.866	1	3	2	4	125.62
.860	1	1	0	9	127.22
•839	5	2	1	8	133.30
.823	1	з	2	5	138.86
.821	5	4	0	6	139.48
.811	1	3	1	7	143.60
.808	1	3	3	0	144.78
.807	5	З	0	8	145.12
.800	5	5	0	з	148.56
.794	1	4	2	0	152.16
.792	5	З	з	2	153.24
	-				

Chromium	Cobalt	Niobium,	CoCrNb -	(continued)
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Ca	lculated P	attern (	Inte	grat	ed)
d (Å)	I	ł	ıkl	λ	20(°) = 1.540598Å
3 700			0	1	23.07
2.879	5	1	0	2	31.04
2.424	50	1	1	0	37.05
2.232	85	1	ō -	र २	40.37
2.100	15	2	0	0	43.04
2.067	100	1	1	2	43.76
2.029	70	2	0	1	44.62
1.977	10	0	0	4	45.87
1.854	5	2	0 3	2	49.09
1.789	5	1	0	4	51.02
1.480	5	1	0	5	62.73
1.473	1	2	1 .	2	63.06
1.400	5	3	0	0	66.77
1.360	25	2	1 :	3	69.02
1.320	20	З	0	2	71.43
1.318	5	0	0	б	71.54
1.263	20	2	0	5	75.15
1.257	1	1	0	6	75.56
1.238	5	2	1 .	4	76.98
1.212	20	2	2	0	78.90
1.120	5	2	1	5	86.88
1.116	5	2	0 (	б	87.28
1.091	1	1	0	7	89.85
1.065	10	3	1	3	92.62
1.050	1	4	0	0	94.40
1.041	5	4	0	1	95.49
1.033	5	2	2 4	4	96.39
1.014	1	2	1 (	6	98.88
1.003	1	3	1 4	4	100.28
•962	5	1	0	8	106.39
.938	5	З	1 :	5	110.45
•920	5	2	1	7	113.65
•916	5	4	1 (	0	114.41
•915	5	1	1	8	114.63
.905	10	3	2	5	116.71
.893	10	4	1	2	119.28
.892	5	2	2	0	127 45
.873	10	4	1	5	123.45
.866	1	3	2	4	125.61
.860	1	1	0	•	127-21
.839	5	2	1	8	133.30
.823	5	3	2	5	138.86
.821	5	4	0	6	139.47
.811	5	3	1	7	143.60
.808	5	3	3	0	144.78
.807	5	3	0	в	145.13
.800	5	5	0	3	148.56
.794	5	4	2	0	152.16
•792	10	З	З :	2	153.24

```
Structure
  Hexagonal, P6_3/mmc(194), Z = 4, a ternary Laves
  phase, isostructural with MgZn2, from powder
  data [Kuo, 1953].
Atom positions
  6(h) 3 chromium(1) and 3 cobalt(1)
  2(a)
         1 chromium(2) and 1 cobalt(2)
  4(f) 4 tantalum
  [Friauf (1927); Faller and Skolnick (1963)]
Lattice constants
  a = 4.856 \text{ Å}
  c = 7.952 [Kuo (1953), table II]
  c/a = 1.6376
Volume
 162.4 Å<sup>3</sup>
Density
 (calculated) 11.94 g/cm<sup>3</sup>
Thermal parameters
 Isotropic: tantalum B = 0.75; chromium B = 1.0;
  cobalt B = 1.0
Scattering factors
Co<sup>0</sup>, Cr<sup>0</sup>, Ta<sup>0</sup> [Cromer and Mann, 1968]
Scale factor (integrated intensities)
 \gamma = 0.599 \times 10^{-3}
References
  Cromer, D.T. and Mann, J.B. (1968). Acta Crys-
    tallogr. A24, 321.
  Faller, J.G. and Skolnick, L.P. (1963). Trans.
    AIME 227, 687.
  Friauf, J. B. (1927). Phys. Rev. 29, 34.
  Kuo, K. (1953). Acta Met. 1, 720.
```

	Calculated	Pattern	(Pea	k he	eights)
d (Å)	I		hkl		$20(^{\circ})$ $\lambda = 1.540598 ^{\circ}$
4.20 3.97	3 20 3 15	1	0 0	0 2	21.12 22.36
3.71	7 20 B 20 B 75	1	0	1 2	23.92 30.94
2.24	3 100	1	0	3	40.18
2.10	3 15 2 90	2	0	0 2	42•98 43•64
2.03	3 45 8 5	2	0	1 4	44•54 45•60
1.79 <sup>-</sup> 1.64	7 5 7 5	1 2	0 0	4 3	50.76 55.76
	9 5 9 5 7 10	2	1 1 0	0 1 5	57.98 59.24 62.38
		•	Ť	0	02000

	0					
	d (A)	I		hkl		20(°)
						$\lambda = 1.540598A$
-				_		
	1.476	5	2	1	2	62.92
	1.402	10	З	0	0	66.66
	1.363	30	2	1	3	68.82
	1.325	5	0	0	6	71.08
	1.322	20	-	0	2	71.28
	1.022	20	5	v	~	71.20
			~	•	_	
	1.269	20	2	0	5	74.78
	1.241	1	2	1	4	76.70
	1.214	15	2	2	0	78.76
	1.166	1	З	1	0	82.66
	1.163	5	1	1	6	82.92
	1.161	5	2	2	2	83.14
	1 150	ĩ	-			07 74
	1.154	1	3	1	1	03.74
	1.124	10	2	1	5	86.50
	1.121	10	2	0	6	86.78
	1.119	5	З	1	2	87.04
	1.097	1	1	0	7	89.24
	1.068	15	्य	1	3	92.36
	1.051	1	~	ā	õ	94.22
	1.051	-	7	~		94.22
	1.042	5	4	0	1	95.30
	1.036	1	2	2	4	96.06
	1.018	1	2	1	6	98.36
	.977	1	4	0	З	104.04
	.967	5	1	0	8	105.56
	-965	1	3	2	0	105.94
	. 96 7	-	-	-	6	106.20
	.903	-	5	v	0	100+24
ł		-	_		-	100.04
	•941	5	3		5	109.90
	•938	5	3	2	2	110.38
	•924	1	2	1	7	112.92
	•920	5	1	1	8	113.72
	.918	10	4	1	0	114.16
	.907	10	з	2	з	116.34
	.890	1	2	0	8	118.00
	005	-	2	2	4	118.74
	•095	5	2	~	2	110.04
	.894	10	4	-	2	118.90
	•877	5	4	0	5	122.88
		_	_			107.04
	.876	5	3	1	6	123.24
	•865	1	1	0	9	125.96
	•843	5	2	1	8	132.12
	.825	5	3	2	5	138.08
	.824	5	4	0	6	138.52
		•		Ť		
	.814	1	٦		7	142.36
	011	-	3	•	6	143 60
	•011	5	5	0	0	143.02
	.809	5	3	3	0	144.28
1	.802	5	5	0	3	147.82
	•795	1	4	2	0+	151.50
	.793	5	З	3	2	152.48
	•791	5	4	2	1	153.82

	Calculated	Pattern	(Int	egra	ated)
d (A)	I		hkl		20(°) 。
					$\lambda = 1.540598A$
		_		_	
4.20	5 20	1	0	0	21.11
3.97	6 10	0	0	2	22.34
3.71	8 15	1	0	1	23.92
2.88	9 15	1	0	2	30.93
2.42	6 70	1	T	0	30.99
2.24	2 100	1	0	з	40.18
2.10	3 15	2	0	0	42.98
2.07	2 90	1	1	2	43.65
2.03	3 45	2	0	1	44.53
1.98	8 5	0	0	4	45.59
1.79	7 5		0	٨	50.76
1.64	7 10	2	0	7	55.76
1.58	9 5	2	ĭ	õ	57.97
1.55	9 5	2	1	1	59.23
1.48	8 15	1	ò	5	62.37
		-	•	-	
1.47	6 5	2	1	2	62.92
1.40	2 10	3	0	0	66.67
1.36	3 35	2	1	З	68.81
1.32	5 5	0	0	6	71.07
1.32	2 20	3	0	2	71.28
1.26	в 20	2	0	5	74.79
1.26	4 5	1	0	6	75.09
1.24	1 1	2	1	4	76.70
1.21	4 15	2	2	0	78.77
1.16	6 1	3	1	0	82.66
1.16	3 1	1	1	6	82.93
1.16	1 1	2	2	2	83.12
1.15	4 1	з	1	1	83.75
1.12	4 10	2	1	5	86.50
1.12	L 5	2	0	6	86.79
1.119	9 1	3	1	2	86.98
1.09	7 1	1	0	7	89.24
1.068	3 15	3	1	з	92.36
1.05	1 1	4	0	0	94.22
1.04	2 5	4	0	1	95.30
1.030	5 1	2	2	4	96.06
1.01	8 5	2	1	6	98.36
.97	7 1	4	0	3	104.04
.96	7 5	1	Ō	8	105.56
•96	5 1	З	2	0	105.96
.96	3 1	7	0	6	106.23
.956	- I	3	2	ĩ	107.08
.94	1 10	3	1	5	109.97
.93	8 1	3	2	2	110.49
•924	¥ 5	2	1	7	112.91
.920	) 10	,	1	8	113,73
.91/	B 10	4	1	0	114.15
.90	7 15		2	3	116.35
.89	9 1	2	0	8	118.00
.895	5 5	2	2	6	118.74

d (Å)	I		hkl		$2\Theta(^{\circ})$ , $\lambda = 1.540598A$
.894	15	4	1	2	118.96
.877	10	4	0	5	122.87
.876	5	3	1	6	123.23
.865	1	1	0	9	125.96
.843	10	2	1	8	132.13
.825	10	ч	2	5	138.08
.824	5	4	0	6	138.52
.823	1	5	ň	2	138.82
.814	5	3	ĭ	7	142.36
-811	10	3	ò	8	143.61
•••••		•	Ŭ	Ŭ	1.000
.809	5	З	З	0	144.27
.802	10	5	0	З	147.83
.795	1	0	0	10	151.25
•795	5	4	2	0	151.50
•793	10	З	З	2	152.47
•791	10	4	2	1	153.84

Cobalt Gallium Niobium,  $Co_{1.5}Ga_{0.5}Nb$ 

Structure Hexagonal, $P6_3/mmc(194)$ , $Z = 4$ , a ternary
Laves phase, isostructural with MgZn <sub>2</sub> , from powder data [Teslyuk et al., 1964].
Atom positions
<pre>6(h) 4.5 cobalt and 1.5 gallium 2(a) 1.5 cobalt and 0.5 gallium 4(f) 4 niobium The positions assigned were those given</pre>
for Ge <sub>0.5</sub> Ni <sub>1.5</sub> Ta [ibid.]
Lattice constants
a = 4.870 A c = 7.893 [ibid., table II]
c/a = 1.6207
Volume
162.1 Å <sup>3</sup>
Density
(calculated) 8.857 g/cm <sup>3</sup>
mb
Isotropic: overall B = 1.0
Scattering factors
Co <sup>v</sup> , Ga <sup>v</sup> , Nb <sup>v</sup> [Cromer and Mann, 1968]
Co°, Ga°, Nb° [Cromer and Mann, 1968] Scale factor (integrated intensities) $\gamma = 0.375 \times 10^{-3}$
Co°, Ga°, Nb° [Cromer and Mann, 1968] Scale factor (integrated intensities) $\gamma = 0.375 \times 10^{-3}$ References
Co <sup>o</sup> , Ga <sup>o</sup> , Nb <sup>o</sup> [Cromer and Mann, 1968] Scale factor (integrated intensities) $\gamma = 0.375 \times 10^{-3}$ References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u> , 321. Teslyuk, M. Yu., Markiv, V. Ya., and Gladyshevs'kii, E. I. (1964). J. Struct. Chem. USSR <u>5</u> , 364.

	Calculated	Pattern	(Pea	ak he	ights)
d (Å)	I		hkl		$2\Theta(\circ) \circ $ $\lambda = 1.540598A$
2.001	E	1	0	2	31.02
2.001	5	1	1	2	36.88
2.232	40	1		3	40.38
2.108		2	Å	0	40.50
2.072	100	1	Ĭ	2	42.60
20072	. 100	•	•	٤	+3+0+
2.037	75	2	0	1	44.44
1.973	15	0	0	4	45.96
1.860	10	2	0	2	48.94
1.787	10	1	0	4	51.06
1.478	5	1	0	5+	62.80
1.406	5	3	0	0	66.46
1.363	25	2	1	3	68.80
1.324	15	3	0	2	71.14
1.316	5	0	0	6	71.68
1.264	20	2	0	5	75.12
1.256	1	1	0	6	75.66
1.240	5	2	ĭ	4	76.80
1.217	15	2	2	0	78.50
1.122	. 5	2	1	5	86 • 74
1.116	5	2	ō	6	87.28
		-	•	-	
1.089	1	1	0	7	90.00
1.069	10	З	1	3	92.22
1.054	1	4	0	0	93.86
1.045	5	4	0	1	94.96
1.036	5 5	2	2	4	96.04
1.015	5 1	2	1	6	98.78
1.006	5 1	3	1	4	99.90
.961	. 5	1	0	8	106.60
•940	) 1	3	1	5	110.10
•920	5	4	1	0+	113.62
.914	5	1	1	8	114.78
.908	5	3	2	З	116.04
.896	5 10	4	1	2	118.50
.894	5	2	2	6	119.08
.877	5	4	0	5	122.94
-875	5 5	з	1	6	123.46
-869	) 1	3	2	4	124.92
.859	- 1	1	0	9	127.56
.839	5	2	1	8	133.32
.825	j 1	3	2	5	138.06
.823	5	4	0	6	138.86
.812	2 5	3	1	7+	143.22
•808	3 1	3	0	8	145.04
.803	5	5	0	3	147.08

Calculated Pattern (Integrated) d (Å) Ι hkl 20(°)  $\lambda = 1.540598A$ 5 2.882 1 0 2 31.01 2.435 45 36.88 1 1 0 2.232 80 1 0 З 40.37 2 0 0 2.109 10 42.85 100 1 1 2.072 2 43.64 2 0 1 0 0 4 2 0 2 2.037 70 44.43 1.973 15 45.96 1.860 10 48.93 1 1.787 4 10 0 51.06 5 1 0 5 1.478 62.80 1.478 2 1 2 1 62.82 3 0 2 1 1.406 5 0 66.45 1.363 25 З 68.80 3 0 1.324 20 2 71.13 0 0 1.316 5 6 71.68 1.264 20 2 0 5 75.11 1 0 6 1.256 1 75.67 2 1 4 1.240 5 76.81 2 2 1.218 20 0 78.50 1.122 5 2 1 5 86.75 5 1.116 2 0 6 87.28 1.089 1 0 7 1 90.01 10 1.069 3 1 3 92.22 4 0 0 1.054 1 93.87 1.045 5 4 0 1 94.96 1.036 5 2 2 4 96.05 1.019 98.26 1 4 0 2 1.015 2 1 6 1 98.79 1.006 3 1 4 1 99.91 .994 1 2 0 7 101.55 .961 5 1 0 8 106.61 .940 1 3 1 5 110.09 .921 5 2 1 7 113.60 .920 5 4 1 0 113.64 .914 5 1 1 8 114.79 .908 10 323 116.04 4 1 2 2 2 6 10 .896 118.50 .894 5 119.10 10 4 0 5 .877 122.93 .874 1 3 1 6 123.58 .869 1 3 2 4 124.92 .859 1 1 0 9 127.56 2 1 8 3 2 5 4 0 6 .839 5 133.32 .825 5 138.06 .823 5 138.87 .812 5 3 1 7 143.20 3 3 2 0 .812 5 0 143.26 .810 1 9 144.08 30 .808 5 8 145.04 5 •803 5 0 З 147.07

Cobalt Gallium Niobium,  $Co_{1.5}Ga_{0.5}Nb$  - (continued)

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Cobalt Gallium Tantalum, Co<sub>1.5</sub>Ga<sub>0.5</sub>Ta

<pre>Structure Hexagonal, P63/mmc(194), Z = 4, a ternary Laves phase, isostructural with MgZn2, from powder data [Teslyuk et al., 1964].</pre>
Atom positions 6(h) 4.5 cobalt and 1.5 gallium 2(a) 1.5 cobalt and 0.5 gallium 4(f) 4 tantalum The positions assigned were those given for Ge <sub>0.5</sub> Ni <sub>1.5</sub> Ta [ibid.]
Lattice constants a = 4.860  Å c = 7.861  [ibid., table II]
c/a = 1.6175
Volume 160.8 A <sup>3</sup>
Density (calculated) 12.57 g/cm <sup>3</sup>
Thermal parameters Isotropic: cobalt B = 1.0; gallium B = 1.0; tantalum B = 0.75
Scattering factors Co <sup>0</sup> , Ga <sup>0</sup> [Cromer and Mann, 1968] Ta <sup>0</sup> [International Tables, 1974]
Scale factor (integrated intensities) $\gamma = 0.632 \times 10^{-3}$
<pre>References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321. International Tables for X-ray Crystallo- graphy IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101. Teslyuk, M. Yu., Markiv, V. Ya., and Glady- shevs'kii, E. I. (1964). J. Struct. Chem. USSR 5, 364.</pre>

	Calculated	Pattern	(Pea	ak he	eights)
d (Å)	I		hkl		20(°) ° λ = 1.540598A
4.207 3.928 3.708 2.872	15 10 15 15	1 0 1	0000	0 2 1 2	21.10 22.62 23.98 31.12
2.430 2.224 2.105 2.067 2.033	100 15 95 50	1 2 1 2 1 2 2 1 2 1 2 2 1	1 0 0 1 0	0 3 0 2 1	36.96 40.52 42.94 43.76 44.54
1.963 1.781 1.641 1.591 1.559 1.473	5 5 1 1 15	1 2 2 1	0 0 1 1 0	4 3 0 1 5+	48.18 51.26 56.00 57.92 59.22 63.06

ł

d (Å)	I		hkl		20(°)
					$\lambda = 1.540598A$
1.403	10	з	0	0	66.60
1.360	30	2	1	3	69.00
1.321	15	З	0	2	71.32
1.310	5	0	0	6	72.02
1.260	20	2	0	5	75.40
1.251	5	1	0	6	76.02
1.237	1	2	1	4	77.06
1.215	15	2	2	0	78.70
1.167	1	3	1	0	82.58
1.161	1	2	2	2	83.14
1.155	1	3	1	1	83.70
1.153	1	1	1	6	83.82
1.118	10	2	1	5	87.08
1.112	5	2	0	6	87.66
1.085	1	.1	0	7	90.46
1.066	15	з	1	з	92.50
1.052	1	4	0	0	94.12
1.043	5	4	0	1	95.22
1.033	1	2	2	4	96.38
1.011	1	2	1	6	99.22
.976	1	4	0	з	104.16
•957	5	1	0	8+	107.22
.937	5	З	1	5	110.54
•918	5	4	1	0	114.00
.917	5	2	1	7	114.20
•911	5	1	1	8	115.46
•906	10	З	2	з	116.46
.894	10	- 4	1	2	118.92
.891	5	2	2	6	119.68
•874	5	4	0	5	123.50
.872	5	з	1	6	124.20
•855	1	1	0	9	128.50
.836	5	2	1	8	134.26
.823	5	З	2	5	138.84
.821	5	4	0	6	139.64
.810	5	з	з	0	143.98
.809	1	з	1	7	144.28
.805	5	З	0	8	146.30
.801	5	5	0	З	147.96
•795	1	4	2	0	151.14
.793	5	з	3	2	152.32
•791	5	4	2	1	153.50
.786	1	0	0	10	156.98

Cobalt	Gallium	Tantalum,	Co	5 Ga	<sub>5</sub> Ta	-	(continued)	
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	Calculated	Pattern	(In	tegr	ated)
	т		hk?		20(°)
U(A)	-		111214		$\lambda = 1.540598A$
4.200	15	1	0	0	21.09
4.209	10	0	ă	2	22.60
3.711	15	1	õ	1	23.96
2.873	15	i	õ	2	31.11
2.430	70		ĩ	0	36.96
		-	-		
2.224	100	1	0	з	40.52
2.104	15	2	0	0	42.94
2.067	100	1	1	2	43.76
2.033	50	2	0	1	44.53
1.965	5	0	0	4	46.15
	-				
1.781	5	1	0	4	51.26
1.641	5	2	0	з	56.00
1.591	1	2	1	0	57.92
1.559	1	2	1	1	59.21
1.475	5	2	1	2	62.98
1.473	10	1	0	5	63.07
1.403	10	3	0	0	66.60
1.360	35	2	1	З	69.01
1.321	20	3	0	2	71.32
1.310	5	0	0	6	72.02
1.260	25	2	0	5	75.41
1.251	5	1	0	6	76.02
1.236	1	· 2	1	4	77.07
1.215	20	2	2	0	78.69
1.167	' 1	З	1	0	82.58
1.161	1	2	2	2	83.15
1.155	1	3	1	1	83.69
1.153	5 1	1	1	6	83.82
1.119	1	3	1	2	87.00
1.118	10	2	1	5	87.08
1.112	2 5	2	0	6	87.67
1.085	5 1	1	0	7	90.46
1.066	5 15	3	1	3	92.51
1.052	2 1	4	0	0	94.12
1.043	5	4	0	1	95.22
			~		04.70
1.033	5	2	2	4	96.38
1.011	5	2	1	0	99.22
1.004	1	3	1	4	100.26
.976		4	0	3	104.10
.958	, 1	3	0	0	107+11
.057		,	0	P	107.22
.070	5	7	2	2	110.47
.930		3	2	5	110.55
.936	3 10	5	1	0	114-00
.910		9	1	7	114.20
•711	5	2		,	114020
.011	10	1	1	8	115.47
-904	5 15	3	2	3	116.47
.894	15	4	1	2	118-92
.891	5	2	2	6	119.69
.890		2	0	8	119.80
1 0000		-	-	~	

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d (Å)	I		hk	l	$20(^{\circ})_{0}$ $\lambda = 1.540598A$
•874	10	4	0	5	123.50
.872	5	3	1	6	124.21
.855	1	1	0	9	128.50
.836	10	2	1	8	134.27
.823	1	5	0	2	138.73
.823	10	з	2	5	138.84
.820	5	4	0	6	139.75
.810	5	З	З	0	143.97
.809	5	3	1	7	144.28
.805	10	3	0	8	146.30
.801	10	5	0	з	147.95
.795	5	4	2	0	151.13
.793	15	З	З	2	152.32
•791	15	4	2	1	153.50
.786	5	0	0	10	156.99

Cobalt Germanium, Co<sub>5</sub>Ge<sub>7</sub>

[Stolz and Schubert, 1962].
Atom positions
2(a) 2 cobalt(1)
8(c) 8 cobalt(2)
2(a) 2 germanium(1)
4(b) 4 germanium(2)
8(d) 8 germanium(3) [ibid.]

Tetragonal, I4mm (107), Z = 2, from powder data

Lattice constants a = 7.641 Å

c = 5.814 [ibid.]

c/a = 0.7609

Volume 339.45 Å<sup>3</sup>

Structure

Density . (calculated) 7.854 g/cm<sup>3</sup>

Thermal parameters Isotropic: overall B = 1.0

Scattering factors Co<sup>0</sup>, Ge<sup>0</sup> [Cromer and Mann, 1968]

Scale factor (integrated intensities)  $\gamma = 0.599 \times 10^{-3}$ 

References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u>, 321. Stolz, E. and Schubert, K. (1962). Chem. Erde

22, 709.

	Calculated	Pattern	(Pea	ak hei	.ghts)
d(Å)	I		hkl	λ	20(°) = 1.540598A
4.624 3.818 2.946	35 1 35	1 2 2	0 0 1	1 0 1	19.18 23.28 30.32
2.701	10	2	2	0	33.14
2.416 2.333 2.313 1.991 1.979	1 10 5 25 100	3 3 2 3 2	1 0 2 2	0 1 2 1 2	37.18 38.56 38.90 45.52 45.82
1.910 1.878 1.765 1.708 1.686	40 10 5 5 1 1 5 5	4 1 4 4 2	0 0 1 2 1	0 3 1 0 3	47.56 48.42 51.74 53.60 54.38
1.596 1.542 1.476 1.474 1.454	5 1 1 5 5 5 5	4 3 4 0	0 0 3 2 0	2 3 1+ 2 4	57.70 59.92 62.82 63.02 64.00
1.379 1.359 1.351 1.339 1.280	9 5 1 10 5 9 1	5 2 4 2	2 0 4 1 2	1 4 0 3 4	67.94 69.08 69.54 70.22 74.00
1.228 1.200 1.195 1.169 1.166	1 5 1 9 1	6 5 5 5 6	1 0 3 4 0	1 3+ 2 1 2	77.72 79.88 80.30 82.44 82.66
1.157 1.145 1.116 1.107 1.101	10 11 15 15 1 1	4 5 6 4 2	0 2 2 2 1	4 3 2 4 5	83.50 84.58 87.34 88.18 88.82
1.073 1.033 1.019 1.016 .996	1 5 5 5 5 5	7 7 3 5 6	0 2 2 4 4	1 1 5 3 2	91.78 96.46 98.16 98.58 101.38
•990 •955 •939 •935 •927		4 8 2 7 8	4 0 0 4 2 2	4 0 6 1+ 0	102.24 107.50 110.20 110.88 112.46

Cobalt Germanium,  $Co_5 Ge_7$  - (continued)

Ca	lculated Pa	ttern (	Integi	rated)
d (Å)	I	hl	kl	$2\Theta(^{\circ}) \\ \lambda = 1.540598 \text{\AA}$
4.627	30	1	0 1	19.17
3.820	1	2	0 0	23.26
2.946	30	2	1 1	30.32
2.907	10	0	0 2	30.73
2.702	10	2	2 0	33.13
2.416	1	3	1 0	37 • 18
2.333	10	3	0 1	38.56
2.313	5	2	0 2	38.90
1.991	20	3	2 1	43.52
1.0313	100	2	~ ~	4 36 62
1.910	45	4	0 0	47.56
1.879	10	1	0 3	48.42
1.766	5	4	1 1	51.73
1.709	1	4	2 0	53.60
1.686	5	2	1 3	54.38
1.596	1	4	0 2	57.70
1.542	1	З	0 3	59.93
1.478	1	5	0 1	62.82
1.478	5	4	31	62.82
1.473	5	4	2 2	63.06
1.453	5	0	0 4	64.01
1.378	5	5	2 1	67.95
1.359	1	2	0 4	69.09
1.351	10	4	4 0	69.54
1.339	5	4	1 3	70.21
1.280	1	2	2 4	74.00
1.228	1	6	1 1	77.71
1.200	5	5	0З	79.87
1.200	1	4	з з	79.87
1.195	1	5	32	80.30
1.169	1	5	4 1	82.44
1.166	1	6	0 2	82.66
1.157	10	4	0 4	83.51
1.145	1	5	2 3	84.57
1.118	1	6	31	87.12
1.116	15	6	2 2	87.33
1.107	1	4	2 4	86.18
1.101	1	2	1 5	88.81
1.073	1	7	0 1	91.78
1.000	1	6	4 0	93.26
1.033	5	7	2 1	96+45
1.019	5	3	2 5	98.16
1.016	5	5	4 3	98.59
•996	1	4	4 2 4	102.25
055		•	0 0	107 51
.955	1	8		110/•51
.939	1	2	4 1	110.97
.927	1	Ŕ	2 0	112.47
.912	5	2	2 6	115.24
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Cobalt	Germanium	Niobium,	Co	5 Ge	۲NP
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Structure Hexagonal,  $P6_3/mmc(194)$ , Z = 4, a ternary Laves phase, isostructural with MgZn2, from powder data [Teslyuk et al., 1964]. Atom positions 4.5 cobalt and 1.5 germanium 6(h) 2(a) 1.5 cobalt and 0.5 germanium 4(f)4 niobium The positions assigned were those given for Ge0.5Ni1.5Ta [ibid.] Lattice constants a = 4.860 Åc = 7.832 [ibid.] c/a = 1.6115Volume 160.2 Å<sup>3</sup> Density (calculated) 9.022 g/cm<sup>3</sup> Thermal parameters Isotropic: overall B = 1.0 Scattering factors Co<sup>0</sup>, Ge<sup>0</sup>, Nb<sup>0</sup> [Cromer and Mann, 1968] Scale factor (integrated intensities)  $\gamma = 0.375 \times 10^{-3}$ References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u>, 321. Teslyuk, M. Yu., Markiv, V. Ya., and Gladyshevs'kii, E. I. (1964). J. Struct. Chem. USSR 5, 364.

	Calculated	Pattern	(Pea	ak he	eights)
d (Å)	I		hkİ		$2\theta$ (°) $\lambda = 1.540598A$
2.866	5	1	0	2	31.18
2.430	45	1	1	0	36.96
2.218	08 8	1	0	З	40.64
2.105	5 15	2	0	0	42.94
2.064	100	1	1	2	43.82
2.033	5 75	2	0	1	44.54
1.958	15	0	0	4	46.34
1.854	10	2	0	2	49+10
1.775	5 10	1	0	4	51.44
1.474	1	2	1	2	63.02
1.468	5	1	0	5	63.30
1.403	5	3	0	0	66.60
1.359	25	2	1	3	69.08
1.321	15	3	0	2	71.36
1.305	5 5	0	0	6	72.34
1.257	20	2	0	5	75.62
1.247	, 1	1	0	6	76.32
1.235	5 5	2	1	4	77.20
1.215	5 15	2	2	0	78.70
1.116	5 5	2	1	5	87.28
1.109	> 5	2	0	6	87.96
1.081	1	1	0	7	90.86
1.066	5 10	3	1	З	92.58
1.052	2 1	4	0	0	94.12
1.043	3 5	4	0	1	95.24
1.032	2 5	2	2	4	96.52
1.009	) 1	2	1	6	99.52
1.003	3 1	3	1	4	100.40
•988	3 1	2	0	7	102.48
•954	5	1	0	8	107.76
.93	5 1	з	1	5	110.76
•918	3 5	4	1	0	114.00
•915	5 1	2	1	7	114.64
•908	3 5	1	1	8	116.06
•906	5 5	3	2	3	116.54
.894	4 10	4	1	2	118.96
.889	9 5	2	2	6	120.02
.87:	3 5	4	0	5	123.74
.87	0 1	З	1	6	124.56
•86	5 1	З	2	4	125.62
.85	2 1	1	0	9	129.36
.83	4 5	2	1	8	135.00
.822	2 1	3	2	5	139.16
.819	9 5	4	0	6	140.20
•810	) 1	3	3	0	143.98
.808	B 1	З	1	7	144.96
.80	3 1	3	0	8	147.26
•80	1 5	5	0	З	148.10

Calculated Pattern (Integrated) d (A) 2⊖(°) Ι hkl  $\lambda = 1.540598A$ 2.867 5 0 2 31.17 1 2.430 45 1 1 0 36.96 2.219 80 1 0 3 40.63 2.104 10 2 0 0 42.94 2.065 100 1 1 2 43.81 2.032 75 2 0 1 44.55 1.958 15 0 0 4 46.33 1.854 10 2 0 2 49.11 10 1 0 4 1.775 51.43 1.474 2 1 2 1 63.02 1.468 5 1 0 5 63.30 1.403 5 66.60 3 0 0 1 25 З 69.09 1.358 2 З 0 2 1.321 20 71.36 1.305 5 0 0 6 72.33 1.257 20 2 0 5 75.62 1.247 1 1 0 6 76.32 1.235 5 2 1 4 77.20 1.215 20 2 2 0 78.69 1.116 5 2 1 5 87.28 5 2 1.109 0 6 87.96 1.081 1 1 0 7 90.86 3 1 1.066 10 З 92.58 1.052 4 0 94.12 1 0 1.043 5 4 0 1 95.23 5 2 2 4 1.032 96.51 1.016 1 4 0 2 98.58 1.009 2 1 6 99.52 1 3 1 1.003 4 100.39 1 2 0 7 .988 1 102.47 .954 5 1 0 8 107.77 .936 1 3 1 5 110.77 .918 5 4 1 0 114.00 .915 5 2 1 7 114.64 .908 5 116.05 1 1 8 .906 10 З 2 3 116.55 .894 15 4 1 2 118.96 .889 5 2 2 6 120.02 .873 10 4 0 5 123.75 1 3 1 .870 6 124.57 .866 2 1 3 4 125.62 .852 1 1 0 9 129.35 .834 10 2 1 8 135.00 .822 5 3 2 5 139.16 .819 5 4 0 6 140.20 .810 5 3 3 0 143.97 5 .808 З 1 7 144.97 .804 1 2 0 9 146.62 .803 5 З 0 8 147.26 .801 5 5 0 З 148.09

Coba 1	tι	Germanium	Niobium,	Col	.5 <sup>Ge</sup> 0.	.5 <sup>ND -</sup>	(continued)
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Structure Hexagonal, P63/mmc(194), Z = 4, a ternary Laves phase, isostructural with MgZn2, from powder data [Teslyuk et al., 1964]. Atom positions 6(h) 4.5 cobalt and 1.5 germanium 2(a) 1.5 cobalt and 0.5 germanium 4 tantalum 4(f)The positions assigned were those given for Ge0.5Ni1.5Ta [ibid.] Lattice constants a = 4.875 Å c = 7.817 [ibid., table II] c/a = 1.6035Volume 160.9 Å<sup>3</sup> Density (calculated) 12.62 g/cm<sup>3</sup> Thermal parameters Isotropic: cobalt B = 1.0; germanium B = 1.0; tantalum B = 0.75Scattering factors Co<sup>0</sup>, Ge<sup>0</sup> [Cromer and Mann, 1968] Ta<sup>0</sup> [International Tables, 1974] Scale factor (integrated intensities)  $\gamma = 0.623 \times 10^{-3}$ References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 231. International Tables for X-ray Crystallography IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101. Teslyuk, M. Yu., Markiv, V. Ya., and Gladyshevs'kii, E. I. (1964). J. Struct. Chem. USSR 5, 364.

_	Calculated	Pattern	(Pea	ak h	eights)
d (Å)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
4.219 3.907 3.714 2.868 2.438 2.217 2.111	15 10 15 15 75 100	1 0 1 1 1 1	0 0 0 1	0 2 1 2 0 3	21.04 22.74 23.94 31.16 36.84 40.66
2.068	100 50	1 2 0	1	2	42.00 43.74 44.42
1.1954	5	Ŭ	v	-	40844

d (Å)	I	hkl	,	$2\Theta(^{\circ}) \\ \lambda = 1.540598 \text{\AA}$
1.774	5	1 0	4	51.48
1.640	5	20	3	56.02
1.596	1	2 1	0	57.72
1.563	1	2 1	1	59 • 04
1.477	5	2 1	2	62.86
1.466	10	1 0	5	63.40
1.407	10	3 0	õ	66.38
1.361	30	2 1	3	68.96
1.324	15	3 0	2	71.16
1.303	5	0 0	6	72.50
			-	
1.256	20	20	5	75.64
1.245	5	1 0	6	76.46
1.236	1	2 1	4	77.10
1.219	15	2 2	0	78.40
1 • 171	1	3 1	0	82.28
1.163	1	22	2	82.92
1.158	1	3 1	1	83.40
1.149	1	1 1	6	84.20
1.122	1	3 1	2	86.74
1.117	10	2 1	5	87.22
	-			
1.109	5	2 0	0	88.02
1.060	1	1 0	4	91.04
1.068	15	3 1	3	92.32
1.055	1	4 0	0	93.74
1.046	5	4 0	1	94.86
1.034	1	22	4	96.30
1.009	1	2 1	6	99.50
1.004	1	31	4	100.16
•978	1	4 0	З	103.90
•956	1	30	6	107.36
.952	5	1 0	8	108.02
.940	1	3 2	2	110.04
.937	5	3 1	5	110.56
.921	5	4 1	ō	113.46
.915	1	2 1	7	114.68
			-	
•908	10	5 2	3	116.06
.907	5	1 1	8	110.20
•897	10	4 1	2	118.42
.890	5	2 2	0	119.88
•887	1	20	8	120.60
.875	5	4 0	5	123.42
.871	1	3 1	6	124.38
-851	1	1 0	9	129.76
.833	5	2 1	8	135.16
-823	5	3 2	5	138.64
	-		-	
•820	1	4 0	6	139.86
.813	1	33	0	142.90
.808	1	31	7	144.80
.803	5	5 0	З	147.08
.803	5	30	8	147.36
.798	1	4 2	0	149.80
.795	5	3 3	2	151.08
.794	5	4 2	1	152-10
	-	-	-	

Cobalt Germanium	Tantalum,	Co,	-Ge	<sub>5</sub> Ta	-	(continued)
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	Calculated	Pattern	(Int	tegr	ated)
d (Å)	I		hkl		$20(^{\circ})$ ° $\lambda = 1.540598A$
4.222 3.908 3.715 2.868	15 10 15	1 0 1	0 0 0	0 2 1 2	21.03 22.73 23.94 31.16
2.438	75	1	1	0	36.84
2.217 2.111 2.068	100 15 100	1 2 1	0 0 1	3 0 2	40.66 42.80 43.73
2.038 1.954	50 5	2	0	1 4	44.42 46.43
1.773	5 5	1 2 2	0	43	51.49 56.02
1.563	1 5	2	1	12	59.03 62.85
1.466	10	1 3	0	5	63•39 66•37
1.361 1.324 1.303	35 20 5	2 3 0	1 0 0	3 2 6	68•95 71•15 72•49
1.256	25 5	2	0	5	75.63 76.45
1.236	1 20 1	2 2 3	1 2 1	4 0 0	77.10 78.40 82.27
1.163	1	2 3	2	2	82.91 83.39
1.149 1.122 1.117	1 1 10	3	1 1	6 2 5	84•20 86•74 87•22
1.109	5 1	2	0	6 7	88.02 91.04
1.055	15 1 5	4	0	0 1	92•31 93•74 94•86
1.034	5	2 2	2	4	96.30 99.51
•978 •956	1	3 4 3	0	4 3 6	100.15 103.89 107.36
•952 •940	5	1 3	02	8 2	108.03 110.04
.937 .921 .915	5 10 5	3 4 2	1 1 1	5 0 7	110.55 113.46 114.69
•908 •907	15	3	2	382	116.09 116.27
•890 •887	10	2	2	6 8	119.87

d(Å)	I		hkl		20(°) 。
					$\lambda = 1.540598A$
•875	10	4	0	5	123.42
•87i	5	З	1	6	124+38
.851	1	1	0	9	129.77
.833	10	2	1	8	135.15
•825	1	5	0	2	137.92
.823	10	З	2	5	138.64
.820	5	4	0	6	139.86
.813	5	3	3	0	142.91
.808	5	3	1	7	144.80
•803	10	5	0	3	147.06
.803	10	з	0	8	147.37
•798	5	4	2	0	149.79
.795	15	З	З	2	151.08
•794	15	4	2	1	152.08

Structure Hexagonal, was deter of the 3 c at random.	$P6_3/m$ (176), Z = 1. The structure mined by Lemaire et al. [1969]. sobalt sites is only partially for	oture One illed
Atom positio 6(h)	ns 6 holmium(1)	
6(h)	6 holmium(2)	
6(h)	6 cobalt(1)	
2(c)	2 cobalt(2)	
2 (b)	1.2 cobalt(3)	
Lattice cons a = 11.411	tants A	
c = 3.984		
(published [ibid., ta	<pre>values: a = 11.410 A, c = 3.984 ble 4])</pre>	
c/a = 0.34	.91	
Volume 449.3 Å <sup>3</sup>		
Density		
(calculate	ed) 9.319 g/cm <sup>3</sup>	
Thermal para Isotropic	meters [Lemaire et al., 1969]	
-		
Scattering f Co <sup>0</sup> , Ho <sup>0</sup> [	actors [Cromer and Mann, 1968]	
Scale factor $\gamma = 0.948$	s (integrated intensities) $\times 10^{-3}$	
I/I corundu	(calculated) = 9.96	
References		
Cromer, D Crystall	). T. and Mann, J. B. (1969). Logr. <u>A24</u> , 321.	Acta
Lemaire, P (1969).	Acta Crystallogr, B25, 710.	os, J.

	Calculated	Pattern	(Pea	ak he	eights)
o d (A)	I		hkl		$20(^{\circ})$ $\lambda = 1.540598A$
4.940	1	2	0	0	17.94
3.693	s /	2	1	0	23.82
3.293 3.266	1 5 2	3	0	0	27.06 27.28
2.852	2 6	2	2	0	31.34
2.740	42           5         100	3 2	1 1	0 1+	32.66 32.84
2.538 2.470	8 23 9 5	3	0	1 0	35.34 36.34
2.319	9 9	2	2	1	38.80
2.266	5 3 8 5	2	3 3	0+ 1+	39•74 39•90
2.156 2.100	5 19 9 4	1 4	4 0	0+ 1	41.86 43.04

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d (A)	I		hkl	;	$20(^{\circ})$ . $\lambda = 1.540598A$
1.992	13	0	0	2	45.50
1.971	5	2	з	1	46.02
1.896	1	1	4	1+	47.94
1.868	5	2	4	0	48.72
1.775	4	1	5	0+	51.44
1.758	3	2	1	2+	51.98
1.716	2	3	З	1	53.34
1.704	1	3	0	2	53.74
1.691	8	2	4	1+	54.20
1.633	3	2	2	2	56.28
1.621	6	1	5	1	56.74
1.611	9	З	1	2	57.12
1.582	5	5	2	0+	58.26
1.550	1	4	0	2	59.58
1.507	2	1	6	0+	61.48
1.496	2	2	з	2+	61.96
1.470	15	5	2	1	63.18
1.463	7	1	4	2+	63.52
1.412	2	3	5	0+	66.14
1.362	З	2	4	2	68.86
1.331	1	5	з	1+	70.74
1.325	3	1	5	2	71.08
1.296	2	6	2	1+	72.94
1.265	З	4	5	0	75.00
1.251	5	2	1	3+	76.00
1.243	2	1	7	1	76.56
1.239	4	5	2	2+	76.88
1.236	3	8	0	0	77.14
1.232	2	З	0	3	77.40
1.204	1	2	2	3	79.58
1.202	2	1	6	2+	79.72
1.188	2	з	6	1	80.82
1.157	1	8	1	0+	83.52
1.152	1	5	З	2+	83.94
1.111	3	1	8	1+	87.82
1.090	2	Å	6	1+	89.90
1.082	2	2	4	3+	90.76
1.078	1	8	2	0	91-18
1.071	2	7	3	1+	92.00
1.068	3	4	5	2	92.30
1.063	1	1	5	з	92.84
1-059	1	9	0	1	93-38
1-050	2	8	0	2	94.40
1.0173	4	5	2	3	98.44

Cobalt Holmium,  $Co_{9.2}Ho_{12}$  - (continued)

	Calculated	Pattern	(Int	egr	ated)
d (A)	I		hkl		$2\Theta(^{\circ}) \circ \\ \lambda = 1.540598A$
4.941	1	2	0	0	17.94
3.735	7	2	1	0	23.80
3.695	7	1	0	1	24.07
3.294	1	3	0	0	27.05
3.200	5	1	1	1	21.28
2.853	8	2	2	0	31.33
2.741	42	3	1	0	32.65
2.725	100	2	1	1	32.84
2.539	23	1	2	1	32.84
20005	51	5	Ŭ	•	55.55
2.471	6	4	Э	0	36.33
2.319	12	2	2	1	38.79
2.258	2	2	3	1	39.13
2.258	5	1	3	1	39.89
0.000					
2.156	5	4	1	0	41.86
2.100	21	1	4	1	41.80
1.992	18	Ŏ,	õ	2	45.50
1.976	1	5	0	0	45.88
1 070	6	2	-		66.00
1.896	1	2	4	1	40.02
1.868	6	2	4	ō	48.72
1.848	1	2	0	2	49.28
1.775	1	5	1	0	51.44
1.775	4	1	5	0	51.44
1.758	4	2	1	2	51.98
1.716	2	3	З	1	53.34
1.705	1	3	0	2	53.73
1.691	3	4	2	1	54.20
1.691	10	2	4	1	54.20
1.633	4	2	2	2	56.28
1.625	1	4	3	0	56.61
1.611	7	1	5	1	56.73
10011	12	3	1	2	57+11
1.582	3	5	2	0	58.26
1.582	3	2	5	0	58.26
1.522	1	4	0	2	59.57
1.507	1	6	1	0	61.48
1.496	2	1	6	0	61.48
1.496	2	3	2	2	61.96
1.471	23	5	2	1	63.17
1.463	1	4	1	2	63.53
1.463	8	1	4	2	63.53
1.426	1	4	4	0	65.37
1.412	1	3	5	0	66.14
1.362	5	2	4	2	68.86
1.325	4	1	5	2	71 09

d (Ă)	I		hkl		$20(^{\circ})$ ° $\lambda = 1.540598A$
1.296	2	6	2	1	72.94
1.296	1	2	6	1	72.94
1.265	4	4	5	ō	75.00
1.251	7	2	1	3	75.99
1.251	1	1	2	3	75.99
1.244	з	1	7	1	76.55
1.239	2	2	5	2	76.88
1.239	3	5	2	2	76.88
1.235	3	8	0	0	77.16
1.232	2	3	0	3	77.42
1.204	1	2	2	з	79.56
1.202	1	6	1	2	79.72
1.202	2	1	6	2	79.72
1.188	3	3	6	1	80.81
1.152	1	5	3	2	83.94
1.152	1	3	5	2	83.94
1.146	1	2	З	З	84.48
1.112	1	7	З	0	87.71
1+111	4	1	8	1	87.81
1.090	1	6	4	1	89.90
1.090	з	4	6	1	89.90
1.082	2	2	4	З	90.75
1.078	1	8	2	0	91.19
1.071	2	7	З	1	91.99
1.071	1	3	7	1	91.99
1.068	4	4	5	2	92.31
1.063	2	1	5	З	92.84
1.059	1	9	0	1	93.39
1.050	3	8	0	2	94.40
1.0172	6	5	2	З	98.44

Cobalt Magnesium, Co<sub>2</sub>Mg

Structure Hexagonal, P6 <sub>3</sub> /mmc(194), Z = 4, a Laves phase, isostructural with MgZn <sub>2</sub> , from powder data [Stadelmaier and Yun, 1961].
Atom positions 4(f) 4 magnesium 2(a) 2 cobalt(1) 6(h) 6 cobalt(2)
The "ideal" parameters and distributions of the Cl4 structure type were used [Friauf, 1927].
Lattice constants a = 4.866  Å c = 7.926 [Smith and Smith, 1964]
c/a = 1.6289
Volume 162.53 Å <sup>3</sup>
Density (calculated) 5.811 g/cm <sup>3</sup>
Thermal parameters Isotropic: overall B = 1.0
Scattering factors Co <sup>0</sup> , Mg <sup>0</sup> [Cromer and Mann, 1968]
Scale factor (integrated intensities) $\gamma = 0.187 \times 10^{-3}$
<ul> <li>References</li> <li>Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u>, 321.</li> <li>Friauf, J. B. (1927). Phys. Rev. <u>29</u>, 34.</li> <li>Smith, J. F. and Smith, M. J. (1964). ASM (Amer. Soc. Metals) Trans. Quart. <u>57</u>, 337.</li> <li>Stadelmaier, H. H. and Yun, T. S. (1961). Z. Metallk. <u>52</u>, 477.</li> </ul>

		Calculated	Pattern	(Pea	k h	eights)
	d (Å)	I		hkl		20 (°)
						$\lambda = 1.540598A$
	4.21	70	1	0	0	21.08
	3.96	35	0	0	2	22.42
	3.72	30	1	0	1	23.90
	2.886	1	1	0	2	30.96
	2.433	10	1	1	0	36.92
	2.238	40	1	0	3	40.26
	2.106	5	2	0	0	42.90
	2.073	85	1	1	2	43.62
	2.036	100	2	0	1	44.46
	1.981	30	0	0	4	45.76
	1.860	40	2	0	2	48.92
	1.793	1 15	1	0	4	50.88
	1.647	20	2	0	З	55.76
	1.593	5	2	1	0	57.84
	1.561	5	2	1	1	59.12
	1.444	1	2	0	4	64.50
	1.405	; 1	3	0	0	66.52
	1.364	10	2	1	З	68.76
	1.324	15	3	0	2	71.16
	1.267	15	2	0	5	74.90
	1.241	5	2	1	4	76.70
	1.216	5 15	2	2	0	78.58
	1.169	) 1	3	1	0	82.46
	1.163	5	2	2	2	82.96
	1.161	5	1	1	6	83.14
	1.156	; <b>1</b>	з	1	1	83.54
	1.119	5	2	0	6	86.98
	1.094	1	1	0	7	89.56
	1.069	) 5	3	1	З	92.22
	1.044	5	4	0	1	95.06
	1.037	10	2	2	۵	95.98
	1-014	3 5	4	0	2	98.32
	1.017	7 1	2	1	6	98.50
	1.007	. 5	3	1	4	99.84
	.997	74 5	2	0	7	101.12
	.001	)8 1	0	0	8	102.06
	.978	36 1	4	ō	3	103.84
	.966	8 1	3	2	Ō	105.64
	.964	4 1	1	0	8	106.02
	.962	22 1	3	0	6	106.36
	.025	0 1	2	1	7	113-16
	.907	79 1	3	2	3	116.08
	-804	58 5	4	1	2	118.62
	.894	19 5	2	2	6	118.80
	.877	74 5	4	0	5	122.78
	.868	39 1	з	2	4	124.88
L						

Cobalt Magnesium,  $Co_2^{(l)}$  - (continued)

	Calculated	Pattern	(Int	egra	ted)
d (Å)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
4.21 3.96 3.72 2.887 2.433	60 30 25 1 5	1 0 1 1	0 0 0 0	0 2 1 2 0	21.06 22.42 23.90 30.95 36.92
2.238 2.107 2.073 2.036 1.981	40 5 85 100 30	1 2 1 2 0	0 0 1 0 0	3 0 2 1 4	40.26 42.89 43.62 44.45 45.75
1.860 1.793 1.647 1.593 1.562	45 15 20 5 5	2 1 2 2 2	0 0 0 1 1	2 4 3 0 1	48.92 50.88 55.76 57.84 59.11
1.443 1.405 1.364 1.324 1.321	1 10 15 1	2 3 2 3 0	0 0 1 0 0	40326	64.50 66.51 68.76 71.16 71.34
1.267 1.261 1.241 1.216 1.169	20 1 10 20 1	2 1 2 3	0 0 1 2 1	5 6 4 0	74.90 75.34 76.70 78.57 82.46
1.163 1.161 1.156 1.119 1.094	5 5 1 10 1	2 1 3 2 1	2 1 1 0 0	2 6 1 6 7	82.96 83.14 83.55 86.98 89.57
1.069 1.044 1.037 1.018 1.017	5 5 15 5 1	3 4 2 4 2	1 0 2 0 1	3 1 4 2 6	92.22 95.05 95.98 98.32 98.50
1.007 .9974 .9907 .9786 .9668	5 5 7 1 5 5 8 1	3 2 0 4 3	1 0 0 2	4 7 8 3 0	99.84 101.12 102.06 103.84 105.65
•9645 •9623 •9229 •9079 •8958	5 5 3 1 9 1 9 5 5 10	1 3 2 3 4	0 0 1 2 1	8 6 7 3 2	106.01 106.35 113.17 116.08 118.61
•8949 •8774 •8753 •8689 •8620	9 5 4 5 3 1 9 5 0 1	2 4 3 3	2 0 1 2 0	6 5 6 4 9	118.81 122.78 123.28 124.89 126.65

Cobalt Molybdenum,  $\mathrm{Co_2Mo_3}$ 

Structure Tetragonal, $P4_2/mnm$ (136), $Z = 6$ , $\sigma$ -phase, iso-	d (Å)	I		hkl		$20(^{\circ})$ , $\lambda = 1.540598A$
structural with $\sigma$ -CrFe. The structure was deter-	2.083	81	2	1	2	43.40
mined by forsyth and d Aite da verga [1965].	2.031	100	4	1	1	44.58
Atom positions	1.983	44	3	3	1	45.72
2(a) 2 cobalt(1)	1.940	9	2	2	2	46.78
8(i) 8 cobalt(2)	1.860	9	Э	1	2	48.94
8(i) 1 cobalt(3) and 7 molybdenum(2)						
8(i) 1 cobalt(4) and 7 molybdenum(4)	1.724	1	4	З	1	53.08
4(a) 4 molybdenum (1)	1.569	1	4	2	2	58.82
1 (g) 1 morphaeman(1)	1.466	4	4	з	2	63.38
Lattice constants	1.459	1	6	2	0	63.72
a = 9.2292(4)Å	1.448	Э	5	1	2+	64.28
c = 4.8271(6)						
(published values: $a = 9.2287(4)$ , $c = 4.8269(6)$	1.442	2	5	4	0	64.60
(juid 1)	1.409	2	Э	1	Э	66.28
[1514.])	1.3971	9	5	2	2+	66.92
c/a = 0.5230	1.3811	2	5	4	1	67.80
o, a 0.0200	1.3236	16	5	з	2	71.18
Volume						
411 16 Å <sup>3</sup>	1.3064	16	4	1	3+	72.26
411.10 A	1.2971	8	6	0	2	72.86
Density	1.2938	10	3	3	3	73.08
$(a)(a)(a)(a) = a^{2}(a)^{3}$	1.2844	5	6	1	2	73.70
(calculated) 5.051 g/cm	1.2677	12	7	2	0	74.84
Thermal parameters		• -		-	Ū	
Testropie: everall P = 2.0	1.2599	4	5	5	1	75.38
isotropic: overall B = 2.0	1.2487	2	6	2	2	76.18
Casthaning Fratan	1.2374	2	5	4	2+	77.00
scattering factors	1.2261	3	7	2	1	77.84
co, Mo [Forsyth and Wells, 1959], corrected	1.2067	6	0	5	à	79.34
for the real part of the anomalous dispersion	102007	Ũ	v	v	•	13031
[Dauben and Templeton, 1955].	1,1224	1	7	2	2	86.68
	1,1103	5	8	2	0	86.98
Scale factors (integrated intensities)	1.0903	7	8	2	ĩ	89.90
$\gamma = 0.231 \times 10^{-5}$	1.0877	्र भ	6	6	0	90-18
corundum (calculated) = 2.97	1.0809	1	6	2	Ä	90.90
D. Commence	1.0003	•	U	2	5	30 • 30
References	1.0623	7	4	1	4	92.96
Dauben, C. H. and Templeton, D. H. (1955). Acta	1.0553	4	7	-	4	93.76
Crystallogr. 8, 841.	1.0408	4	8	0	2	95.48
Forsyth, J. B. and d'Alte da Veiga, L. M. (1962).	1.0343	7	7	<u>م</u>	2	96.28
Acta Crystallogr. <u>15</u> , 543.	1.0136	1	5	5	7	98.92
Forsyth, J. B. and Wells, M. (1959). Acta Crys-	1.0150	•	5	5	5	50 <b>•</b> 52
tallogr. <u>12</u> , 412.						
	•9959	1	7	2	з	101.34
	•9247	3	7	6	2+	112.82
Calculated Pattern (Peak heights)	•9188	2	8	2	3+	113.94
0	•9065	1	8	6	1+	116.36
$d(A)$ I $hk\ell$ $2\Theta(0)$	•9023	З	9	3	2+	117.24
$\lambda = 1.540598A$						
	•9011	2	6	6	3	117.48
4.275 5 1 0 1 20.76	.8964	1	9	5	0	118.48
4.126 3 2 1 0 21.52	•8864	4	4	1	5+	120.68
3.880 2 1 1 1 22.90	•8824	1	3	3	5	121.60
3.262 2 2 2 0 27.32	•8740	6	7	2	4+	123.60
3.136 1 2 1 1 28.44						
	•8620	1	8	6	2+	126.66
2.917 6 3 1 0 30.62	•8583	1	10	1	2	127.66
2.593 5 3 0 1 34.56	.8532	2	9	6	0	129.06
2.559 4 3 2 0 35.04	•8402	1	9	6	1	132.92
2.497 18 3 1 1 35.94	.8356	2	11	1	0	134.40
2.414 18 0 0 2 37.22						
	•8255	1	10	5	0	137.86
2.306 3 4 0 0 39.02	•8233	1	11	1	1	138.64
2.262 9 1 1 2+ 39.82	.8206	З	8	2	4	139.66
2.238 95 4 1 0 40.26	•8137	1	10	5	1	142.42
2.175 46 3 3 0 41.48	.8079	1	6	6	4	144.90
2.139 47 2 0 2 42.22						

Cal	lculated P	attern	ı (Ir	ntegi	cated)							
d (Å)	I		hk	2	$20(^{\circ})$ ° $\lambda = 1.540598A$		d (Å)	I		hkl		$20(^{\circ})_{\circ}$ $\lambda = 1.540598A$
4.277	4	1	0	1	20.75	] [	1 0553	A	7	7	4	93.77
4.127	3	2	1	ĥ	21.51	1	1.0400	4	2	0	5	95.47
3.881	2	1	1	1	22.00		1.0767	4	7	~	2	95.47
3.263	2	2	2		22.90		1.0176	0	, ,	4	2	90.20
3,137	2	~	1	•	27.031		1.0136	2	5	5	3	90.92
20137	-	2	1	1	20.43		•9958	2		2	5	101+35
2.919	6	3	1	0	30.61		•9389	1	9	1	2	110.25
2.594	5	3	0	1	34.55		•9247	2	9	2	2	112.83
2.560	4	3	2	0	35.03		•9247	2	7	6	2	112.83
2.498	18	3	1	1	35.93		• 9188	2	8	2	3	113.94
2.414	18	0	0	2	37.22		•9065	1	8	6	1	116.37
2.307	2	4	0	0	39.01		•90 23	З	9	з	2	117.23
2.264	5	1	1	2	39.79		.9022	1	10	1	1	117.26
2.261	2	3	2	1	39.83		.9011	2	6	6	3	117.48
2.238	92	4	1	0	40.26		.8964	1	9	5	0	118.48
2.175	44	З	З	0	41.48		.8865	4	4	1	5	120.67
6 170	45			-				_	_	_		
2.139	45	2	0	2	42.22		.8861	3	5	5	4	120.76
2.083	79	2	1	2	43.40		.8824	2	3	3	5	121.60
2.031	100	4	1	1	44.58		.8741	9	7	2	4	123.59
1.983	44	3	3	1	45.71		•8736	3	9	4	2	123.72
1.940	9	2	2	2	46.78		.8620	2	8	6	2	126.65
1.860	9	з	1	2	48.93		.8583	1	10	1	2	127.65
1.724	1	4	3	1	53.08		.8532	З	9	6	0	129.06
1.569	1	4	2	2	58.83		.8402	1	9	6	1	132.92
1.466	4	4	З	2	63.39		.8356	з	11	1	0	134.41
1.459	1	6	2	0	63.72		-8255	З	10	5	0	137.86
1.448	3	5	1	2	64.28		. 8233	2	11	1	1	138.65
1.441	1	5	4	0	64.61		. 8206	6	2 A A	2	Å	139.67
1.409	2	3	1	3	66.28		-8137	3	10	5	1	142.42
1.3974	8	5	2	2	66.91		- 8065	1	11	3	Ô	144.21
1.3968	3	6	2	1	66.93		.8079	3	6	6	4	144.89
		_										
1.3811	2	5	4	1	67.80		•8052	1	6	2	5	146.15
1.3236	17	5	3	2	71.18		8045	1	9	6	2	146.49
1.3065	15	4	1	3	72.26		•8006	1	8	6	3	148.39
1.3052	5	5	5	0	72.34		•7983	1	11	3	1	149.56
1.2972		6	0	2	72.86		•7976	1	10	1	3	149.94
1.2936	7	з	з	з	73.09		•7926	2	2	0	6	152.78
1.2845	5	6	1	2	73.69		.7897	5	2	1	6	154.58
1.2677	14	7	2	0	74.84		.7896	2	11	1	2	154.62
1.2600	4	5	5	1	75.38		.7888	1	10	2	З	155.14
1.2488	3	6	2	2	76.17							
1.2375	2	6	~	2	76.00	-						
1.2261	2	7	4	2	77.04							
1.20.68	7	6	2	4	70 77							
1.1223	1	7	2	4	19.55							
1.1192	5	8	2	2	86-98							
		Ŭ	-	Ĵ	000,00							
1.0903	4	8	2	1	89.90							
1.0877	2	6	6	0	90.18							
1.0809	1	6	2	З	90.90							
1.0622	8	4	1	4	92.97							
1.0611	2	6	6	1	93.10							

Cobalt	Molybdenum,	Co_Mo3 -	(continued)
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Cobalt Molybdenum, Co<sub>7</sub>Mo<sub>6</sub>

Structure Hexagonal, $\overline{B_{m}}$ (166), $\overline{Z} = 3$ , u-phase isostruc-	d (Å)	I		hkl	$20(^{\circ})$ $\lambda = 1.540598A$
tural with $Fe_7W_6$ . The structure was determined					
by Forsyth and d'Alte da Veiga [1962].	1.7965	13	0	27	50.78
	1.7782	4	1	0 1 3	51.34
Atom positions	1.7336	5	2	08	52.76
3(a) $3 cobalt(1)$	1.6061	3	0	2 10	57.32
$18(n) \qquad 18 \text{ cobalt}(2)$	1.5439	1	2	0 1 1	59.86
6(c) $6  molybdenum(2)$	1 4026			0.16	<b>60.14</b>
6(c) $6  molybdenum (3)$	1.4015	1	1	2 8	66.68
	1.3876	2	1	1 15	67-44
Lattice constants	1.3747	12	3	0 0	68.16
a = 4.762(1)  Å c = 25.617(5)	1.3317	20	2	1 10	70.68
(published values: $a = 4.762(1)A$ , $c = 25.615(5)$	1.3086	15	0	3 6+	72.12
[ibid.])	1.2953	18	1	2 11	72.98
	1.2814	1	1	0 1 9	73.90
c/a = 5.3795	1.2645	7	0	2 16	75.06
	1.2379	2	З	0 9+	76.96
Volume ·					
503.1 A <sup>3</sup>	1.2216	12	1	1 18+	78.18
Dengitu	1.2198	9	0	0 21	78.32
(a) (a) (a) (b) $(a)$ (b) $(a)$ (c)	1.2167	10	2	0 17	78.56
(carcurated) 9.785 g/cm <sup>2</sup>	1.1905	20	2	2 0	80.64
Thermal narameters	1.1168	I	2	1 16	87.22
Isotropic: overall $B = 1.0$	1 0990	2	2	0.20	00.14
	1.0856	5	2	1 21	90.40
Scattering factors	1.0752	1		1 23	91.52
Co <sup>2+</sup> , Mo <sup>+</sup> [Forsyth and Wells, 1959], corrected	1.0708	1		0 15+	92.00
for the real part of the dispersion effects	1.0674	1	õ	0 24	92.38
[Dauben and Templeton, 1955].		-	Ŭ	0 2 .	2000
	1.0445	9	1	3 10	95.04
Scale factors (integrated intensities)	1.0398	5	2	2 12	95.60
$\gamma = 0.223 \times 10^{-3}$	1.0301	2	4	0 1	96.80
$I/I_{corundum}$ (calculated) = 3.15	1.0266	8	З	1 11	97.24
	1.0197	1	2	1 19	98.12
References		_			
Dauben, C. H. and Templeton, D. H. (1955). Acta	1.0179	2	4	0 4	98.36
Crystallogr. 6, 641.	1.0139	1	0	2 22	98.88
(1962) Acta Crystallogr 15 543	1.0108	2	0	4 5	99.30
Forsyth, J B and Wells, M (1959) Acta Crys-	• 9923	1	4	2 20	102.24
tallogr. <u>12</u> , 412.	•9095	5	-	2 20	102024
	.9888	6	0	3 18+	102.34
Calculated Pattern (Peak heights)	•9739	1	1	1 24	104.54
	•9564	1	4	0 10	107.30
$d(A)$ I hkl $2\Theta(^{\circ})$	• 9124	З	0	3 21+	115.18
$\lambda = 1.540598 \lambda$	•9063	1	1	2 23	116.42
	•8999	7	4	1 0	117.74
8.532 4 0 0 3 10.36	.8875	6	З	2 10	120.44
4.267 1 0 0 6 20.80	-8806	9	4	1 6+	122.04
	.8765	6	2	3 11	123.00
2.529 5 0 1 8 35.46	•8723	1	1	3 19	124.04
	-8669	2	۵	0.16	125.40
2.381 98 1 1 0 37.76	• 638	1	ō	1 29	126.20
2.293 5 1 1 3 39.26	.8581	1	ĩ	4 9+	127.72
2.176 72 1 0 10 41.46	.8531	З	3	1 20	129.10
2.135 18 0 0 12 42.30	.8520	8	2	2 21	129.40
2.080 100 1 1 6 43.48					
	.8510	4	0	4 17	129.70
	•8363	2	0	2 28	134.18
	•8329	1	1	2 26	135.30
	.8120	4	2	0 29	143.12
	•8101	3	1	0.31	143.92

Cobalt Molybdenum, Co<sub>7</sub>Mo<sub>6</sub> - (continued)

d (Å)	I	hkl	$2\Theta(^{\circ})$ $\lambda = 1.540598 ^{\circ}$
.8031 .8012 .7980 .7961 .7947 .7937	2 1 1 3 3	0 4 20 2 3 17 3 1 23 1 4 15+ 2 2 24 3 3 0 0 5 10	147.12 148.08 149.74 150.76 151.52 152.12 157.70
	5		

Ca	lculated Pa	ttern	(Integ	rated)
d (Å)	I		hkl	$20(^{\circ})$ $\lambda = 1.540598A$
8.539	3	0	03	10.35
4.270	1	0	06	20.79
4.072	4	1	0 1	21.81
3.467	4	1	0 4	25.67
2.529	5	0	1 8	35.46
2.381	95	1	1 0	37.75
2.294	4	1	1 3	39.25
2.176	72	1	0 10	41.46
2.135	17	0	0 12	42.30
2.079	100	1	16	43.48
2.055	39	0	2 1	44.02
2.036	8	2	0 2	44.47
2.028	58	0	1 11	44.65
1.9628	21	0	2 4	46.21
1.9129	32	2	0 5	47.49
1.8263	12	1	19	49.89
1.7965	13	0	2 7	50.78
1.7780	4	1	0 13	51.35
1.7337	5	2	0 8	52.76
1.6063	3	0	2 10	57.31
1.5438	1	2	0 11	59.86
1.4925	1	1	0 16	62.14
1.4015	1	1	28	66.68
1.3877	2	1	1 15	67.43
1.3747	13	3	0 0	68.16
1.3316	23	2	1 10	70.69
1.3085	8	3	06	72.13
1.3085	8	0	36	72.13
1.2954	20	1	2 11	72.98
1.2815	1	1	0 19	73.90
1.2646	8	0	2 16	75.05
1.2379	1	3	0 9	76.97
1.2379	1	0	39	76.97
1.2232	3	0	1 20	78.06
1.2225	2	2	1 13	78.12
1.2216	11	1	1 18	78.19
1.2199	4	0	0 21	78.32
1.2166	8	2	0 17	78.56
1.1905	24	2	2 0	80.64
1.1169	1	2	1 16	87.21

d (Å)	I	hkl	20(°)
			$\lambda = 1.540598A$
			00.11
1.0880	4	2 0 20	90+14
1.0857	5	1 1 21	90.39
1.0753	1	0 1 23	91.51
1.0674	1	0 0 24	92.39
1.0444	10	1 3 10	95+04
1 0707	6	2 2 12	95-61
1.0397	5		96.79
1.0302	3	3 1 1 1	97.23
1.0107	9	2 1 19	98-12
1.6179	2	4 0 4	98.36
1001/3	-		
1.0139	1	0 2 22	98.88
1.0107	2	0 4 5	99.30
•9924	1	4 0 7	101.83
•9896	4	1 2 2 0	102.23
•9892	1	1 3 13	102.28
•9887	3	0 3 18	102.35
•9887	3	3 0 18	102.35
•9740	1	1 1 24	104.53
•9564	1	4 0 10	107+29
• 9124	2	0 3 21	112.18
•9124	2	3 0 21	115.18
.9062	2	1 2 23	116.43
.8999	9	4 1 0	117.73
.8875	9	3 2 10	120.44
.8814	3	1 1 27	121.85
•8806	6	1 4 6	122.03
•8806	6	4 1 6	122.03
.8765	8	2 3 11	123.00
•8722	1	1 3 19	124.05
•8668	3	4 0 16	125.41
.8638	2	0 1 29	126.20
.8581	1	4 1 9	127.72
.8581	1	1 4 9	127.72
. 8531	4	3 1 20	129.08
.8520	12	2 2 2 1	129.41
•8509	3	0 4 17	129.72
• 8363	4	0 2 28	134.18
•8328	1	1 2 26	135.31
.8145	1	3 2 16	142.06
.8120	8	2 0 29	143.13
-8102	4	1 0 31	143.87
.80.31	4	0 4 20	147.12
.8013	1	2 3 17	148.04
•7980	3	3 1 23	149.74
.7962	1	1 4 15	150.71
• 7962	1	4 1 15	150.71
•7947	7	2 2 24	151.52
•7937	8	3 3 0	152.12
•7890	1	2 1 28	154.99
•7851	9	0 5 10	15/•/1

.

Cobalt Molybdenum Silicide, Co<sub>3</sub>Mo<sub>2</sub>Si

Structure Hexagonal,  $P6_3/mmc(194)$ , Z = 2, a ternary Laves phase, isostructural with MgZn2, from powder data [Bardos et al., 1961]. Atom positions 6(h) 6 cobalt 4(f) 4 molybdenum 2(a) 2 silicon The positions assigned were those given for Co<sub>3</sub>Nb<sub>2</sub>Si [Kuz'ma et al., 1964] Lattice constants a = 4.70 Åc = 7.67 [Bardos et al., (1961), table III] c/a = 1.6319Volume 146.7 Å<sup>3</sup> Density (calculated) 8.98 g/cm<sup>3</sup> Thermal parameters Isotropic: overall B = 1.0 Scattering factors  $Co^0$ ,  $Mo^{\bar{0}}$ ,  $Si^0$  [Cromer and Mann, 1968] Scale factor (integrated intensities)  $\gamma = 0.304 \times 10^{-3}$ References Bardos, D. I., Gupta, K. P. and Beck, P. A. (1961). Trans. AIME 221, 1087. Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321. Kuz'ma, Yu. B., Gladyshevs'kii, E. I. and Byk, D. S. (1964). J. Struct. Chem. USSR 5, 518.

	Calculated	Pattern	(Pea	k hei	lghts)
d (Å)	I		hkl	λ	20(°) = 1.540598A
4 07	10		_	~	21 82
4.07	10	1	0	0	21.02
3.83	1	1	0	2	23.10
3.59	1	1	0	2	24010
2.79	25	1		2	32.04
2.35	40	1		0	30.20
2.17	100	1	0	з	41.68
2.04	25	2	õ	0	44.48
2.00	90	1	1	2	45.22
1.97	80	2	Ô	1	46.12
1.92	10	-	õ	4	47.38
	2.5				
1.80	5	2	0	2	50.74
1.73	5	1	0	4	52.72
1.54	1	2	1	0	60.10
1.44	5	1	0	5	64.92
1.43	5	2	1	2	65.30
1.40	1	2	0	4	67.00
1.36	5	3	0	0	69.18
1.32	30	2	1	з	71.52
1.28	15	3	0	2+	74.06
1.23	20	2	0	5	77.92
1.20	1	2	1	4	79.88
1.18	15	2	2	0	81.92
1.09	5	2	1	5	90.32
1.08	5	2	0	6+	90.72
1.06	1	1	0	7	93.44
1.03	10	з	1	з	96.48
1.02	1	4	0	0	98.40
1.01	5	4	0	1	99.56
1.00	5	2	2	4	100.50
•983	3 1	2	1	6	103.16
.933	3 1	1	0	8	111.26
.909	9 5	З	1	5	115.82
.907	7 1	З	2	2	116.24
.892	2 1	2	1	7	119.34
.888	3 5	1	1	8+	120.38
.877	7 10	3	2	з	122.86
.865	5 15	4	1	2+	125.82
.848	B 10	4	0	5	130.58
.834	1	1	0	9	134.88
.814	4 5	2	1	8	142.42
.798	в 1	3	2	5	149.92

Cobalt Molybdenum Silicide,  $Co_3Mo_2Si - (continued)$ 

0					
d (A)	I		hkl		20(°)
<del></del>	· · · ·				$\lambda = 1.540598A$
4.07	10	1	0	0	21-82
3.84	10	0	ő	2	23.17
3.60	1	1	ō	1	24.74
2.79	25	1	ō	2	32.04
2.35	40	1	1	0	38.27
2.17	100	1	0	3	41.68
2.04	25	2	0	0	44.48
2.00	90	1	1	2	45.22
1.97	85	2	0	1	46.11
1.92	10	0	0	4	47.37
1.80	5	2	0	2	50.74
1.73	5	1	0	4	52.73
1.54	1	2	1	0	60.09
1.44	5	1	0	5	64.91
1.43	5	2	1	2	65.30
1.40	1	2	0	4	67.00
1.36	5	3	0	0	69.19
1.32	30	2	1	3	71.52
1.28	15	3	0	2	74.06
1.28	5	0	0	6	74.11
1.22	25	2	0	5	77.93
1.22	1	1	0	6	78.34
1.20	1	2	1	4	79.87
1.18	20	2	2	0	81.93
1.09	5	2	1	5	90.33
1.08	1	3	1	2	90.68
1.08	5	2	0	6	90.73
1.06	1	1	0	7	93.44
1.03	15	3	1	3	96.47
1.02	I	4	0	0	98.40
1.01	5	4	0	1	99.57
1.00	5	2	2	4	100.50
.903	1	2	1	0	103.10
•965	1	2	0	7	105.96
.933	5	1	0	8	111.26
.909	5	3	1	5	115.82
.907	1	3	2	2	116.21
.892	5	2	1	7	119.33
•888	5	4	1	<b>0</b> i	120.28
.888	5	1	1	8	120.39
.877	10	З	2	3	122.85
.865	15	4	1	2	125.80
.865	10	2	2	6	125.86
•848	15	4	0	5	130.57
.846	1	3	1	6	131.10
.840	1	3	2	4	133.13
.834	1	1	0	9	134.88
	10			24	147.41

<pre>Structure Tetragonal, I4/mmm (139), Z = 4, isostructural with NiTiSi<sub>2</sub>. The structure was determined by Yarmolyuk and Kripyakevich [1969].</pre>
Atom positions 16(k) 12 cobalt and 4 silicon(5) 8(j) 8 niobium(1) 8(h) 8 niobium(2) 8(i) 8 silicon(1) 8(h) 8 silicon(2) 4(e) 4 silicon(3) 4(c) 4 silicon(4)
Lattice constants a = 12.56  Å c = 4.984
c/a = 0.3968
Volume 786.2 Å <sup>3</sup>
Density (calculated) 6.294 g/cm <sup>3</sup>
Thermal parameters Isotropic: overall B = 3.4
Scattering factors Co <sup>0</sup> , Nb <sup>0</sup> , Si <sup>0</sup> [Cromer and Mann, 1968]
Scale factors (integrated intensities) $\gamma = 0.191 \times 10^{-3}$ I/I <sub>corundum</sub> (calculated) = 1.99
<pre>References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u>, 321. Yarmolyuk, Ya. P. and Kripyakevich, P.I. (1969). Sov. Phys. Crystallogr. <u>13</u>, 862.</pre>

	Calculated	Pattern	(Pea	ak h	eights)
d (Å)	I		hkl		$20(^{\circ})$ ° $\lambda = 1.540598 ^{\circ}$
8.874 6.276 4.440 3.969	45 10 10 5	1 2 2 3	1 0 2 1	0 0 0 0	9.96 14.10 19.98 22.38
3.204 3.140 2.959	10 15 30	3 4 3 3	032	1 0 0 1	27.82 28.40 30.18 31.30
2.693	5 5 35	4	2 1	0	31.84 34.48
2 •491 2 •464 2 • 399 2 • 243 2 • 220	10 15 100 40	5 1 4 4	1 1 3 4	0 2 1+ 0	36.44 37.46 40.18 40.60

_							
	d (Å)	I	-	hkl		20(°)	
						× = 1:540550A	_
	2.173	10	2	2	2	41.52	
	2.111	65	З	1	2	42.80	
	2.093	35	6	0	0	43.18	
	1.986	1	6	2	0	45.64	
	1.952	5	4	0	2	46.48	
	1 907	E	7	7	<b>2</b> +	47 66	
	1 964	5	5	2	27	47.00	
	1 776	5	-	5	~	40.02	
	1 688	5	7	0	1	54 30	
	1 6 5 9	1	6	~	• 2	54.50	
	1.000	1	4	4	2	22.20	
	1.630	1	7	2	1+	56.40	
	1.570	5	8	0	0	58.76	
	1.530	5	6	5	1	60.44	
	1.524	1	8	2	0	60.74	
	1.500	1	3	2	3	61.82	
	1.487	5	8	1	1+	62.40	
	1.480	5	6	6	0	62.72	
	1.459	5	4	1	3	63.76	
	1.446	5	7	1	2+	64.36	
	1.428	1	6	4	2	65.30	
	1.404	5	8	4	0	66.54	
	1.386	10	4	З	3+	67.54	
	1.375	15	7	З	2	68.12	
	1.324	5	9	З	0	71.16	
1	1.300	1	8	2	2	72.70	
	1.260	1	7	5	2	75.40	
	1.246	5	0	0	4	76.38	
	1.223	1	8	4	2	78.04	
	1.219	1	7	0	3	78.38	
	1.212	1	10	1	1+	78.92	
	1.169	1	10	з	1+	82.40	
	1.166	5	10	4	0	82.68	
	1.155	- 1	6	5	3	83.62	
	1.150	-	8	7	1	84.14	
	1.136	1	8	1	- 3+	85.36	
		•					
	1.131	1	7	7	2	85.88	
	1.122	1	10	0	2	86.76	
	1.113	1	11	0	1	87.60	
	1.096	1	10	5	1	89.32	

## Cobalt Niobium Silicide, $Co_3Nb_4Si_7$ - (continued)

	Calculated	Pattern	(Int	tegr	ated)
d (Å)	I		hkl		20(°)
					$\lambda = 1.540598A$
8.881	55	1	1	0	9.95
6.280	15	2	0	0	14.09
4.441	10	2	2	0	19.98
3.972	5	3	1	1	22.31
3.200	, 10	5	Ŭ	•	27.001
3.140	15	4	0	0	28.40
2.960	20	3	3	0	30.16
2.855	5 45	3	2	1	31.30
2.809	5	4	2	0	31.84
2.599	45	4	1	1	34+40
2.492	2 15	0	0	2	36.01
2.463	1	5	1	0	36.45
2.399	20	1	1	2	37.45
2.243	60	5	0	1	40.17
2.243	s 90	4	3	1	40.17
2.220	50	4	4	0	40.60
2.173	15	2	2	2	41.52
2.111	100	3	1	2	42.80
2.093	50	6	0	0	43.18
1.986	. 1	6	2	0	45.65
1.952	2 10	4	0	2	46.49
1.908	5	6	1	1	47.63
1.906	5 10	3	3	2	47.66
1.864	5	4	2	2	48.82
1.825	5 1	5	4	1	49.92
1.776	5 5	5	5	0	51.40
1.742	2 1	6	4	0	52.50
1.688	3 10	7	0	1	54.29
1.658	3 1	4	4	2	55.38
1.630	) 1	(	2	T	20.33
1.603	3 1	6	0	2	57.45
1.570	) 5	8	0	0	58.76
1.530	) 10	6	5	1	60.44
1.523		8	2	3	61.82
1.500	, 5	J	-	5	01002
1.487	7 5	8	1	1	62.40
1.487	1	7	4	1	62.40
1.480	) 5	6	6	0	62.72
1.459	9 5 : E	4	1	3	64 76
1 .440	5	(	1	2	04.00
1.446	5 1	5	5	2	64.36
1.428	3 5	6	4	2	65.31
1.404	+ 5	8	4	0	67.54
1.38	5 10	4	0	3	67.54
	, in the second s				
1.375	5 25	7	З	2	68.12
1.324	4 5	9	3	0	71.16
1.314	4 1	7	6	1	72.70
1.260		7	2	2	75-39
1 10200			9	-	

d (Å)	I		hkl		$20(°)$ $\lambda = 1.540598A$
•					
1.246	5	0	0	4	76.37
1.223	5	8	4	2	78.05
1.219	1	7	0	З	78.38
1.212	5	10	1	1	78.90
1.212	1	9	1	2	78.93
1.169	1	10	З	1	82.40
1.166	5	10	4	0	82.68
1.155	5	6	5	З	83.62
1.150	5	8	7	1	84.14
1.136	1	8	1	З	85.35
1.131	1	7	7	2	85.89
1.122	5	10	0	2	86.75
1.113	1	11	0	1	87.59
1.096	1	10	5	1	89.32
	-			-	

Cobalt Niobium Tin, Co<sub>2</sub>NbSn

Structure Cubic, Fm3m (225), Z = 4, a Heusler alloy, isostructural with AlCu2Mn, from powder data (x-ray and neutron) [Ziebeck and Webster, 1974]. Atom positions 8(c) 8 cobalt 4(b) 4 niobium 4(a) 4 tin Lattice constant a = 6.153 Å [ibid.] Volume 233.0 Å<sup>3</sup> Density (calculated) 9.394 g/cm<sup>3</sup> (measured) 9.80 [Ziebeck and Webster, 1974] . Thermal parameters Isotropic: overall B = 1.0 Scattering factors Co $^0,\ \mathrm{Nb}^0,\ \mathrm{Sn}^0$  [Cromer and Mann, 1968], corrected for dispersion [Cromer and Liberman, 1970]. Scale factor (integrated intensities)  $\gamma = 1.008 \times 10^{-3}$ References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u>, 321. Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891. Ziebeck, K. R. A. and Webster, P. J. (1974). J. Phys. Chem. Solids 35, 1.

	Calculated	Pattern	(Pea	k hei	ights)
d (Å)	I		hkl	)	20(°) a = 1.540598A
3.551 3.077 2.175 1.855 1.776 1.538 1.375 1.255 1.087	1 15 100 1 5 7 5 9 20 7 5	1 2 3 2 4 4 4	1 0 2 1 2 0 2 2 4	1 0 1 2 0 0 2 0	25.06 29.00 41.48 49.06 51.40 60.10 68.10 75.66 90.18
1.025 .972 .927 .888 .853 .822	5 1 9 10 6 1 1 1 3 1 2 10	4 6 4 6 6	4 2 2 4 4 4	2+ 0 2 4 0 2	97.38 104.70 112.28 120.30 129.04 139.06
	Calculated	Pattern	(Int	egra	ted)
d (Å)	I		hkl	,	2⊖(°) ° \ = 1.540598A

	Calculated	Pattern	(Int	egr	ated)
o d (A)	I		hkl		20(°) λ = 1.540598Å
3.552 3.076 2.175 1.855 1.776 1.538 1.375 1.256 1.087 1.025 .972 .927 .888 .853	$ \begin{array}{c} 1\\ 15\\ 100\\ 1\\ 5\\ 9\\ 5\\ 0\\ 25\\ 7\\ 5\\ 1\\ 9\\ 10\\ 6\\ 1\\ 5\\ 3\\ 1 \end{array} $	1 2 3 2 4 4 4 4 4 4 4 6 6 4 6	1 0 2 1 2 0 2 2 4 4 2 2 4 4	1 0 0 2 0 2 0 2 4 0	25.05 29.00 41.48 49.07 51.40 60.10 68.09 75.66 90.18 97.38 104.70 112.28 120.30 129.05
.822	2 25	6	4	2	139.06

Structure Tetragonal, P4/mmm (123), Z=1, disordered, [van Laar, 1964]. An ordered phase also exists, with a very similar tetragonal cell [Newman and Hren, 1967].
Atom positions The probability of a Co-site being occupied by a Pt atom is 0.076(8) [van Laar, 1964] 1(a) 0.924 cobalt and 0.076 platinum 1(d) 0.924 platinum and 0.076 cobalt
Lattice constants a = 2.677  Å c = 3.685 [Newman and Hren, 1967]
c/a = 1.3/65 Volume 26.41 Å <sup>3</sup>
Density (calculated) 15.97 g/cm <sup>3</sup>
Thermal parameters Isotropic: overall B = 1.0
Scattering factors Co <sup>0</sup> , Pt <sup>0</sup> [Cromer and Mann, 1968]
Scale factor (integrated intensities) $\gamma = 1.321 \times 10^{-3}$
<pre>References Cromer, D. T. and Mann, J. B. (1968). Acta Crys- tallogr. A24, 321. van Laar, B. (1964). J. Phys. Paris 25, 600. Newman, R. W. and Hren, J. J. (1967). Surface Sci. 8, 373.</pre>

				•				
	Calc	ulated H	Pattern	(Pea	k he	eight	s)	
d (2	A)	I		hkl		λ =	20(°) 1.540598	° A
3. 2. 2. 1. 1.	684 676 165 893 843	25 20 100 30 15	0 1 1 1 0 1 1 1 0 1 1 1 1 0 1 1 1 1 1 0 1	0 0 1 0	1 0 1 0 2		24.14 33.46 41.68 48.02 49.42	
1 • 1 • 1 • 1 •	518 3386 3204 2579	5 10 15 5	1 2 1 2	0 0 1 0	2 0 2 1		61.00 70.26 71.38 75.52	
1 • 1 • 1 • 1 •	1971 1387 1164 0830 0304	1 15 10 5 1	2 2 1 2 1	1 1 0 0 1	0 1 3 2 3		80.10 85.14 87.26 90.68 96.76	

d (Å)	I		hkl		2Θ(°) 。 λ = 1.540598A
1.0039	5	2	1	2	100.22
.9464	1	2	2	0	108.96
.9212	1	0	0	4	113.48
.9167	1	2	2	1	114.34
•9050	1	2	0	з	116.68
.8711	1	1	0	4	124.32
.8672	5	з	0	1	125.30
.8573	10	2	1	з	127.92
.8465	5	З	1	0	131.00
•8419	5	2	2	2	132.40
.8284	5	1	1	4	136.84
.8250	1	З	1	1	138.02
.8031	1	З	0	2	147.14

	Calculated	Pattern	(Int	tegr	ated)
d (Å)	I		hkl		$2\Theta(^{\circ})$ . $\lambda = 1.540598A$
7 605					04.17
3.685	20	0	0	1	24.13
2.0//	20	1	0	0	33.45
2.100	100	1	1		41.07
1.693	30	1	1	2	40.03
1.843	15	0	0	2	49.43
1.684	10	1	1	1	54.45
1.518	5	1	0	2	61.00
1.338	5 10	2	0	0	70.27
1.320	3 15	1	1	2	71.38
1.258	1 5	2	0	1	75.51
1.228	3 1	0	0	з	77.67
1.197	2 5	2	1	0	80.09
1.138	6 20	2	1	1	85.15
1.116	4 10	1	0	з	87.26
1.082	9 10	2	0	2	90.69
1.030	4 1	1	1	з	96.76
1.003	9 5	2	1	2	100.23
.946	5 5	2	2	0	108.95
.921	31	0	0	4	113.47
•916	7 1	2	2	1	114.34
.905	0 1	2	0	3	116.67
. 892	3 1	3	0	0	119.37
•871	1 1	1	0	4	124.32
.867	3 5	з	0	1	125.29
.857	3 15	2	1	З	127.92
-846	5 5	ч	1	0	130,99
.841	9 5	2	2	2	132-40
.828	4 5	2	1	4	136-84
825	1 5	3	1	1	138.02
.803	1 1	3	ò	2	147.13
			, in the second s	-	

```
Structure
  Tetragonal, P4/mmm (123), Z = 1, ordered [van
  Laar, 1964]. This is the arrangement described
  as face-centered tetragonal by Newkirk et al.
  [1951]. There is also a disordered phase with
  a very similar tetragonal cell.
Atom positions
           l cobalt
  1(a)
  1(d)
           1 platinum
Lattice constants
  a = 2.682 \text{ Å}
  c = 3.675
  [Newman and Hren, 1967]
  c/a = 1.3702
Volume
  26.44 A<sup>3</sup>
Density
  (calculated) 15.96 g/cm<sup>3</sup>
Thermal parameters
  Isotropic: overall B = 1.0
Scattering factors
Co<sup>0</sup>, Pt<sup>0</sup> [Cromer and Mann, 1968].
Scale factor (integrated intensities)
  \gamma = 1.321 \times 10^{-3}
References
  Cromer, D. T. and Mann, J. B. [1968].
                                                Acta
   Crystallogr. A24, 321.
  van Laar, B. (1964). J. Phys. Paris 25, 600.
  Newkirk, J. B., Smoluchowski, R., Geisler,
    A. H., and Martin, D. L. (1951). J. Appl.
    Phys. 22, 290.
  Newman, R. W. and Hren, J. J. (1967). Surface
    Sci. 8, 373.
         Calculated Pattern (Peak heights)
```

d(Å)	I		hkl		$2\Theta(^{\circ}) \circ $ $\lambda = 1.540598A$
7 675	70		_		24.20
3 40 3	30		Ň		27 20
2.082	25	4	0	•	33.30
2.100	100	1	0	1	41.00
1.896	30	1	1	0	47.94
1.837	15	0	0	2	49.58
1.685	10	1	1	1	54.40
1.516	10	1	0	2	61.08
1.3410	10	2	0	0	70.12
1.3197	15	1	1	2	71.42
1.2596	5	2	0	1	75.40
1.2251	1	0	0	з	77.92
1.1994	5	2	1	0	79.92
1.1402	15	2	1	1	85.00
1.1143	10	1	0	7	87.46
1.0071	-	2	~	2	00.66
1•1143 1•0831	10 5	1 2	0 0	3 2	87•46 90•66

d(Å)	I	hk	ςl λ	20(°) 。 = 1.540598A
1.0290	1	1 1	3	96.94
1.0044	5	2 1	2	100.16
.9482	1	2 2	2 0	108.66
•9182	1	2 2	2 1+	114.06
•9044	1	2 (	) 3	116.80
.8940	1	3 (	0	119.00
.8687	5	3 (	) 1+	124.94
.8570	10	2 1	3	128.00
.8481	5	3 1	LO	130.52
•8427	5	2 2	2 2	132.16
.8268	5	1 1	4+	137.40
.8039	1	3 (	) 2	146.76

	Calculated	Pattern	(In	tegr	ated)
d (Å)	I		hkl		20(°) λ = 1.540598A
_	7.6	•	•	•	24 20
3.675	30	0	0	1	24.20
2.682	25	1	0	0	33.38
2.166	100	1	0	1	41.00
1.896	30	1	1	0	47.93
1.838	15	0	0	2	49.57
1.685	10	1	1	1	54.40
1.516	10	1	0	2	61.08
1.341	0 10	2	0	0	70.12
1.319	7 15	1	1	2	71.42
1.259	85	2	0	1	75.39
1.225	0 1	0	0	з	77.93
1.199	4 5	2	1	0	79.92
1.140	<b>2</b> 20	2	1	1	85.00
1.114	3 10	1	0	3	87.47
1.083	2 10	2	0	2	90.65
1.029	0 1	1	1	з	96.94
1.004	4 5	2	1	2	100.16
.948	2 5	2	2	0	108.65
.918	8 1	0	0	4	113.95
•918	2 1	2	2	1	114.06
.904	4 1	2	0	з	116.79
.894	0 1	3	0	0	119.00
.869	2 1	1	0	4	124.81
-868	7 5	3	0	1	124.94
.857	0 15	2	1	З	128.00
.848	1 5	3	1	0	130.53
.842	6 5	2	2	2	132.17
-826	8 10	1	1	4	137.38
.826	4 5	3	1	1	137.53
.803	9 5	3	0	2	146.75

```
Structure
  Cubic, Fm3m (225), Z=1, disordered, from powder
  data. It occurs when the material is heated
  above 800 °C, then quenched. There is also an
  ordered phase with a similar size and structure
  [Geisler and Martin, 1952].
Atom positions
  4(a)
       l cobalt
  4(a)
         3 platinum
Lattice constant,
  a = 3.8532(3) A
  (published value, 3.8530(3) [Berg and Cohen,
  1972]).
Volume
  57.209 Å<sup>3</sup>
Density
  (calculated) 18.694 g/cm<sup>3</sup>
Thermal parameters
  Isotropic: cobalt B = -0.1; platinum B = 0.337
  [Berg and Cohen, 1972].
Scattering factors
  Co^0, Pt<sup>0</sup> [Cromer and Mann, 1968] corrected for
  dispersion [Cromer and Liberman, 1970].
Scale factor (integrated intensities)
  \gamma = 1.632 \times 10^{-3}
References
  Berg, H. and Cohen, J. B. (1972). Metall. Trans.
    <u>3</u>, 1797.
  Cromer, D. T. and Liberman, D. (1970). J. Chem.
    Phys. 53, 1891.
  Cromer, D. T. and Mann, J. B. (1968). Acta Crys-
    tallogr. <u>A24</u>, 321.
```

Geisler, A. H. and Martin, D. L. (1952). J. Appl. Phys. <u>23</u>, 375.

	Calculated	Pattern	(Pe	ak h	eights)
d(Å)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598 \text{\AA}$
2.224	100	1	1	1	40.52
1.926	45	2	ō	0	47.14
1.362	4 25	2	2	0	68.86
1.161	8 30	З	1	1	83.06
1.112	3 10	2	2	2	87.66
•963	3 5	4	0	0	106.20
.884	0 15	3	з	1	121.24
.861	6 15	4	2	0	126.76
•786	5 20	4	2	2	156.68

Calculated Pattern (Integrated)							
d(Å)	I		hkl		20(°) $\lambda = 1.540598A$		
2.225	100	1	1	1	40.52		
1.927	50	2	0	0	47.13		
1.362	з зо	2	2	0	68.87		
1.161	8 35	З	1	1	83.06		
1.112	3 10	2	2	2	87.66		
• 963	<b>3</b> 5	4	0	0	106.19		
.884	0 25	3	з	1	121.24		
.861	6 25	4	2	0	126.77		
•786	5 55	4	2	2	156.68		

Structure	
Cubic, Pm3m (221), $Z = 1$ , isostructural with AuCu <sub>3</sub> , from powder data. There is also a dis- ordered phase with very similar size and structure, found when the sample is heated to 800 °C, then quenched [Geisler and Martin, 1952].	
Atom positions	
l(a) l cobalt	
3(c) 3 platinum	
Lattice constant。	
a = 3.8541(4) A	
(published value, a = 3.8539(4) [Berg and Cohen,	
1972]).	

Volume 57.249 Å<sup>3</sup>

Density

(calculated) 18.686 g/cm<sup>3</sup>

```
Thermal parameters
Isotropic: cobalt B = -0.1; platinum B = 0.337
[Berg and Cohen, 1972].
```

```
Scattering factors
Co<sup>0</sup>, Pt<sup>0</sup> [Cromer and Mann, 1968], corrected for
dispersion [Cromer and Liberman, 1970].
```

```
Scale factor (integrated intensities)

\gamma = 1.633 \times 10^{-3}
```

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References
```

```
Berg, H. and Cohen, J. B. (1972). Metall. Trans.
3, 1797.
```

```
Cromer, D. T. and Liberman, D. (1970). J. Chem.
Phys. <u>53</u>, 1891.
```

- Cromer, D. T. and Mann, J. B. (1968). Acta Crysstallogr. <u>A24</u>, 321.
- Geisler, A. H. and Martin, D. L. (1952). J. Appl. Phys. 23, 375.

	Cal	culated	Pattern	(Pea	ak h	eights)
d (A)	)	I		hkl		$2\theta(^{\circ})$ , $\lambda = 1.540598 ^{\circ}$
3.8	54	15	1	0	0	23.06
2.7	25	10	1	1	0	32.84
2.22	24	100	1	1	1	40.52
1.92	27	45	2	0	0	47.12
1.7	23	5	2	1	0	53.10
1.5	74	5	2	1	1	58.62
1.30	527	25	2	2	0	68.84
1.2	B47	1	2	2	1+	73.68
1.2	188	1	3	1	0	78.40
1.10	520	30	3	1	1	83.04
1.1	125	10	2	2	2	97 64
1 04	12J 600	10	2	2	2	07.04
1.0	201	1	נ ד	2	1	92.022
1.04	575	1	5	2	1	90.00
•90	240	5	4	0	0	100+10
• 7.	340	+	3	2	24	110.98
•90	084	1	4	1	1+	115.98
.88	342	15	3	з	1	121.20
.86	518	15	4	2	0	126.72
.84	+11	1	4	2	1	132.66
. 82	217	1	3	З	2	139.26
.78	367	20	4	2	2	156.54

	Calculated	Pattern	(In	tegi	rated)
d (A)	I		hkl		$2\Theta(^{\circ})$ ° $\lambda = 1.540598A$
3.854	15	1	0	0	23.06
2.725	10	1	1	0	32.84
2.225	100	1	1	1	40.51
1.927	50	2	0	0	47.12
1.724	5	2	1	0	53.09
1.573	5	2	1	1	58.62
1.3626	5 30	2	2	0	68.85
1.2847	7 1	2	2	1	73.68
1.2188	3 1	3	1	0	78.40
1.1621	35	3	1	1	83.04
1.1126	5 10	2	2	2	87.63
1.0689	) 1	3	2	0	92.21
1.0301	5	3	2	1	96.80
•9635	5 5	4	0	0	106.16
• 9348	3 1	4	1	0	110.99
.9348	3 1	3	2	2	110.99
.9084	+ 1	4	1	1	115.98
.8842	2 25	3	З	1	121.19
.8618	3 25	4	2	0	126.72
.8410	) 5	4	2	1	132.67
.8217	1	3	З	2	139.26
.7867	55	4	2	2	156.55

## Cobalt Plutonium, CoPu<sub>3</sub>

Structure	Cal	culated Pat	tern	(Pea	k he	eights)
Orthorhombic, Cmcm (63), $2 = 4$ , isostructural with BRe <sub>3</sub> and Al <sub>2</sub> CuMg. The structure was refined by Larson, Cromer, and Roof [1963].	d (A)	I	}	nkl		$2\Theta(\circ) \circ \\ \lambda = 1.540598A$
Atom positions						
4(c) 4 cobalt	4.61	2	0	0	2	19.24
4(c) 4 plutonium(1)	3.53	5	0	2	2	25.22
8(f) 8 plutonium(2) [ibid.]	3.312	3	1	1	0	26.90
	3.116	16	1	1	1	28.62
Lattice constants a = 3.475(4) Å	2.745	24	0	4	0	32.60
b = 10.977(10)	2.688	88	1	1	2	33.30
c = 9.221(8)	2.682	100	0	2	3	33.38
	2.630	14	0	4	1	34.06
(published values: $a = 3.475(4)A$ , $b = 10.976(10)$ ,	2.520	19	1	3	0	35.60
c = 9.220(8) [Larson et al., 1963]).	2.430	35	1	3	1	36.96
CD cell: a=9.221(8)Å, b=10.977(10), c=3.475(4);	2.358	11	0	4	2	38.14
sp. qp. Amam; $a/b = 0.8400$ ; $c/b = 0.3166$	2.305	7	0	0	4	39.04
	2.253	11	1	1	3	39.98
Volume .	2.211	15	1	з	2	40.78
351.7 A <sup>3</sup>	2.047	2	0	4	3	44.22
Density	1.892	2	1	1	4	48.04
(calculated) 14.823 g/cm <sup>3</sup>	1.795	1	0	6	1	50.84
(massured) 14.82 g/cm <sup>3</sup> [Larson et al., 1963]	1.765	1	0	4	4	51.76
(medsureu) 14.02 g/om (marson ee ure, 1903)	1.748	3	0	2	5	52.30
Thormal narameters	1.737	10	2	0	õ	52.64
Isotropic [Larson et al., 1963]	101.01	1.	-	Ũ	Ũ	52104
	1.722	7	1	5	2	53.16
Scattering factors	1.700	4	0	6	2	53.88
Co <sup>0</sup> [Forsyth and Wells, 1959], corrected for	1.611	8	1	1	5	57.12
dispersion by $\Delta f' = -2.2$	1.589	10	1	5	3	58.00
Pu <sup>0</sup> [Larson et al., 1963], modified for use	1.572	3	0	6	3	58.68
with tu A.	1.559	1	2	2	2	59.22
Scale factors (integrated intensities)	1.537	3	0	0	6	60.16
$v = 0.413 \times 10^{-3}$	1.531	3	0	4	5	60.42
T/T (calculated) 8 07	1-488	10	1	3	5	62.34
corundum (carculated, 5.0)	1.468	4	2	4	0	63.30
References			2	2	-	( 7 70
Forsyth, J.B. and Wells, M. (1959). Acta Crystal-	1.458	11	2	2	3	63.78
logr. <u>12</u> , 412.	1.450	3	2	4	1	64.18
Larson, A. C., Cromer, D. T., and Roof, R. B., Jr.	1.429	7	1	-	0	65.22
(1963). Acta Crystallogr. <u>16</u> , 835.	1.399	2	2	4	2	66.82
	1.388	2	2	0	4	67.44
	1.341	1	0	4	6	70.12
	1.315	2	0	8	2	71.72
	1.312	2	1	3	6	71.90
	1.308	2	1	5	5	72.14
	1.299	2	0	6	5	72.76
	1.281	2	0	2	7	73.94
	1.232	1	2	2	5	77.38
	1.215	3	2	6	2+	78.68
	1.166	1	2	6	з	82.72
	1.151	2	2	0	6+	84.00
	1.149	2	2	4	5	84.24
	1-118	2	3	1	2	87.14
	1.104	1	3	3	0	88-46
	1.096	1	3	3	1	89.26
	1.089	2	1	1	8	90-08
		-	•		Ŭ	

Cobalt Plutonium, C	CoPu <sub>3</sub> - (	continued)
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	Calculated	Pattern	(Int	egr	ated)
(A) b	Ť		hkl		2 <u>9</u> (°)
u(11)	-		11122		$\lambda = 1.540598A$
				_	
4.61	2	0	0	2	19.24
3.53	, 0		2	2	20.21
3.119		1	1	1	28.61
2.744	32	0	4	0	32.60
	. 52	· ·		Ŭ	02000
2.690	) 100	1	1	2	33.27
2.682	2 78	0	2	З	33.39
2.630	18	0	4	1	34.06
2.520	) 26	1	З	0	35.60
2.431	. 49	1	З	1	36.95
2.358	3 15	0	4	2	38.13
2.305	5 10	0	0	4	39.04
2.253	3 15	1	1	З	39.98
2.211	21	1	З	2	40.78
2.047	7 3	0	4	3	44.21
1.892	2 4	1	1	4	48.04
1.856	5 1	1	5	0	49.04
1.795	5 1	0	6	1	50.84
1.765	5 1	0	4	4	51.75
1.748	3 4	0	2	5	52.29
1.737	7 14	2	0	0	52.63
1.722	2 11	1	5	2	53.15
1.701	. 6	0	6	2	53.87
1.611	12	1	1	5	57.12
1.589	9 15	1	5	З	58.00
1.572	2 5	0	6	з	58.68
1.559	9 1	2	2	2	59.22
1.537	7 4	0	0	6	60.16
1.53	1 3	0	4	5	60.43
1.488	3 16	1	З	5	62.34
1.468	3 7	2	4	0	63.30
1.45	8 16	2	2	З	63.78
1.450	0 4	2	4	1	64.19
1.43	31	0	6	4	65.03
1.429	9 10	1	7	0	65.22
1.39	9 4	2	4	2	66.83
1.38	в З	2	0	4	67.44
1.34	1 1	0	4	6	70.13
1.32	5 1	2	4	З	71 • 11
1.31	5 4	0	8	2	71.71
1.31	2 1	1	з	6	71.90
1.30	8 2	1	5	5	72.15
1.29	9 3	0	6	5	72.75
1.28	1 3	0	2	7	73.94
1.23	2 2	2	2	5	77.37
1.21	5 3	2	6	2	78.67
1.21	5 2	1	7	4	78.71
1.16	6 2	2	6	З	82.72
1.15	1 2	2	0	6	84.00
1.14	9 2	2	4	5	84.24

d (Å)	I	hkl		$20(^{\circ})$ $\lambda = 1.540598A$
1.130	1	1 7	5	85.97
1.118	З	31	2	87.14
1.106	1	26	4	88.34
1.104	1	33	0	88.46
1.096	2	33	1	89.26
1.090	1	0 10	1	89.93
1.089	3	1 1	8	90.08
## Cobalt Samarium, Co<sub>2</sub>Sm

Structure
Cubic, Fd3m(227), Z=8, isostructural with Cu <sub>2</sub> Mg,
from powder data [Harris et al., 1965].
Atom positions
16(d) 16 cobalt
8(a) 8 samarium
origin at 43m
Lattice constants
a = 7.2627 A
(published value, a = 7.2476 kX [Harris et al.,
1965])
Volume
383.08 A <sup>3</sup>
Density

(calculated) 9.301 g/cm<sup>3</sup>

Thermal parameters Isotropic: overall B = 1.0

### Scattering factors Co<sup>0</sup> [Cromer and Mann, 1968] Sm<sup>0</sup> [International Tables, 1974].

- Scale factor (integrated intensities)
  - $\gamma = 0.569 \times 10^{-3}$

## References

- Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u>, 321.
- Harris, I. R., Mansey, R. C. and Raynor, G. V. (1965). J. Less-Common Metals 9, 270.
- International Tables for X-ray Crystallography, <u>IV</u> (1974). (The Kynoch Press, Birmingham, Eng.) p. 100.

Ca	lculated Pat	ttern	(Pea	ık he	eights)
d (Å)	I		hkl		$20(^{\circ})$ $\lambda = 1.540598A$
4.191	15	1	1	1	21.18
2.567	70	2	2	0	34.92
2.189	100	3	1	1	41.20
2.096	15	2	2	2	43.12
1.6660	5	З	З	1	55.08
1 40.07			-	_	
1.4823	20	4	2	2	62.62
1.3978	25	5	1	1+	66.88
1.2838	15	4	4	0	73.74
1.2277	1	5	З	1	77.72
1.1483	5	6	2	0	84.26
1.1075	5	5	з	з	88,14
1.0949	5	6	2	2	89.42
1.0170	1	7	1	1+	98.48
.9706	10	6	4	2	105-06
•9455	10	7	3	1+	109.12
•9078	1	8	0	0	116.10
.8559	5	8	2	2+	128.30
.8386	10	7	5	1+	133.42
.8331	1	6	6	2	135.22
•7972	1	7	5	3+	150.16
Ca	lculated Pa	ttern	(Int	egra	ated)
å (Å)	I		hkl		20(°) 。

d(A)	I	hkl			$2\Theta(^{\circ}) \\ \lambda = 1.540598 A$
			_		
4.193	10	1	1	1	21 + 17
2.568	65	2	2	0	34.91
2.190	100	3	1	1	41.19
2.097	15	2	2	2	43.11
1.6662	5	3	3	1	55.07
1.4825	20	4	2	2	62.61
1.3977	20	5	1	1	66.89
1.3977	5	З	З	З	66.89
1.2839	20	4	4	0	73.74
1.2276	1	5	3	1	77.73
1.1483	10	6	2	0	84.26
1.1076	10	5	3	3	88.13
1.0949	5	6	2	2	89.42
.9705	10	6	4	2	105.06
.9455	10	7	З	1	109.11
- 9455	5	5	5	3	109-11
-9078	5	Ř	õ	õ	116.10
- 8559	5	6	6	ñ	128.31
- 8559	5	e B	2	2	128.31
9796	10	7	5	1	133.42
.0300	10	•	Ŭ	•	
.8386	1	5	5	5	133.42
.8331	5	6	6	2	135.23
.7972	1	7	5	З	150.15
•7972	1	9	1	1	150.15

.

Cobalt Tin Vanadium, Co<sub>2</sub>SnV

```
Structure
Cubic, Fm3m(225), Z = 4, a Heusler alloy iso-
structural with AlCu<sub>2</sub>Mn, from powder data
[Kripyakevich and Markiv, 1963].
```

Atom pos	siti	ons
8(c)	8	cobalt
4(a)	4	tin
4(b)	4	vanadium

Lattice constant a = 5.994 Å [ibid.]

```
Volume
215.35 Å<sup>3</sup>
```

```
Density
```

```
(calculated) 8.867 g/cm<sup>3</sup>
```

```
Thermal parameters
Isotropic: overall B = 1.0
```

```
Scattering factors
Co<sup>0</sup>, Sn<sup>0</sup>, V<sup>0</sup> [Cromer and Mann, 1968]
```

```
Scale factor (integrated intensities) \gamma = 0.835 \times 10^{-3}
```

```
References
```

```
Cromer, D. T. and Mann, J. B. (1968). Acta
Crystallogr. <u>A24</u>, 321.
Kripyakevich. P. I. and Markiv, V.Ya. (1963).
Dopov. Akad. Nauk Ukr. RSR <u>12</u>, 1606.
```

	Calculated	Pattern	(Pea	ak he	eights)
d (Å)	I		hkl		$2\Theta(°)$ $\lambda = 1.540598A$
3.458	15 5 5	1 2	1	1 0	25.74 29.80
1.807	5	2 3 2	2 1 2	1 2	42.64 50.46 52.88
1.499 1.379 1.340	15 5 1 1	4 3 4	0 3 2	0 1 0	61.86 68.14 70.16
1.223	20 3 1	<b>4</b> 5	2 1	2 1+	78.04 83.80
1.060 1.013 .948	5 1 10	4 5 6	4 3 2	0 1 0	93.26 98.98 108.74
•865 •839		47	4	4 1+	125.84 133.20
•801	15	6	4	2	148.18

	Calculated	Pattern	(Int	tegr	ated)
d (Å)	I		hkl		$20(^{\circ})$ $\lambda = 1.540598A$
3.461	15	1	1	1	25.72
2.99	7 5	2	0	0	29.79
2.119	9 100	2	2	0	42.63
1.80	7 5	3	1	1	50.46
1.73	0 1	2	2	2	52.87
1.499	9 15	4	0	0	61.87
1.379	5 5	З	З	1	68.14
1.34	0 1	4	2	0	70.16
1.224	25	4	2	2	78.04
1.154	4 1	5	1	1	83.79
1.060	) 5	4	4	0	93.27
1.013	3 1	5	3	1	98.98
.94	в 10	6	2	0	108.74
.914	4 1	5	3	З	114.85
.86	5 5	4	4	4	125.84
.839	9 1	5	5	1	133.20
.83	9 1	7	1	1	133.20
.80	1 30	6	4	2	148.18

Cobalt Tin Zirconium, Co<sub>2</sub>SnZr

```
Structure
  Cubic, Fm3m (225), Z = 4, a Heusler alloy, iso-
  structural with AlCu2Mn, from x-ray and neutron
  powder data [Ziebeck and Webster, 1974].
Atom positions
  8(c)
          8 cobalt
             4 tin
  4(a)
  4(b)
             4 zirconium
Lattice constant
  a = 6.249 A [Ziebeck and Webster, 1974]
Volume
  244.0 Å<sup>3</sup>
Density
  (calculated) 8.921 g/cm<sup>3</sup>
  (measured) 8.90 g/cm<sup>3</sup> [Ziebeck and Webster, 1974]
Thermal parameters
  Isotropic: overall B = 1.0
Scattering factors
  Co<sup>0</sup>, Sn<sup>0</sup>, Zr<sup>0</sup> [Cromer and Mann, 1968], corrected
  for anomalous dispersion [Cromer and Liberman,
  1970]
Scale factor (integrated intensities)
  \gamma = 1.009 \times 10^{-3}
References
  Cromer, D.T. and Mann, J.B. (1968). Acta Crystal-
    logr. A24, 321.
  Cromer, D. T. and Liberman, D. (1970). J. Chem.
    Phys. <u>53</u>, 1891.
  Ziebeck, K. R. A. and Webster, P. J. (1974). J.
    Phys. Chem. Solids 35, 1.
```

Ca	alculated	Pattern	(Pea	k he:	ights)
d (Å)	I		hkl	,	$2\Theta(^{\circ})$ = 1.540598A
3.607	1	1	1	1	24.66
3.123	15	2	0	0	28.56
2.209	100	2 3	2	1	40.02
1.804	5	2	2	2	50.56
1.562	15	4	0	0	59.08
1.397	5	4	2	0	66.90
1.276	20	4	2	2	74.30
1.1047	5	4	4	0	88.42
1.0415	1	4	4	2+	95.40
.9880	10	6	2	0	102.46
.9421	1	6	2	2	109.70
.9020	1	4	4	4	117.30
.8666	1	6	4	0	125.46
.8350	10	6	4	2	134.58

	Calculated	Pattern	(In	tegr	ated)
d(Å)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
3.608 3.124 2.209 1.884 1.804 1.562 1.397 1.276 1.104 1.041 .988 .942 .902 .866	3       1         5       100         1       15         1       100         1       5         2       15         5       25         5       25         5       1         31       10         21       1         20       5         56       1         36       1	1 2 2 3 2 4 4 4 4 4 4 6 6 4 6	1 0 2 1 2 0 2 2 4 4 2 2 4 4	1 0 1 2 0 0 2 0 2 0 2 4 0 2	24.66 28.55 40.81 48.26 50.56 59.09 66.91 74.30 88.42 95.40 102.45 109.70 117.30 125.47 136.57
•835	51 20	6	4	2	134.57

```
Structure
  Cubic, Fm3m(225), Z=4, a Heusler alloy, iso-
  structural with AlCu2Mn, from powder data
  [Gladyshevs'kii, 1962].
Atom positions
  8(c) 8 cobalt
  4(b)
         4 vanadium
  4(a)
         4 silicon
Lattice constant
  a = 5.659 Å [ibid.]
Volume
  181.2 Å<sup>3</sup>
Density
  (calculated) 7.216 g/cm<sup>3</sup>
Thermal parameters
  Isotropic: overall B = 1.0
Scattering factors
  Co^0, V^0, Si^0 [Cromer and Mann, 1968]
Scale factor (integrated intensities)
 \gamma = 0.606 \times 10^{-3}
References
  Cromer, D. T. and Mann, J. B. (1968). Acta
  Crystallogr. <u>A24</u>, 321.
Gladyshevs'kii, E. I. (1962). Porosh. Met.
    2, 46.
```

(	Calculated	Pattern	(Pe	ak 1	heights)
d (Å)	I		hkl		$2\Theta(^{\circ})$ , $\lambda = 1.540598A$
	<u></u>				
3.266	5	1	1	1	27.28
2.829	10	2	0	0	31.60
2.000	100	2	2	0	45.30
1.7061	1	З	1	1	53.68
1.6338	1	2	2	2	56.26
1.4147	10	4	0	0	65.98
1.2654	. 1	4	2	0	75.00
1.1552	20	4	2	2	83.64
1.0004	5	4	4	0	100.70
.8947	10	6	2	0	118.84
•8168	3 1	4	4	4	141.14

	Calculated	Pattern	(I	ntegi	cated)
d (A)	I		hk	l	20(°) ° λ = 1.540598A
3.267	5	1	1	1	27.27
2.829	10	2	0	ō	31.60
2.001	100	2	2	0	45.29
1.7063	3 1	З	1	1	53.67
1.6336	5 1	2	2	2	56.27
1.4147	15	4	0	0	65.98
1.2654	+ 1	4	2	0	75.00
1.1551	20	4	5	2	83.65
1.0004	5	4	4	0	100.71
. 8948	3 10	6	2	0	118.83
.8168	3 5	4	4	4	141.14
•7845	• 1	6	4	0	157.97
	-				

Synonyms	Cal	lculated	Pattern	(Pea	k he	ights)
1-Methy1-5,5-diethylbarbituric acid	0					
N-Methylbarbital Gemonil	d (A)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
Structure	8.61	100	0	1	1	10.26
Monoclinic, $P2_1/c$ (14), $Z = 4$ . The structure was	6.79	36	1	0	0	13.02
determined by Wunderlich [1973].	6.59	90	O	0	2	13.42
	5.83	16	1	1	0	15.18
Atom positions	5.70	94	С	2	0+	15.54
All atoms are in general positions 4(e) [ibid.].						
	5.33	97	1	1	1+	16.62
Lattice constants	5.23	21	0	2	1	16.94
a = 6.798(2) A	4.74	4	-1	0	2	18.70
h = 11, 398(3)	4.380	31	-1	1	2	20.26
c = 13, 191(3)	4.312	8	0	2	2	20.58
$R = 90.29(1)^{\circ}$	40012	-	•	-	-	
p = 50.25(1)	4.141	1.0	1	2	1	21.44
(published values, $a = 6.798(2)$ ) $b = 11.397(3)$	4.100	12	-	1	3	21.66
(published values: a = 0.790(2)A, b = 11.537(5),	3.642	14	- 1	2	2+	24.42
C = 13.190(3), p = 90.29(1) [wunderlich, 1973])	3.490	63		2		25.58
	3.400		2	2	0	26.20
CD cell: $a = 13.191(3)A$ , $b = 11.398(3)$ ,	2.399	3	2	U	U	20.20
$c = 6.798(2), \beta = 90.29(1)^\circ; \text{ sp. gp. } P2_1/a;$		0.5	0	-	2	27.06
a/b = 1.1573; c/b = 0.5964	3.293	25	0	3	2	27.00
	3.213	4	1	5	1	27.74
Volume	3.164	20	-2	1	1	28.18
1022.07 A <sup>3</sup>	3.093	15	1	2	3+	28.24
	3.014	3	2	0	2	29.62
Density				_	<b>.</b> .	
(calculated) 1.288 g/cm <sup>3</sup>	2.961	3	-1	3	2+	30.16
(measured) 1.273 g/cm <sup>3</sup> [Wunderlich, 1973]	2.915	14	2	1	2+	30.64
	2.873	29	0	3	3	31.10
Thermal parameters	2.852	12	-2	2	1+	31.34
For hydrogen atoms: isotropic B's [Wunderlich,	2.665	3	2	2	2	33.60
1973]. For other atoms isotropic B, were esti-						
mated from $\beta_{11}$ , $\beta_{22}$ , $\beta_{33}$ for each atom.	2.651	3	-1	3	3	33.78
	2.617	9	0	4	2+	34.24
Scattering factors	2.570	3	0	1	5	34.88
$C^0$ , $H^0$ , $N^0$ , $O^0$ [International Tables, 1962]	2.486	2	2	З	1+	36.10
	2.439	З	1	4	2	36.82
Scale factors (integrated intensities)						
$\gamma = 1.503 \times 10^{-3}$	2.408	3	-1	1	5	37.32
I/I _ (calculated) 0.601	2.400	5	1	1	5	37.44
corundum	2.393	4	0	4	3	37.56
References	2.372	2	-2	0	4	37.90
International Tables for X-ray Crystallography,	2.368	2	- 2	З	2	37.96
III (1962), (The Kynoch Press, Birmingham, Eng.)						
p. 202.	2.335	3	1	З	4	38.52
Wunderlich, H. (1973), Acta Crystallogr, B29,	2.253	8	1	4	з	39.98
168	2.192	9	-3	1	1+	41.14
100.	2.167	5	0	з	5	41.64
	2.162	4	0	1	6	41.74
	2.132	2	1	5	1	42.36
	2.108	2	-3	1	2	42.86
	2.104	2	3	1	2	42.96
	2.081	2	-3	2	1	43.46
	2.062	2	1	3	5+	43.88
		-	•	-		
	2.056	2	0	2	6+	44.00
	2.034	2	0	5	3	44.74
	2.005	3	2	7	4	45.18
	1.009	2	-7	1	7	45.60
	1.986	1	-5	2	5	46.26
	1.961	1	1	2	07	40.20

Metharbital,  $C_{9}H_{14}N_{2}O_{3}$  - (continued)

d (Å)	I	ł	nkl	λ	20(°) = 1.540598A
1.954	1	2	4	з	46.44
1.903	1	-3	2	3+	47.76
1.893	1	2	5	0	48.02
1.873	1	2	5	1+	48.56
1.864	2	З	З	2	48.82
1.860	2		٨	5.	49.04
1.850	2	-2	7	5	40.30
1.007	2	-2	~	6 6 -	49.20
1.810	3	-2	~	4	49.90 E0 10
1 004	1	2		4	50.12
1.000	•	T	5	4	50.48
1.796	1	-1	1	7	50.80
1.760	1	-2	2	6+	51.92
1.740	3	-2	5	3+	52.54
1.725	2	С	5	5	53.06
1.700	1	4	0	0	53.90
1.679	1	- 3	٦	4+	54.60
1.658	1	2	6	0	55.36
1.645	1	= 2	6	14	55.84
1.628	1	2	1	7+	56.48
1.583	2	2	-	6.	59.24
1.000	2	Ŭ	5	0+	50.24
1.579	2	4	2	2+	58.38
1.572	1	1	7	1+	58.68
1.565	1	-3	4	4	58.98
1.542	1	1	2	8+	59.96

	Calculated	Pattern	(In	tegr	ated)
d (Å)	I		hkl		$2\Theta(°)$ $\lambda = 1.540598 Å$
8.62	100	0	1	1	10.25
6.80	34	1	0	0	13.01
6.60	91	0	0	2	13.41
5.84	13	1	1	0	15.16
5.71	15	0	1	2	15.51
5.70	84	0	2	0	15.54
5.35	27	-1	1	1	10004
5.33	83	- 1	1	1	16.50
5.23	19		2	1	16 67
4.75	10	-1	2	-	10.95
4075	*	-1	Ŭ	2	10.00
4.72	1	1	0	2	18.78
4.381	l 32	- 1	1	2	20.25
4.367	7 3	1	2	0	20.32
4.362	2 1	1	1	2	20.34
4.312	2 7	0	2	2	20.58
4.142	, 10	1	2	1	21.44
4.102	13	-	1	-	21.65
3.651	1	ő	3	ĩ	24.36
3.647	12	-1	2	2	24.39
3.636	5 5	1	2	2	24.46
		-	-	-	2.10.10
3.520	) 2	-1	1	з	25.28
3.505	5 8	1	1	з	25.39
3.481	72	0	2	З	25.57
3.399	2	2	0	0	26.20
3.316	5 <b>7</b>	1	З	0	26.86

d(Å)	I	hkl		$20(^{\circ})$ $\lambda = 1.540598A$
3.298	2	0 0	4	27.02
3.292	27	0 3	2	27.06
3.257	2	2 1	0	27.36
3.215	3	1 3	1	27.73
3.166	22	-2 1	1	28.16
3.104	7	-1 2	3	28.74
3.094	14	1 2	3	28.84
3.015	3	2 0	2	29.60
2.966	2	-1 3	2	30.11
2.961	1	1 0	4	30.16
2.926	1	-2 1	2	30.53
2.919	4	2 2	0	30.60
2.915	13	2 1	2	30.65
2.877	1	-1 1	4	31.06
2.875	33	0 3	3	31.08
2.854 2.853 2.848 2.665 2.651	3 7 3 3 2	0 2 -2 2 2 2 2 2 -1 3	4 1 2 3	31.31 31.33 31.39 33.60 33.79
2.628	6	1 4	03235	34.09
2.623	2	-2 1		34.15
2.616	7	0 4		34.25
2.611	2	2 1		34.31
2.570	3	0 1		34.88
2.486	1	2 3	12553	36.10
2.440	4	1 4		36.81
2.408	3	-1 1		37.31
2.400	4	1 1		37.44
2.391	3	0 4		37.58
2.373	2	-2 0	4 2 4 0 3	37.89
2.368	1	-2 3		37.97
2.336	3	1 3		38.51
2.266	1	3 0		39.75
2.254	10	1 4		39.97
2.199	3	-2 3	3	41.02
2.193	7	-3 1	1	41.12
2.190	5	3 1	1	41.19
2.181	2	2 2	4	41.36
2.167	6	0 3	5	41.64
2.159	1	0 1	6	41.81
2.156	1	0 4	4	41.86
2.132	2	1 5	1	42.35
2.109	1	-3 1	2	42.84
2.103	2	3 1	2	42.97
2.081 2.067 2.062 2.060 2.024	2 1 1 3	-3 2 -1 3 1 3 -1 1 0 5	1 5 5 6 3	43.45 43.76 43.87 43.91 44.74
2.005	2	2 3	4	45.18
1.987	1	-3 1	3	45.61
1.961	1	1 2	6	46.26
1.953	1	2 4	3	46.45
1.893	1	2 5	0	48.02

Metharbital,  $C_9H_{14}N_2O_3$  - (continued)

d (Å)	Ι,	hkl			$2\Theta(\circ) \circ \\ \lambda = 1.540598 \text{\AA}$
1.873	1	2	5	1	48.56
1.864	2	З	з	2	48.81
1.850	2	-2	0	6	49.20
1.824	1	2	З	5	49.97
1.823	2	-2	4	4	49.98
1.818	2	2	4	4	50.14
1.806	1	1	5	4	50.48
1.796	2	- 1	1	7	50.81
1.760	1	-2	2	6	51.92
1.741	2	-2	5	З	52.53
1.741	2	0	4	4	50 57
1.725	2	õ	-	5	52.05
1.699	2	<u> </u>	5	0	53.05
1.663	1	-2	2	4	53.91
1.659	1	-2	2	0	00017
1.050	1	2	0	0	22.00
1.628	1	2	1	7	56.49
1.582	1	ō	5	6	58.26
1.572	1	1	7	1	58+68
1.565	1	-3	4	4	58.99

Structure

Tetragonal,  $P4_12_12$  (92) or  $P4_32_12$  (96), Z = 4. The structure was studied by Dollase [1965] and by Peacor [1973].

#### Polymorphism

Low cristobalite is one of many  $\mathrm{SiO}_2$  forms, many of them metastable. Polymorphic changes occur with variations in purity, water inclusion, temperature, and pressure. Of the more nearly pure forms, the ordinary ones are low quartz (trigonal), high quartz (hexagonal), high cristobalite (cubic) and the low cristobalite described here. One or two forms of tridymite may be present when impurities or a flux are involved. The inversion from high to low cristobalite takes place readily at 268 °C for the pure material.

Atom positions

4(a) 4 silicon

8(b) 8 oxygen

The parameter values were taken from Peacor [1973].

Lattice constants a = 4.971 A

c = 6.918 [Swanson et al., 1960 and on PDF card 11-695]

c/a = 1.3917.

Volume . 171.0 Å<sup>3</sup>

\_.\_...

```
Density
(calculated) 2.335 g/cm<sup>3</sup>
```

Thermal parameters Isotropic: silicon B = 0.747, oxygen B = 1.247 [Peacor, 1973].

Scattering factors
Si<sup>3+</sup> [International Tables, 1962]
O<sup>-</sup> [Cromer and Mann, 1968]
The silicon factors were corrected for dispersion
[Cromer and Liberman, 1970].

Scale factors (integrated intensities)  $\gamma = 2.152 \times 10^{-3}$ I/I (calculated) = 4.64

The values, of  $\gamma$  and  $I/I_C$  will change with different conditions of ionization and dispersion. The range for this problem was about  $\pm 7$ % of the values given. The relative scaled intensities did not vary more than  $\pm 1$ %.

Additional patterns 1. PDF card 11-695 [Powder Diffraction Data, 1976]

References Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891. Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321. Dollase, W.A. (1965). Z. Kristallogr. Kristall-

geometrie Kristallphys. Kristallchem. 121,369.

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Peacor, D. R. (1973). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. <u>138</u>,274.

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Swanson, H. E., Cook, M. I., Evans, E. H., and de Groot, J. H. (1960). Nat'l Bur. Std. U. S. Circ. 539 #10, 48.

		Calculated	Pattern	(Pea	k h	eights)
	d (Å)	I		hkl		$20(^{\circ})$ , $\lambda = 1.540598A$
	4.033	100	1	0	1	22.02
	3.515	1	1	1	0	25.32
	3.134	9	1	1	1	28.46
	2.840	11	1	0	2	31.48
	2.485	14	2	0	0	36.12
	2.465	5	1	1	2	36.42
1	2.117	3	2	1	1	42.68
	2.092	1	1	0	З	43.22
	2.018	2	2	0	2	44.88
	1.928	5	1	1	3	47.10
	1.870	5	2	1	2	48.64
	1.757	1	2	2	0	52.00
	1.729	1	0	0	4	52.90
	1.690	2	2	0	3	54.22
	1.633	1	1	0	4	56.28
	1.611	4	3	0	1	57.12
	1.600	1	2	1	3	57.54
1	1.572	1	3	1	0	58.68
	1.567	1	2	2	2	58.88
	1.533	3	3	1	1	60.34
	1.494	3	3	0	2	62.06
	1.431	2	3	1	2	65.14
	1.420	1	2	0	4	65.72
	1.398	1	2	2	3	66.88
	1.365	2	2	1	4	68.70
	1.352	1	3	2	1	69.46
	1.346	1	3	0	3	69.84
	1.333	2	1	0	5	70.EO
	1.299	0 2	3	1	3	72.74
	1.280	92	3	2	2	73.94
	1.232	8 1	2	2	4	77.34
	1.223	2 1	4	0	1	78.06
	1.208	7 1	2	0	5	79.18
	1.205	7 1	4	1	0	79.42
	1 • 187	8 1	4	1	1	80.86
	1.183	4 1	3	2	3	81.22
	1.174	6 1	2	1	5	81.96
	1+171	8 1	3	3	0	82.20
	1.169	4 1	4	0	2	82.40
	1.163	2 1	3	1	4	82.94

Silicon Oxide (Low Cristobalite),  $SiO_2$  - (continued)

d(Å)	I		hkl		$2\Theta(^{\circ})$ $\lambda = 1.540598A$
1.1552	1	З	З	1	83.64
1.1385	1	4	1	2	85.16
1.1097	1	З	З	2	87.92
1.0974	1	4	2	1	89.16
1.0955	2	1	1	6	89.36
1.0871	1	2	2	5	90.24
1.0781	1	З	2	4	91.20
1.0685	1	4	1	З	92.26
1.0583	1	4	2	2	93.42
1.0446	1	3	З	З	95.02
1.0387	1	з	1	5	95.74
1.0013	1	4	2	З	100.58
•9941	1	4	З	0	101.58
•9891	1	4	1	4	102.30
•9841	1	4	3	1	103.02
.9766	1	з	2	5	104.14
.9747	1	5	1	0	104.42
.9700	1	3	З	4	105.14
.9694	1	1	0	7	105.24
•9654	1	5	1	1	105.86

	Calculated	Pattern	(Integr	cated)
d (Å)	I		hkl	$20(^{\circ})$ $\lambda = 1.540598A$
4.037	100	1	0 1	22.00
4.037	100	-1	0 -1	22.00
3.515	100	1	1 0	25.32
3.515	1	-1	-1 0	25.32
3.134	9	1	1 1	28.46
3.134	9	-1	-1 -1	28.46
2.839	12	1	0 2	31.48
2.839	12	-1	0 -2	31.48
2.486	16	2	0 0	36.11
2.486	16	-2	0 0	36.11
2.465	4	1	1 2	36.41
2.465	4	-1	-1 -2	36.41
2.117	3	2	1 1	42.69
2.117	3	-2	-1 -1	42.69
2.092	1	1	03	43.21
2.092	1	-1	0 -3	43.21
2.018	3	2	0 2	44.87
2.018	3	-2	0 -2	44.87
1.928	6	1	1 3	47.10
1.928	6	-1	-1 -3	47.10
1.870	6	2	1 2	48.65
1.870	6	-2	-1 -2	48.65
1.758	1	2	2 0	51.99
1.758	1	-2	-2 0	51.99
1.729	1	0	0 4	52.90
1.729	1	0	0 -4	52.90
1.690	3	2	0 3	54.22
1.690	3	-2	0 -3	54.22
1.633	1	1	0 4	56.27
1.633	1	-1	0 -4	56.27

d (A)	I	hkl	2⊖(°) 。
			$\lambda = 1.540598A$
	_		
1.611	5	3 0 1	57.11
1.611	5	-3 0 -1	57.54
1.600	1	-2 -1 -3	57.54
1.572	1	3 1 0	58.68
1.512	•	• · · ·	
1.572	1	-3 -1 0	58.68
1.567	1	2 2 2	58.89
1.567	1	-2 -2 -2	58.89
1.533	3	3 1 1	60.33
1.533	3	-3 -1 -1	60.33
1.494	4	302	62.06
1.494	4	-3 0 -2	62.06
1.431	З	3 1 2	65.13
1.431	З	-3 -1 -2	65.13
1.420	2	204	65.72
1.420	2	-2 0 -4	65.72
1.398	2	2 2 3	66.88
1.398	2	-2 -2 -3	66.88
1.365	З	2 1 4	68.71
1.365	З	-2 -1 -4	68.71
1.352		3 2 1	69.46
1.352	1	-3 -2 -1	69.46
1.346	1	3 0 3	69.84
1.346	1	-3 0 -3	69.84
1.333	2	1 0 5	70.61
	2	-1 0 -5	70.61
1.2989	3	3 1 3	72.75
1.2989	3	-3 -1 -3	72.75
1.2807	3	322	73.95
1.2807	З	-3 -2 -2	73.95
1.2429	1	<b>A</b> O O	76.61
1.2428	1	-4 0 0	76.61
1.2327	1	2 2 4	77.35
1.2327	1	-2 -2 -4	77.35
1.2232	1	4 0 1	78.06
1.2232	1	-4 0 -1	78.06
1.2089	1	2 0 5	79.16
1.2089	1	-2 0 -5	79.16
1.2056	2	4 1 0	79.42
1.2056	2	-4 -1 0	79.42
1.1077		A 1 1	80.96
1.1977	1	-4 -1 -1	80.86
1.1833	2	3 2 3	81.23
1.1833	2	-3 -2 -3	81.23
1.1747	2	2 1 5	81.95
1.1747	2	-2 -1 -5	81.05
1.1717	2	3 3 0	82.21
1.1717	1	-3 -3 0	82.21
1.1696	1	4 0 2	82.39
1.1696	1	-4 0 -2	82.39

		the second second second	
d (A)	I	hkl	$2\Theta(^{\circ})$ $\lambda = 1.540598\lambda$
	· · · · · · · · · · · · · · · · · · ·		
1.1633	1	3 1 4	82.93
1.1633	1	-3 -1 -4	82.93
1.1552	1	3 3 1	83.64
1.1552	1	-3 -3 -1	83.64
1.1385	1	4 1 2	85.16
1.1385	1	-4 -1 -2	85.16
1.1097	1	3 3 2	87.92
1.1097	1	-3 -3 -2	87.92
1.0975	1	4 2 1	89.16
1.0975	1	-4 -2 -1	89.16
1 0050			
1.0950	2	1 1 0	89.35
1.0956	2	-1 -1 -6	89.35
1.0940	1	4 0 3	89.52
1.0940	1	-4 0 -3	89.52
1.0871	1	2 2 5	90.24
1.0871	1	-2 -2 -5	90.24
1.0781	1	324	91.21
1.0781	1	-3 -2 -4	91.21
1.0684	1	4 1 3	92.27
1.0684	1	-4 -1 -3	02.27
1.0004	•	-4 -1 -5	72.021
1.0583	1	4 2 2	93.42
1.0583	1	-4 -2 -2	93.42
1.0446	1	333	95.03
1.0446	1	-3 -3 -3	95.03
1.0386	1	315	95.75
1.0386	1	-3 -1 -5	95.75
1.0013	1	4 2 3	100.58
1.0013	-	-4 -2 -3	100.58
.9942	-	A 7 0	101.57
.9942	1	-4 -3 0	101.57
	•		
•9890	2	4 1 4	102.31
•9890	2	-4 -1 -4	102.31
•9841	1	4 3 1	103.03
.9841	1	-4 -3 -1	103.03
.9766	1	325	104.14
9766	1	-1 -2 -5	104-14
.9740	1	5 1 0	104.40
0740	1	-5 -1 0	104 40
0700	1	-5-1 0	104+40
.9700	1	3 3 4	105.14
.9700	1	-3 -3 -4	105.14
•9693	1	1 0 7	105.25
•9693	1	-1 0 -7	105.25
•9654	1	5 1 1	105.87
•9654	1	-5 -1 -1	105.87

Silicon Oxide (Low Cristobalite),  $SiO_2$  - (continued)

Зm

11m

5m

7m

8m

	Vol. or		,	Vol. or	
	Sec.	Page		Sec.	Page
Aluminum, Al	1	11	Ammonium aluminum sulfate,		
Aluminum antimony, AlSb	4	72	$\mathrm{NH}_{4}\mathrm{Al}(\mathrm{SO}_{4})_{2}$	10m	5
Aluminum bismuth oxide, Al <sub>4</sub> Bi <sub>2</sub> O <sub>9</sub>	11m	5	Ammonium aluminum sulfate hydrate		
Aluminum chloride, AlCl <sub>3</sub>	9m	61	(tschermigite), $NH_4A1(SO_4)_2 \cdot 12H_2O$	6	3
Aluminum chloride hydrate			Ammonium azide. NHAN2	9	4
(chloraluminite), AlCla.6Ha0	7	3	Ammonium bervllium fluoride.		
Aluminum copper. Al Cuo	11m	79	(NH <sub>4</sub> ) <sub>o</sub> BeF <sub>4</sub>	3m	5
Aluminum fluoride hydroxide silicate			Ammonium boron fluoride NH.BF.	3m	6
topag Al. (F. OH) SiO.	, ]m	4	Ammonium bromide NH.Br	2	49
Aluminum inon oxido AlFoO	15m	7	Ammonium codmium bromido (NH.). CdBr	- 15m	رب م
Aluminum lithium Al Li	10m	08	Ammonium cadmium chloride, (MI4)4001	6 1.5m	6
Aluminum fithium, Al4L19	1011	90	Amanium cadmium cultoride, Mi4cuci3	Ju	0
Aluminum nickel, Alvi	1.2-	0Z E	(MIL) CA (CO.)	7	F
Aluminum nitride, AIN	1211	5	$(N\pi_4)_2 \cup (2(5)_4)_3 \dots	/ 111	5
Aluminum nitrate nydrate,	11	(	Ammonium cadmium suffate hydrate,	0	-
$A1(NU_3)_3 \cdot 9H_2U$	11m	6	$(NH_4)_2 Ld(SU_4)_2 \cdot 6H_2U$	om	С
Aluminum oxide (corundum), $\alpha$ -Al <sub>2</sub> O <sub>3</sub>	9	3	Ammonium calcium sulfate,	0	-
Aluminum oxide hydrate (boehmite),	•		$(NH_4)_2 Ca_2 (SO_4)_3 \dots	Sm	/
$\alpha$ -Al <sub>2</sub> O <sub>3</sub> ·H <sub>2</sub> O	3	38	Ammonium chlorate, NH <sub>4</sub> ClO <sub>4</sub>		
Aluminum oxide hydrate, diaspore,			(orthorhombic)	7	6
$\beta$ -A1 <sub>2</sub> 0 <sub>3</sub> ·H <sub>2</sub> 0	3	41	Ammonium chloride (salammoniac),		
Aluminum phosphate, $Al(PO_3)_3$	2m	3	NH <sub>4</sub> Cl	1	59
Aluminum phosphate (berlinite),			Ammonium chromium sulfate hydrate,		
A1P0 <sub>4</sub> (trigonal)	10	3	$\mathrm{NH}_4\mathrm{Cr}(\mathrm{SO}_4)_2\cdot 12\mathrm{H}_2\mathrm{O}$	6	7
Aluminum phosphate, AlPO <sub>4</sub>			Ammonium cobalt (II) chloride,		
(orthorhombic)	10	4	NH <sub>4</sub> CoCl <sub>3</sub>	6m	5
Aluminum plutonium, Al <sub>3</sub> Pu	15m	77	Ammonium cobalt fluoride, NH <sub>4</sub> CoF <sub>3</sub>	8m	9
Aluminum rhenium, AlRe	15m	79	Ammonium copper bromide hydrate,		
Aluminum rhenium, Al <sub>12</sub> Re	15m	80	$(NH_4)_2 CuBr_4 \cdot 2H_2 0 \dots$	10m	6
Aluminum rhodium, AlRh	15m	82	Ammonium copper chloride, NH4CuCl3	7m	7
Aluminum ruthenium, AlRu	15m	83	Ammonium copper chloride hydrate,		
Aluminum ruthenium, AleRu	15m	84	$(\mathrm{NH}_4)_2\mathrm{CuCl}_4\cdot 2\mathrm{H}_2\mathrm{O}$	12m	6
Aluminum samarium, AlSm <sub>2</sub>	15m	86	Ammonium copper fluoride, NH <sub>4</sub> CuF <sub>3</sub>	11m	8
Aluminum samarium, AlSm <sub>3</sub>	15m	88	Ammonium gallium sulfate hydrate,		
Aluminum samarium, Al <sub>2</sub> Sm	15m	90	$\mathrm{NH}_{4}\mathrm{Ga}(\mathrm{SO}_{4})_{2}\cdot12\mathrm{H}_{2}\mathrm{O}$	6	9
Aluminum samarium, Al <sub>3</sub> Sm	15m	91	Ammonium germanium fluoride.		
Aluminum silicate (mullite).			$(NH_{4})_{2}GeF_{6}$	6	8
AleSi2013	Зm	3	Ammonium hydrogen carbonate		
Aluminum sulfate, Al <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub>	15m	8	(teschemacherite), (NH <sub>4</sub> )HCO <sub>3</sub> ,	9	5
Aluminum technetium. AleTc	15m	93	Ammonium hydrogen phosphate.		
Aluminum terbium. AleTb	15m	95	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>	4	64
Aluminum terbium, AlaTba	15m	96	Ammonium iodate. NH 102	10m	7
Aluminum thorium uranium AlcThI	15m	98	Ammonium iodide. NHAI	4	56
Aluminum tungsten. Al-W. &-phase	15m	100	Ammonium iridium chloride		50
Aluminum tungsten oxide. $Al_{2}(WO_{4})_{2}$	11m	7	(NH <sub>4</sub> )alrClc	8	6
Aluminum vanadium. Al. V	15m	102	Ammonium iron chloride hydrate.	Ŭ	Ŭ
Aluminum vanadium Alio orV	15m	104	(NH <sub>4</sub> ) <sub>o</sub> FeCl <sub>-</sub> ·H <sub>o</sub> O	14m	7
Aluminum vanadium AlooV	15m	106	Ammonium iron fluoride (NH4) FeFo	9m	ģ
Aluminum vanadium AlusVa ( - phase	15m	108	Ammonium iron sulfate $NH_Fe(SO_4)$	10m	8
Aluminum vtterhium Al-Vh	15m	111	Ammonium iron sulfate bydrate	TOW	0
Aluminum yttrium Al-V	15m	112	NH $F_{0}(S_{0}) \rightarrow 12H_{0}$	6	10
Ammonium aluminum fluorido	TOUL	112	Ammonium load chlorido (NW )-PhCl	11m	10
(NH.). AIF.	0	5	Ammonium magnacium aluminum fluorida	TTU	10
Ammonium aluminum colonate hydrote	911	5	NH.Malle.	, 10m	0
NH.Al(So(.). 12H-0	0	6	Ammonium magnacium chromium orrida	TOUL	9
m4m (0004)2 12h20	211	0	hydrate (NH.) Mg(CrO.) - •6H_O	8m	10
				UII I	TO

Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the cumulative index here is not necessarily the concluding index for the project.

m - Monograph 25.

A mineral name in () indicates a synthetic sample.

Ammonium magnesium phosphate hydrate

(struvite), NH<sub>4</sub>MgPO<sub>4</sub>·6H<sub>2</sub>O .....

Ammonium manganese chloride hydrate,  $(NH_4)_2MnCl_4 \cdot 2H_2O$  .....

 $NH_4MnF_3$  ....

 $(\mathrm{NH}_4)_2 \mathrm{Mn}_2 (\mathrm{SO}_4)_3 \ldots \ldots \ldots$ 

Ammonium manganese sulfate hydrate,  $(NH_4)_2 Mn(SO_4)_2 \cdot 6H_2 O \dots \dots$ 

Ammonium manganese(II) fluoride,

Ammonium manganese sulfate,

Vol	•	or	
0		_	

		0	
Ammonium mercury chloride, NH <sub>4</sub> HgCl <sub>3</sub>	8m	14	Antimony s
Ammonium molybdenum oxide phosphate hydrate (NH.) (MoO.) = PO. (HeO.)	8	10	Antimony s
Ammonium nickel(II) chloride.	0	10	(cubic).
NH <sub>4</sub> NiCl <sub>3</sub>	6m	6	Antimony s
Ammonium nickel chromium oxide	0	14	AgSbS <sub>2</sub> (
hydrate, $(NH_4)_2N1(CrO_4)_2 \cdot 6H_2O$	8m	16	Antimony s
NHANO2	7	4	Aggobog Antimony s
Ammonium osmium bromide, $(NH_4)_2OsBr_6$	3	71	Antimony(I
Ammonium osmium chloride,			$Sb_2S_3$
$(\mathrm{NH}_4)_2\mathrm{OsCl}_6$	lm	6	Antimony t
Ammonium palladium chloride,	6	6	Antimony t
Ammonium palladium chloride.	U	0	Antimony t
(NH <sub>4</sub> ) <sub>2</sub> PdCl <sub>6</sub>	8	7	Antimony y
Ammonium platinum bromide,			Antimony y
$(\mathrm{NH}_4)_2\mathrm{PtBr}_6$	9	6	Arsenic, A
Ammonium platinum chloride,	5	3	Arsenic Ce
Ammonium potassium iron chloride	J	J	Arsenic ox
hydrate (kremersite),			$As_20_3$ (cu
$(NH_4,K)_2$ FeCl <sub>5</sub> ·H <sub>2</sub> O	14m	8	Arsenic ox
Ammonium rhenium oxide, NH <sub>4</sub> ReO <sub>4</sub>	9	7	(monoclin
Ammonium selenium bromide,	0	1.	Barium, Ba
(Mn <sub>4</sub> ) <sub>2</sub> Sebr <sub>6</sub>	٥	4	Barium alu
(cryptohalite), (NH <sub>4</sub> ) <sub>2</sub> SiF <sub>6</sub>	5	5	Barium ars
Ammonium strontium chromium oxide,			Barium bor
$(\mathrm{NH}_4)_2 \mathrm{Sr}(\mathrm{CrO}_4)_2 \ldots \ldots \ldots$	14m	9	Barium bor
Ammonium strontium sulfate,	15		Barium bor
$(NH_4)_2 Sr(SU_4)_2$	TOW	11	Barium Dro
$(NH_A)_2SO_A$	9	8	Barium bro
Ammonium tellurium bromide,	-		Barium bro
(NH <sub>4</sub> ) <sub>2</sub> TeBr <sub>6</sub>	8	5	Barium bro
Ammonium tellurium chloride,	0	0	Barium cad
$(NH_4)_2$ let $I_6$	8 5	8 /	BacdCl <sub>4</sub> •4
Ammonium vanadium oxide. NH <sub>4</sub> VO <sub>2</sub>	8	9	Ba osCa o
Ammonium zinc chloride, (NH4) 3ZnCl5	15m	12	Barium cal
Ammonium zinc fluoride, NH <sub>4</sub> ZnF <sub>3</sub>	8m	18	Ba <sub>.50</sub> Ca.s
Ammonium zirconium fluoride,		1/	Barium cal
$(NH_4)_3ZrF_7$	6	14	Ba 75Ca 2
Antimony bromide. $\alpha$ -SbBr	15m	13	BacCaWOc
Antimony cerium, CeSb	4m	40	Barium can
Antimony cobalt, CoSb	15m	121	(orthorho
Antimony cobalt, CoSb <sub>2</sub>	15m	122	Barium can
Antimony cobalt titanium, CoSbTi	15m	124	at 1075 °
Antimony cobalt vanadium, cosbv	15m 4m	41	Barium chi Ba(ClO <sub>4</sub> )
Antimony erbium, ErSb	4m	41	Barium chl
Antimony(III) fluoride, SbF <sub>3</sub>	2m	4	Ba(C10 <sub>3</sub> ) <sub>2</sub>
Antimony gadolinium, GdSb	4m	42	Barium chl
Antimony gallium, GaSb	6	30	Barium chl
Antimony gold (aurostibite), AuSb <sub>2</sub>		18 73	(orthorho
Antimony(III) iodide. Sbla	6	16	Barium chi
Antimony lanthanum, LaSb	4m	42	Barium chi
Antimony neodymium, NdSb	4m	43	$Ba_3(CrO_4)$
Antimony(III) oxide (senarmontite),			Barium flu
Sb <sub>2</sub> O <sub>3</sub> (cubic)	3	31	Barium hyd
Sholo (orthorhombic)	10	6	Barium io
Antimony(IV) oxide (cervantite),	10	, in the second s	Barium lea
Sb <sub>2</sub> 0 <sub>4</sub>	10	8	Barium lea
Antimony(V) oxide, Sb <sub>2</sub> 0 <sub>5</sub>	10	10	Ba.33Pb.
Antimony praseodymium, PrSb	4m	43	

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Antimony scandium, SbSc	4m	44
Antimony selenide, Sb <sub>2</sub> Se <sub>3</sub>	3m	7
(cubic)	5m	48
Antimony silver sulfide (miargyrite),	_	1.0
AgSbS <sub>2</sub> (monoclinic)	5m	49
AgoShSo (trigonal)	, 5m	51
Antimony silver telluride, AgSbTe <sub>2</sub> .	3m	47
Antimony(III) sulfide (stibnite),		
Sb <sub>2</sub> S <sub>3</sub>	5	6
Antimony telluride, Sb <sub>2</sub> Te <sub>3</sub>	3m	8
Antimony terbium, SbTb	5m //m	61
Antimony thorium, SDIn	40	44
Antimony vtterbium. SbYb	4m	45
Antimony vttríum. SbY	4m	46
Arsenic, As	3	6
Arsenic cerium, AsCe	4m	51
Arsenic(III) iodide, AsI <sub>3</sub>	13m	7
Arsenic oxide (arsenolite),	-	- 1
$As_2O_3$ (cubic)	T	51
Arsenic oxide, claudetite, $As_2O_3$	2-	0
(monoclinic)		9
Barium aluminum oxide BaAloO4	5m	11
Barium aluminum oxide, BasAlaOc	12m	7
Barium arsenate, Ba <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>	2m	6
Barium borate, BaB407	4m	6
Barium borate, high form, BaB <sub>2</sub> O <sub>4</sub>	4m	4
Barium borate, BaB <sub>8</sub> O <sub>13</sub>	7m	10
Barium bromate hydrate,		
$Ba(BrO_3)_2 \cdot H_2 O \dots D D$	8m	19
Barium bromide, BaBr <sub>2</sub>	10m	63
Barium bromide Hudrate BaBra HaO	3m	10
Barium cadmium chloride hydrate.	Jui	10
BaCdCl <sub>4</sub> ·4H <sub>2</sub> O	15m	14
Barium calcium nitrate,		
$Ba_{25}Ca_{75}(NO_3)_2$	12m	38
Barium calcium nitrate,	7.0	
$Ba_{50}Ca_{50}(NO_3)_2$	12m	38
Barium calcium nitrate,	10-	20
Barium calcium tungsten ovide	1 Zui	20
BasCaWOs	9m	10
Barium carbonate (witherite), BaCO <sub>3</sub>		
(orthorhombic)	2	54
Barium carbonate, BaCO <sub>3</sub> (cubic)		
at 1075 °C	10	11
Barium chlorate hydrate,	0	7
$Ba(CIO_4)_2 \cdot 3H_2O$	Zm	/
$B_2(Clo_2) \rightarrow H_2O$	8m	21
Barium chloride, BaClo, (cubic)	9m	13
Barium chloride, BaCl <sub>2</sub> ,		
(orthorhombic)	9m	11
Barium chloride fluoride, BaClF	10m	11
Barium chloride hydrate, $BaCl_2 \cdot 2H_2O$	12m	9
Barium chromium oxide,	15	17
$Ba_3(UrU_4)_2$	15m	10
Barium Iluoride, Bar	T	70
$Ba_{E}(OH)(PO_{A})_{2}$	11m	12
Barium iodíde. BaI2	10m	66
Barium lead chloride, BaPbCl <sub>4</sub>	llm	13
Barium lead nitrate,		
Ba $_{33}Pb _{67}(NO_3)_2$	12m	40

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Barium lead nitrate,	10	
$Ba_{67}Pb_{33}(NO_3)_2$	12m	40
Barium manganese oxide,	15m	17
Barium molybdenum oxide BaMoO.	1311	7
Barium molybdenum oxide, Banoo4	, 12m	10
Barium nitrate (nitrobarite).	12	10
$Ba(NO_3)_2$	llm	14
Barium nitrite hydrate,		
$Ba(NO_2)_2 \cdot H_2O$	15m	18
Barium oxide, BaO	9m	63
Barium oxide, BaO <sub>2</sub>	6	18
Barium phosphate, $Ba_3(PO_4)_2$	12m	12
Barium selenide, Base	12m	01
Barium silicate (caphornite)	1.200	0
B-BaSioOr	13m	10
Barium silicate BasSiO	13m	12
Barium silicate. BasSisOe	13m	13
Barium silicate. Ba <sub>2</sub> SiO <sub>5</sub>	13m	15
Barium silicate, Ba <sub>3</sub> Si <sub>5</sub> O <sub>13</sub>	13m	17
Barium silicon fluoride, BaSiF <sub>6</sub>	4m	7
Barium strontium nitrate,		
$Ba_{25}Sr_{75}(NO_3)_2$	12m	42
Barium strontium nitrate,		
$Ba_{.50}Sr_{.50}(NO_3)_2$	12m	42
Barium strontium nitrate,		
$Ba_{75}Sr_{25}(NO_3)_2$	12m	42
Barium sulfate (baryte), $BaSO_4$	10m	12
Barium sulfide, BaS		8
Barium tin oxide, BaSnU <sub>3</sub>	3m 2	11
Barium titanium oxide, Bariug	3	45
Bastision	Qm	14
Barium tungsten oxide. BaWO4	7	9
Barium tungsten oxide, BasWOs	12m	14
Barium vanadium oxide. $Ba_2(VO_4)_2$ .	14m	10
Barium zirconium oxide, BaZrO <sub>3</sub>	5	8
Beryllium, alpha, Be	9m	64
Beryllium aluminum oxide		
(chrysoberyl), BeAl <sub>2</sub> 0 <sub>4</sub>	9	10
Beryllium aluminum silicate, beryl,		
$Be_3Al_2(SiO_3)_6$	9	13
Beryllium calcium oxide,		0.0
$\operatorname{Be}_{17}\operatorname{Ca}_{12}\operatorname{O}_{29}$	/m	89
Beryllium chromium oxide, $Betr_2U_4$	10	12
Beryllium cormanium oxide Be-GeO.	10	13
Beryllium lanthanum oxide Bealaola	Qm	65
Bervllium nichium BeeNh	7m	92
Beryllium oxide (bromellite). Be0	1	36
Bervllium palladium. BePd	- 5m	62
Beryllium silicate, phenakite,	0	
Be <sub>2</sub> SiO <sub>4</sub>	8	11
Beryllium sulfate, BeSO <sub>4</sub>	15m	20
Bismuth, Bi	3	20
Bismuth bromide oxide, BiOBr	8	14
Bismuth cerium, BiCe	4m	46
Bismuth chloride oxide (bismoclite),		
BiOC1	4	54
Bismuth dysprosium, Biby	4m	4/
Bismuth flueride Bir	4m	4/
Bismuth holmium RiHo	1111 /um	1.0
Rismuth(III) indide Rila		20
Bismuth iodide oxide. Biol	9	16
Bismuth lanthanum, BiLa	4m	48
Bismuth neodymium, BiNd	4m	49
Bismuth oxide (bismite), $\alpha$ -Bi <sub>2</sub> O <sub>3</sub>	3m	16

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Bismuth phosphate, BiPO <sub>4</sub>		
(monoclinic)	3m	11
Bismuth phosphate, BiPO <sub>4</sub> (trigonal)	3m	13
Bismuth praseodymium, BiPr Bismuth sulfide (bismuthinite)	4m	49
Bi <sub>2</sub> S <sub>2</sub>	.5m	13
Bismuth telluride, BiTe	4m	50
Bismuth telluride (tellurobis-		
muthite), Bi <sub>2</sub> Te <sub>3</sub>	3m	16
Bismuth vanadium oxide, low form,	3m	17
Bismuth vanadium oxide, high form.	JUL	14
BiVO <sub>4</sub> (monoclinic)	3m	14
Boron oxide, B <sub>2</sub> O <sub>3</sub> , phase 1	10m	70
Cadmium, Cd	3	10
Cadmium ammine chloride,	10-	14
Cadmium bromide CdBro	2 Q	14
Cadmium bromide, Cdbr2	11m	15
Cadmium carbonate (otavite), CdCO3	7	11
Cadmium cerium, CdCe	5m	63
Cadmium chlorate hydrate,	0	10
$Cd(CIO_4)_2 \cdot 6H_2O$	3m	19
Cadmium chromium oxide CdCro0.	9 5m	16
Cadmium copper. $Cd_{2}Cu_{5}$	11m	81
Cadmium cyanide, Cd(CN) <sub>2</sub>	2m	8
Cadmium fluoride, CdF <sub>2</sub>	10m	15
Cadmium iron oxide, CdFe <sub>2</sub> O <sub>4</sub>	9m	16
Cadmium Lanthanum, CdLa	5m 10m	63
Cadmium manganese oxide, $\operatorname{CdMn}_2O_4$	1011	21
Cadmium nitrate hydrate,	U	21
$Cd(NO_3)_2 \cdot 4H_2O$	7m	93
Cadmium oxide, CdO	2	27
Cadmium oxide, CdO (ref. standard)	8m	2
Cadmium praseodymium, CdPr	Sm	64
CdSe (hexagonal)	7	12
Cadmium silicate, Cd <sub>2</sub> SiO <sub>4</sub>	13m	19
Cadmium silicate, Cd <sub>3</sub> SiO <sub>5</sub>	13m	20
Cadmium sulfate, CdSO <sub>4</sub>	3m	20
Cadmium sulfate hydrate,	(	0
$30050_4 \cdot \delta \Pi_2 \cup \ldots \ldots$	om 6m	10
Cadmium sulfide (greenockite). CdS	4	15
Cadmium telluride, CdTe	3m	21
Cadmium titanium oxide, CdTiO <sub>3</sub>	15m	21
Cadmium tungsten oxide, CdWO <sub>4</sub>	2m	8
Calcium, Ca	9m	68
$Ca_2Al_2(GeO_4)_2$	10	15
Calcium aluminum hydroxide,	10	
Ca <sub>3</sub> Al <sub>2</sub> (OH) <sub>12</sub>	11m	16
Calcium aluminum oxide, Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub>	5	10
Calcium aluminum oxide (mayenite),	0	20
Calcium aluminum sulfate hydrate	9	20
(ettringite), CacAl <sub>2</sub> S <sub>3</sub> O <sub>18</sub> ·31H <sub>2</sub> O	8	3
Calcium borate, CaB <sub>2</sub> O <sub>4</sub>	15m	136
Calcium bromide, CaBr <sub>2</sub>	llm	70
Calcium bromide hydrate, CaBr <sub>2</sub> ·6H <sub>2</sub> O	8	15
CaCO <sub>2</sub> (orthorhombic)	3	53
Calcium carbonate (aragonite).	5	55
$CaCO_3$ (orthorhombic,		
. calculated pattern)	14m	44
Calcium carbonate (calcite),	0	<b>F 1</b>
CaCO <sub>3</sub> (hexagonal)	2	51
100		

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Calcium chloride (hydrophilite),			Cerium copper, CeCu <sub>6</sub>	7m	99
CaCl <sub>2</sub>	11m	18	Cerium(III) fluoride, CeF <sub>3</sub>	8	17
Calcium chloride fluoride, CaClF	10m	17	Cerium gallium, CeGa <sub>2</sub>	13m	54
Calcium chloride hydrate,			Cerium magnesium, CeMg	5m	65
$CaCl_2 \cdot 4H_2O$	11m	73	Cerium magnesium, CeMg <sub>3</sub>	13m	56
Calcium chloride hydrate			Cerium nickel, CeNi <sub>2</sub>	13m	58
(antarcticite), CaCl <sub>2</sub> •6H <sub>2</sub> O	12m	16	Cerium niobium titanium oxide		
Calcium chromium germanium oxide,			(aeschynite), CeNbTiO <sub>6</sub>	3m	24
$Ca_3Cr_2(GeO_4)_3$	10	16	Cerium nitride, CeN	4m	51
Calcium chromium oxide (chromatite),			Cerium(IV) oxide (cerianite), CeO <sub>2</sub>	1	56
CaCrO <sub>4</sub>	7	13	Cerium phosphide, CeP	4m	52
Calcium chromium oxide, $Ca_3(CrO_4)_2$	15m	22	Cerium thallium, CeTl	13m	59
Calcium chromium silicate	1.0	1 -	Cerium thallium, CeTl <sub>3</sub>	13m	60
(uvarovite), $Ca_3Cr_2(SiO_4)_3$	10	1/	Cerium thallium, $Ce_3TI$	13m	61
Calcium fluoride (fluorite), Car <sub>2</sub> .	T	69	Cerium(III) vanadium oxide, $CeVO_4$	Lm	9
(fluence tite) Con E(DO)	2	22	Cerium zinc, CeZn	Sm 1/m	65
(fluorapatite), $\operatorname{Cast}(\operatorname{PO}_4)_3$	310	22	Carium zinc, CeZn <sub>3</sub>	14m	50
CoFPO +24.0	15m	24	Corium zinc, Co.Zn	14m	55
Calcium callium cormanium ovide	1.200	24	Cesium aluminum culfate hydrate	140	55
CasGas (GeO <sub>4</sub> )	10	18	CsAl(SO <sub>4</sub> ) <sub>0</sub> ·12H <sub>0</sub> O	6	25
Calcium hydrogen phosphate hydrate.	10	10	Cesium antimony fluoride. CsSbFc	4m	9
$Ca_{e}H_{e}(PO_{e})c^{*}5H_{e}O_{e}$	13m	21	Cesium bervllium fluoride. CsBeFa	9m	69
Calcium hydroxide (portlandite).	101		Cesium boron fluoride. CsBF4	8	22
Ca(OH) <sub>2</sub>	1	58	Cesium bromate. CsBrO <sub>2</sub>	8	18
Calcium iodate (lautarite),		-	Cesium bromide, CsBr	3	49
$Ca(IO_3)_2$	14m	12	Cesium cadmium bromide, CsCdBr3		
Calcium iodate hydrate,			(hexagonal)	10m	20
$Ca(IO_3)_2 \cdot 6H_2O$	14m	13	Cesium cadmium chloride, CsCdCl <sub>3</sub>		
Calcium iron germanium oxide,			(hexagonal)	5m	19
Ca <sub>3</sub> Fe <sub>2</sub> (GeO <sub>4</sub> ) <sub>3</sub>	10	19	Cesium calcium chloride, CsCaCl <sub>3</sub>	5m	21
Calcium iron silicate (andradite),			Cesium calcium fluoride, CsCaF <sub>3</sub>	8m	25
Ca <sub>3</sub> Fe <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>	9	22	Cesium calcium sulfate,		
Calcium iron silicate			$Cs_2Ca_2(SO_4)_3$	/m	12
hydroxide, julgoldite,	10	70	Cesium cerium chloride, $Cs_2CeCl_6$	14m	58
$La_2 Fe_3 Si_3 U_{10} (OH, U)_2 (OH)_2 \dots \dots$	IUm	72	Continue chlorate, $Collog$	8	20
Co Ph (NO)	1.0m	1.1.	(arthorhombic)	lm	10
Calcium lead nitrate	1211		Cesium chloride CsCl	2	44
Ca caPh as (NOa) a	12m	44	Cesium chromium oxide. CsoCrO4	3m	25
Calcium magnesium silicate	1.770		Cesium chromium sulfate hydrate,		
(diopside), CaMg(SiO <sub>3</sub> ) <sub>2</sub>	5m	17	$CsCr(SO_4)_2 \cdot 12H_2O$	8	21
Calcium molybdenum oxide			Cesium cobalt(II) chloride, CsCoCl <sub>3</sub>	6m	11
(powellite), CaMoO <sub>4</sub>	6	22	Cesium cobalt chloride, Cs <sub>2</sub> CoCl <sub>4</sub>	llm	19
Calcium nitrate, Ca(NO <sub>3</sub> ) <sub>2</sub>	7	14	Cesium copper(II) chloride, CsCuCl <sub>3</sub>	5m	22
Calcium oxide (lime), CaO	1	43	Cesium copper chloride, Cs <sub>2</sub> CuCl <sub>4</sub>	11m	20
Calcium oxide (lime), CaO			Cesium copper sulfate hydrate,		
(calculated pattern)	14m	49	$Cs_2Cu(SO_4)_2 \cdot 6H_2O$	7m	14
Calcium oxide phosphate, $Ca_40(PO_4)_2$	12m	17	Cesium fluoride, CsF	3m	26
Calcium phosphate, $\beta$ -Ca <sub>2</sub> P <sub>2</sub> O <sub>7</sub>	7m	95	Cesium gallium sulfate hydrate,		
Calcium platinum oxide, Ca <sub>4</sub> PtO <sub>6</sub>	10m	18	$CsGa(SO_4)_2 \cdot 12H_2O$	8	23
Calcium selenide, CaSe	5m	64	Cesium germanium fluoride, $Cs_2Ger_6$	15	1/
Calcium strontium nitrate,	10		Cesium iodate, $CsIO_3$	15m	20
$Ca_{33}Sr_{67}(NO_3)_2$	12m	46	Continue indiana hermida Cal Pr	4 7m	103
Calcium strontium nitrate,	10-	10	Conjum iodine plonide, CSI2DI	7.00	50
$Ca_{67}Sr_{33}(NO_3)_2$	1210	40	Cesium iron chloride hydrate	5	50
Calcium sulfide (aldhamite), Caso4	4	15	CsoFeCle • HoO	14m	14
Calcium telluride CaTe	4m	50	Cesium iron sulfate hydrate.		
Calcium titanium oxide		50	$Cs_2Fe(SO_4)_2 \cdot 6H_2O$	7m	16
(perovskite), CaTiO <sub>2</sub>	9m	17	Cesium iron sulfate hydrate,		
Calcium tungsten oxide, Ca <sub>3</sub> WO <sub>6</sub>	9m	19	$CsFe(SO_4)_2 \cdot 12H_2O$	6	28
Calcium tungsten oxide, scheelite,			Cesium lead(II) chloride, CsPbCl <sub>3</sub>		
CaW04	6	23	(tetragonal)	5m	24
Carbon, diamond, C	2	5	Cesium lead fluoride, CsPbF <sub>3</sub>	8m	26
Cerium arsenate, CeAsO <sub>4</sub>	4m	8	Cesium lithium cobalt cyanide,	10	70
Cerium(III) chloride, CeCl <sub>3</sub>	lm	8	USLILO(UN) <sub>6</sub>	10m	105
Cerium cobalt, CeCo <sub>2</sub>	13m	50	cesium fichium fluoride, CsLif <sub>2</sub>	/m	102
cerium codait, $Ce_{24}Co_{11}$	13m	51			

Cesium magnesium chromium oxide,			Cobalt gadolinium, Co <sub>2</sub> Gd	13m	71
$Cs_2Mg_2(CrO_4)_3$	8m	27	Cobalt gadolinium, Co <sub>7</sub> Gd <sub>2</sub>	13m	72
Cesium magnesium chromium oxide			Cobalt gallium hafnium, Co <sub>2</sub> GaHf	14m	65
hydrate, $Cs_2Mg(CrO_4)_2 \cdot 6H_2O$	8m	29	Cobalt gallium manganese, Co <sub>2</sub> GaMn	13m	75
Cesium magnesium sulfate hydrate,			Cobalt gallium niobium,		
$Cs_2Mg(SO_4)_2 \cdot 6H_2O$	7 m	18	Co <sub>1.5</sub> Ga <sub>0.5</sub> Nb	15m	144
Cesium manganese fluoride, CsMnF <sub>3</sub>	10m	21	Cobalt gallium niobium, Co <sub>2</sub> GaNb	14m	66
Cesium manganese sulfate hydrate,			Cobalt gallium oxide, CoGa <sub>2</sub> O <sub>4</sub>	10	27
$Cs_2Mn(SO_4)_2 \cdot 6H_2O$	7m	20	Cobalt gallium tantalum,		
Cesium mercury chloride, CsHgCl <sub>3</sub>	7 m	22	$Co_{1,5}Ga_{0,5}Ta$	15m	146
Cesium nickel(II) chloride, CsNiCl <sub>3</sub>	6m	12	Cobalt gallium tantalum, Co <sub>2</sub> GaTa	13m	76
Cesium nickel sulfate hydrate,			Cobalt gallium titanium, Co <sub>2</sub> GaTi	13m	77
$Cs_2Ni(SO_4)_2 \cdot 6H_2O$	7 m	23	Cobalt gallium vanadium, Co <sub>2</sub> GaV	13m	78
Cesium nitrate, CsNO <sub>3</sub>	9	25	Cobalt germanium, Co <sub>3</sub> Ge <sub>2</sub>	14m	67
Cesium osmium(IV) bromide, Cs <sub>2</sub> OsBr <sub>6</sub>	2m	10	Cobalt germanium, Co <sub>5</sub> Ge <sub>7</sub>	15m	148
Cesium osmium chloride, Cs <sub>2</sub> OsCl <sub>6</sub>	2m	11	Cobalt germanium hafnium.		
Cesium platinum bromide, Cs2PtBr6	8	19	Co <sub>16</sub> Ge <sub>7</sub> Hf <sub>6</sub>	14m	69
Cesium platinum chloride, Cs2PtCl6	5	14	Cobalt germanium manganese,		
Cesium platinum fluoride, Cs <sub>2</sub> PtF <sub>6</sub>	6	27	Co <sub>2</sub> GeMn	13m	79
Cesium selenium bromide, Cs <sub>2</sub> SeBr <sub>6</sub>	8	20	Cobalt germanium niobium.		
Cesium silicon fluoride, Cs <sub>2</sub> SiF <sub>6</sub>	5	19	$C_{01}$ = $Ge_0$ = $Nb$	15m	150
Cesium strontium chloride. CsSrCl <sub>2</sub>	бm	13	Cobalt germanium niobium.		
Cesium sulfate. CsoSO4	7	17	CoaccesNba	14m	71
Cesium tellurium bromide. CsoTeBro	ģ	24	Cobalt germanium oxide CoofeO	10	27
Cesium tin chloride (SoSnClo	5	16	Cobalt germanium tantalum	10	2,
Cesium vanadium sulfate hydrate	5	10	CoGeTa	15m	152
CeV(SO.) - 12H-O	lm	11	Cohalt cormanium tantalum	1.511	152
Casium zinc sulfate hydrate	TW		Co. Co. Ta-	1/m	73
$C_{c} = \frac{7n}{2} \left( \frac{c}{c} \right) + \frac{6H}{2} 0$	7m	25	Coholt cormonium titonium Co-CoTi	13m	80
$Cs_2 z_{11} (so_4)_2 \cdot o_{12} \cdots	, 111	20	Cobalt befrium tin Co Uffer	1/m	75
Chromium chlorido CrCl	11m	20	Coholt holmium Co Ho	1411	75
Chromium coholt nichium CoCrNh	15m	1/0	Coholt holmium, Cogno	14/II 15m	154
Chromium cobalt dilicido	TOm	140	Cohalt hydroxide $R_{-}Co(OH)$	15m	20
Co Cr. Si	1/m	62	Cobalt hydroxide, $p=Co(OH)_2$	12-	29
Charging ashalt testalum CoCrTs	1411	142	Cohelt indium, Coln <sub>3</sub>	1.5m	50
Changing flucuide CoE	10-	142	$\begin{array}{c} \text{cobalt iodide, } \text{col}_2 \ \dots \ $	4 <b>m</b>	52
Chromium fluoride, CrF <sub>2</sub>	TOW 2	100	Cobalt iron arsenide	10	0.0
Chromium fluoride, Cr <sub>2</sub> F <sub>5</sub>	/m	108	$(safflorite), CoreAs_4 \dots$	10	28
Chromium(III) fluoride hydrate,	_	0.5	Cobalt iron oxide, $CoFe_2O_4$	9m	22
$CrF_3 \cdot 3H_2O$	5m	25	Cobalt iron sulfide, Co <sub>8</sub> FeS <sub>8</sub>	14m	//
Chromium iridium, $Cr_3 lr$	6m	14	Cobalt iron vanadium,		
Chromium(III) oxide, $Cr_2O_3$	5	22	$Co_{4,35}Fe_{13,47}V_{12,18}$	14m	/9
Chromium phosphate, $\alpha$ -CrPO <sub>4</sub>	2m	12	Cobalt lanthanum, CoLa <sub>3</sub>	13m	83
Chromium phosphate, $\beta$ -CrPO <sub>4</sub>	9	26	Cobalt lutetium, Co <sub>2</sub> Lu	13m	86
Chromium phosphate hydrate,			Cobalt magnesium, Co <sub>2</sub> Mg	15m	156
$CrPO_4 \cdot 6H_2O$	15m	27	Cobalt manganese silicide, Co <sub>2</sub> MnSi	14m	81
Chromium rhodium, Cr <sub>3</sub> Rh	6m	15	Cobalt mercury thiocyanate,		
Chromium silicide, Cr <sub>3</sub> Si	6	29	Co[Hg(CNS) <sub>4</sub> ]	2m	13
Cobalt, Co (cubic)	4m	10	Cobalt molybdenum, Co <sub>2</sub> Mo	14m	82
Cobalt aluminum oxide, CoAl <sub>2</sub> O <sub>4</sub>	9	27	Cobalt molybdenum, Co <sub>2</sub> Mo <sub>3</sub>	15m	158
Cobalt ammine iodide, $Co(NH_3)_6I_3$	10m	83	Cobalt molybdenum, Co <sub>7</sub> Mo <sub>6</sub>	15m	160
Cobalt antimony oxide, CoSb <sub>2</sub> 0 <sub>6</sub>	5m	26	Cobalt molybdenum silicide,		
Cobalt arsenide, CoAs <sub>2</sub>	4m	10	Co <sub>3</sub> Mo <sub>2</sub> Si	15m	162
Cobalt arsenide (skutterudite),			Cobalt neodymium, Co <sub>2</sub> Nd	13m	87
CoAs <sub>3</sub>	10	21	Cobalt nickel tin,		
Cobalt borate, $Co_3(BO_3)_2$	12m	20	Co <sub>.75</sub> Ni <sub>.75</sub> Sn <sub>.75</sub>	13m	88
Cobalt bromide hydrate, CoBr <sub>2</sub> ·6H <sub>2</sub> O	12m	21	Cobalt niobium silicide, Co <sub>3</sub> Nb <sub>4</sub> Si <sub>7</sub>	15m	164
Cobalt(II) carbonate (sphaero-			Cobalt niobium tin, Co <sub>2</sub> NbSn	15m	166
cobaltite), CoCO <sub>3</sub>	10	24	Cobalt nitrate hydrate,	•	
Cobalt chlorate hydrate, Co(ClO <sub>4</sub> ) <sub>2</sub> .6	$H_2O$ 3m	28	$\alpha$ -Co(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	12m	22
Cobalt chloride hydrate, CoCl <sub>2</sub> ·2H <sub>2</sub> O	11m	22	Cobalt(II) oxide, CoO	9	28
Cobalt chloride hydrate, CoCl <sub>2</sub> ·6H <sub>2</sub> O	11m	23	Cobalt(II.III) oxide. Co <sub>2</sub> O <sub>4</sub>	9	29
Cobalt chromium oxide. CoCr <sub>2</sub> O <sub>4</sub>	9m	21	Cohalt phosphate. $Co(PO_2)_2$	13m	23
Cobalt copper tin, CoCu <sub>2</sub> Sn	14m	64	Cobalt phosphide. CoP	14m	83
Cobalt dysprosium, Co <sub>2</sub> Dv	13m	63	Cobalt phosphide. CoP	14m	85
Cobalt erbium. CosEr	13m	64	Cobalt platinum, CoPt (disordered)	15m	167
Cobalt erbium. CozEro	13m	65	Cobalt platinum, CoPt (ordered)	1.5m	168
Cobalt fluoride. CoFe	10m	85	Cohalt platinum, CoPt.	1011	200
Cobalt fluoride hydrate CoFo.4HoO	11m	24	(disordered)	15m	169
Cobalt gadolinium. CoGdo	13m	68	Cohalt nlatinum CoPts (ordered)	15m	170
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Cobalt plutonium, CoPu <sub>2</sub>	14m	8
Cobalt plutonium, CoPu <sub>2</sub>	15m	17
Cobalt plutonium. CoPus	14m	89
Cobalt plutonium, CooPu	14m	9
Cobalt plutonium, Co <sub>3</sub> Pu	14m	92
Cobalt plutonium, Co <sub>17</sub> Pu <sub>2</sub>	14m	94
Cobalt praseodymium, Co2Pr	14m	9
Cobalt rhodium sulfide, CogRhSg	14m	98
Cobalt ruthenium sulfide, CogRuSg	14m	10
Cobalt samarium, Co <sub>2</sub> Sm	15m	17:
Cobalt samarium, Co <sub>5</sub> Sm	13m	90
Cobalt silicate, Co <sub>2</sub> SiO <sub>4</sub>		
(orthorhombic)	4m	1
Cobalt silicon fluoride hydrate,		
CoSiF <sub>6</sub> •6H <sub>2</sub> 0	Зm	2
Cobalt sulfate, $\beta$ -CoSO <sub>4</sub>	2m	14
Cobalt tantalum silicide,		
Co <sub>16</sub> Ta <sub>6</sub> Si <sub>7</sub>	14m	102
Cobalt thorium, Co <sub>17</sub> Th <sub>2</sub>	12m	64
Cobalt tin, Co <sub>3</sub> Sn <sub>2</sub>	13m	92
Cobalt tin oxide, $Co_2SnO_4$	15m	- 30
Cobalt tin vanadium, Co <sub>2</sub> SnV	15m	174
Cobalt tin zirconium, Co <sub>2</sub> SnZr	15m	17
Cobalt titanium oxide, CoTiO <sub>3</sub>	4m	1;
Cobalt titanium silicide,	7/	10
$Co_{16}T1_6S1_7$	14m	104
Cobalt tungsten oxide, $Cow0_4$	4m	17
Contraction Silicide, Co <sub>2</sub> vS1	TOW	1/1
Copper, Cu	T	Τ.
$C_{\rm W}(\rm NH)$ soo	10m	Q.
Connor ammino sulfato hydrato	TOW	0
Cu(NH <sub>2</sub> ) SO . • H <sub>2</sub> O	10m	9
Copper antimony oxide CuSbola	5m	2
Copper(I) bromide CuBr	4	3
Copper(I) chloride (nantokite).	-	
CuCl	4	3
Copper fluoride hydrate, $CuF_2 \cdot 2H_2O$	11m	2
Copper hydrogen phosphite hydrate,		
CuHPO <sub>3</sub> •2H <sub>2</sub> O	llm	83
Copper hydroxide carbonate,		
azurite, $Cu_3(OH)_2(CO_3)_2$	10	30
Copper hydroxide carbonate		
(malachite), $Cu_2(OH)_2CO_3$	10	3
Copper(I) iodide (marshite), CuI	4	3
Copper(1) oxide (cuprite), $Cu_20$	2	2:
Copper(11) oxide (tenorite), CuO	1/	4
Copper phosphate, $Cu(PO_3)_2$	14m	1:
Copper phosphate, $\alpha$ - $u_2P_2U_7$	/m	11,
comper sufface (charcocyanice),	2 m	20
Coppor(II) sulfide (covallite) (us	500	2:
Copper uranium exide Cullo	10m	0 ·
Dysprosium arsenate DyAs0.	3m	30
Dysprosium arsenide. DyAs	4m	5
Dysprosium gallium oxide.		0.
$Dv_3Ga_5O_{12}$	2m	15
Dysprosium gold, DyAu	5m	6
Dysprosium nitride, DyN	4m	53
Dysprosium oxide, Dy <sub>2</sub> 0 <sub>3</sub>	9	30
Dysprosium silver, DyAg	5m	60
Dysprosium telluride, DyTe	4m	54
Dysprosium vanadium oxide, DyVO <sub>4</sub>	4m	1
Erbium arsenate, ErAsO <sub>4</sub>	3m	3
Erbium arsenide, ErAs	4m	54
Erbium gallium oxide, $Er_3Ga_5O_{12}$	lm	12
Erbium manganese oxide, ErMnO <sub>3</sub>	2m	10
ErDium nitride, ErN	4m	55
Erblum oxide, $Er_2O_3$	8	2

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Erbium phosphate ErPO.	q	31
Erbium silver, ErAg	5m	67
Erbium telluride, ErTe	4m	55
Erbium vanadium oxide, ErVO <sub>4</sub>	5m	29
Europium arsenate, EuAsO <sub>4</sub>	3m	32
Europium(III) chloride, EuCl <sub>3</sub>	lm	13
Europium chloride oxide, EuOCl	lm	13
Europium gallium oxide,		
$Eu_3Ga_5O_{12}$	2m	17
Europium nitride, EuN	4m	56
Europium phosphate EuPO	4400 ]]m	26
Furopium (III) vanadium ovide FuVO.	4m	16
Gadolinium arsenate. GdAsO4	4m	17
Gadolinium arsenide. GdAs	4m	57
Gadolinium chloride hydrate,		
GdCl <sub>3</sub> ·6H <sub>2</sub> O	7m	118
Gadolinium chloride oxide, GdOCl	lm	17
Gadolinium fluoride, GdF <sub>3</sub>	lm	14
Gadolinium gallium oxide,		
Gd <sub>3</sub> Ga <sub>5</sub> O <sub>12</sub>	2m	18
Gadolinium indium, Gdin	50	67
Gadolinium nitride, GdN	411	5/
Gadolinium oxide, $Gd_2O_3$	1111 6m	87
Gadolinium titanium ovide	ош	07
GdaTiOr	8m	32
Gadolinium vanadium oxide. GdVO4	5m	30
Gallium, Ga	2	9
Gallium arsenide, GaAs	Зm	33
Gallium lutetium oxide, Ga <sub>5</sub> Lu <sub>3</sub> O <sub>12</sub>	2m	22
Gallium magnesium, Ga <sub>2</sub> Mg	12m	48
Gallium magnesium, Ga <sub>5</sub> Mg <sub>2</sub>	12m	51
Gallium neodymium oxide, Ga <sub>5</sub> Nd <sub>3</sub> O <sub>12</sub>	lm	34
Gallium oxide, $\alpha$ -Ga <sub>2</sub> O <sub>3</sub>	4	25
Gallium phosphate ( $\alpha$ -quartz type),	0	27
$GaPU_4$	0	27
GaPO. •2H-O	8m	34
Gallium samarium oxide. GarSmoO12	lm	42
Gallium vtterbium oxide. GasYb <sub>2</sub> O <sub>12</sub>	lm	49
Gallium yttrium oxide, Ga <sub>5</sub> Y <sub>3</sub> O <sub>12</sub>	lm	50
Germanium, Ge	1	18
Germanium iodide, Gel <sub>2</sub>	4m	58
Germanium(IV) iodide, GeI <sub>4</sub>	5	25
Germanium oxide, GeO <sub>2</sub> (hexagonal)		
(low form)	1	51
(totmoscal) (bish form)	Q	28
Cold Au	1	20
Gold(I) cvanide AuCN	10	33
Gold holmium. AuHo	5m	68
Gold magnesium, AuMg	бm	83
Gold niobium, AuNb <sub>3</sub>	6m	16
Gold potassium cyanide, AuK(CN) <sub>2</sub>	8m	36
Gold tin, AuSn	7	19
Gold titanium, AuTi <sub>3</sub>	6m	17
Gold vanadium, $AuV_3$	6m	18
Hainium, Hi	3	18
Holmium arsenate, HoAsU <sub>4</sub>	10m	24
Holmium nitride HoN	10m 4m	58
Holmium oxide. Ho202	9	32
Holmium selenide, HoSe	4m	59
Holmium silver, HoAg	5m	68
Holmium vanadium oxide, HoVO <sub>4</sub>	4m	18
Hydrogen amidosulfate, H <sub>2</sub> NSO <sub>3</sub> H	7	54
Hydrogen arsenate, $H_5As_3O_{10}$	7m	84
Hydrogen borate, $\beta$ -HBO <sub>2</sub> (monoclinic)	9m	71

Hydrogen borate (metaborite),			Lead hydrogen arsenate (schultenite),		
HBO <sub>2</sub> (cubic)	4m	27	PbHAs0 <sub>4</sub>	14m	18
Hydrogen iodate, HIO <sub>3</sub>	5	28	Lead hydrogen phosphate, PbHPO <sub>4</sub>	15m	37
Hydrogen iodate, HI <sub>3</sub> 0 <sub>8</sub>	8m	104	Lead hydroxide phosphate,	0	
Hydrogen phosphate hydrate,	1.0	- /	$Pb_5(PO_4)_3OH$	8	33
$H_3PO_4 \cdot 0.5H_2O$	12m	56	Lead(11) 10dide, $Pbl_2$	5	34
Hydrogen tellurate, H <sub>6</sub> TeU <sub>6</sub>	12m	34	Lead molybdenum oxide (wulfenite),	_	
Indium, In	3	12	$PDMOU_4$	/	23
Indium arsenide, InAs	3m	35	Lead nitrate, $PD(NU_3)_2$	5	30
Indium oxide, $In_2U_3$	2	20	Lead oxide (litharge), PDU (red,	2	20
Indium phosphate, InPU <sub>4</sub>	8	29	Letragonal)	2	30
Indian Suffide, In <sub>2</sub> 5 <sub>3</sub>	TTW	30	Lead Oxide (massicot), PDU (yellow,	2	2.2
Taidine, 12	3	10	orthornomble)	2	32
Iridium, Ir	4	10	Lead $(11,111)$ oxide $(minium)$ , $PD_3U_4$	10-	32
Iridium avida Iro	0III /m	19	Lead oxide sufface, PD505504	TOW	27
Inidium titanium InTi	40	20	Lead strentium nitrate	2	20
Inidium vanadium IrV.	6m	20	$Pb = Sr = (NO_{2})$	12m	5.2
Iron W-Fe	6	21	Lead strontium nitrate	1211	22
Iron arcenide FeAs	1	10	Ph a-Sr as(NOa)a	12m	53
Iron arsenide (loellingite) FeAso	10	34	Lead sulfate (anglesite) PbS0.	12111	67
Iron bromide FeBro	4m	59	Lead sulfide (galena) PhS	2	18
Iron carbonate siderite FeCO	15m	32	Lead tin oxide PhoSnO.	10m	20
Iron chloride hydrate FeClo 2Ho0	11m	32	Lead titanium ovide (macedonite)	TOW	29
Iron fluoride hydrate, FeFe •4He0	11m	90	PhTiO <sub>2</sub>	5	30
Iron hydroxide sulfate hydrate	1111		Lead tungsten oxide (stolzite)	5	55
butlerite. $Fe(OH)SO_4 \cdot 2H_0O$	10m	95	PbWO4 (tetragonal)	5m	34
Iron iodide. Felo	4m	60	Lead uranium oxide. Pholloc	8m	109
Iron(II.III) oxide (magnetite)			Lithium aluminum fluoride	0 III	107
Fe <sub>2</sub> O <sub>4</sub>	5m	31	$\alpha$ -LiaAlFc	8m	111
Iron phosphate. FePO4	15m	33	Lithium arsenate LioAsO	2m	19
Iron sulfate hydrate (melanterite).	1.5	55	Lithium azide. LiNo	8m	113
FeSO <sup>4</sup> ·7H <sub>2</sub> O	8m	38	Lithium barium fluoride, LiBaF2	5m	35
Iron sulfide (pyrite), FeS <sub>2</sub>	5	29	Lithium beryllium fluoride, Li2BeF4	7m	126
Iron thorium, FeizTha	12m	67	Lithium borate, $Li_2B_4O_7$	8m	114
Iron titanium oxide (ilmenite).		•,	Lithium bromide, LiBr	4	30
FeTiO <sub>2</sub>	15m	34	Lithium carbonate, Li <sub>2</sub> CO <sub>2</sub>	8m	42
Lanthanum arsenate, LaAsO4	3m	36	Lithium chlorate hydrate,		
Lanthanum arsenide, LaAs	4m	60	LiCl0 <sub>4</sub> •3H <sub>2</sub> O	8	34
Lanthanum borate, LaBO3	lm	20	Lithium chloride, LiCl	1	62
Lanthanum chloride, LaCl3	lm	20	Lithium fluoride, LiF	1	61
Lanthanum chloride oxide, LaOC1	7	22	Lithium gallium oxide, LiGaO <sub>2</sub>	10m	31
Lanthanum fluoride, LaF3	7	21	Lithium hydroxide hydrate, LiOH·H <sub>2</sub> O	11m	92
Lanthanum magnesium, LaMg	5m	69	Lithium iodate, LiIO <sub>3</sub> (hexagonal)	7	26
Lanthanum niobium titanium oxide,			Lithium iodate, LiIO <sub>3</sub> (tetragonal)	10m	33
LaNbTiO <sub>6</sub>	3m	37	Lithium molybdenum oxide, Li <sub>2</sub> MoO <sub>4</sub>		
Lanthanum nitrate hydrate,			(trigonal)	lm	23
$La(NO_3)_3 \cdot 6H_2O$	8m	40	Lithium niobium oxide, LiNbO3	6m	22
Lanthanum nítride, LaN	4m	61	Lithium nitrate, LiNO <sub>3</sub>	7	27
Lanthanum oxide, La <sub>2</sub> 0 <sub>3</sub>	3	33	Lithium oxide, Li <sub>2</sub> 0	lm	25
Lanthanum phosphide, LaP	5m	69	Lithium phosphate hydrate,		
Lanthanum selenide, LaSe	4m	61	$Li_3P_3O_9 \cdot 3H_2O$	2m	20
Lanthanum titanium oxide, La <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub>	15m	35	Lithium phosphate, low form		
Lanthanum zinc, LaZn	5m	70	(lithiophosphate), Li <sub>3</sub> PO <sub>4</sub>	4m	21
Lead, Pb	1	34	Lithium phosphate, high form,		
Lead borate, PbB <sub>4</sub> 07	4m	19	Li <sub>3</sub> PO <sub>4</sub>	3m	39
Lead bromide, PbBr <sub>2</sub>	2	47	Lithium potassium sulfate, KLiSO $_4$	3m	43
Lead bromide chloride, PbBrCl	llm	33	Lithium rubidium fluoride, LiRbF <sub>2</sub>	7m	128
Lead bromide fluoride, PbBrF	10m	25	Lithium selenide, Li <sub>2</sub> Se	10m	100
Lead bromide oxide, Pb <sub>3</sub> 0 <sub>2</sub> Br <sub>2</sub>	5m	32	Lithium silicate, Li <sub>2</sub> SiO <sub>3</sub>	14m	19
Lead carbonate (cerussite), PbCO <sub>3</sub>	2	56	Lithium silver bromide,		
Lead chloride (cotunnite), PbCl <sub>2</sub>	12m	23	Li 2Ag 8Br	12m	55
Lead chloride fluoride (matlockite),			Lithium silver bromide,	10	
PDCIF	13m	25	L1 4Ag.6Br	12m	55
Lead chromium oxide, Pb <sub>2</sub> CrO <sub>5</sub>	14m	16	Lithium silver bromide,	10	
Lead fluoride, $\alpha$ -PbF <sub>2</sub>			Li <sub>6</sub> Ag <sub>4</sub> Br	12m	55
(orthorhombic)	5	31	Lithium silver bromide,	10	
Lead fluoride, p-PbF <sub>2</sub> (cubic)	5	33	L1,8Ag,2Br	12m	55
Lead Huoride lodide, PDF1	TOW	26			

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Lithium sodium aluminum fluoride,		
cryolithionite, $Li_3Na_3Al_2F_{12}$	9m	23
Lithium sulfate $Li_{0}SO_{4}$	6m	24
Lithium sulfate hydrate.	OIII	20
$Li_2SO_4 \cdot H_2O$	4m	22
Lithium sulfide, Li <sub>2</sub> S	10m	101
Lithium tantalum oxide, LiTaO3	14m	20
Lithium telluride, Li <sub>2</sub> Te	10m	102
Lithium tungsten oxide, $Li_2WO_4$	1	0.5
(trigonal)	TW	25
LioW0. 0. 5Ho0	2m	20
Lithium uranium fluoride, LiUF <sub>5</sub>	7m	131
Lutetium arsenate, LuAs04	5m	36
Lutetium manganese oxide, LuMnO3	2m	23
Lutetium nitride, LuN	4m	62
Lutetium oxide, Lu <sub>2</sub> 0 <sub>3</sub>	lm	27
Lutetium vanadium oxide, LuVO <sub>4</sub>	5m	37
Magnesium aluminum ovide (spinel)	T	10
MgAl <sub>2</sub> O <sub>4</sub>	9m	25
Magnesium aluminum silicate (low	2111	25
cordierite), Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub>		
(orthorhombic)	lm	28
Magnesium aluminum silicate		
(indialite) Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub>		
(hexagonal)	lm	29
(purepa) Ma Al (SiO)	/	24
Magnesium horate $Mg_B_0$	410	24
(triclinic)	4m	25
Magnesium bromide, MgBr <sub>2</sub>	4m	62
Magnesium bromide hydrate,		
$MgBr_2 \cdot 6H_2O$	llm	35
Magnesium carbonate (magnesite),	_	~ ~
MgCU <sub>3</sub>	/	28
Magnesium cerium nitrate nyurate, Magnesium cerium nitrate nyurate,	10	20
Magnesium chlorate hydrate	10	20
$M_g(C10_4)_2 \cdot 6H_20$	7m	30
Magnesium chloride (chloro-		
magnesite), MgCl <sub>2</sub>	11m	94
Magnesium chloride hydrate,		
$MgCl_2 \cdot 12H_2O$	7m	135
(hischofite) Macle (H-O	11m	37
Magnesium chromium oxide	T T III	57
(magnesiochromite), MgCr <sub>2</sub> O <sub>4</sub>	9	34
Magnesium chromium oxide hydrate,		
MgCr0 <sub>4</sub> ·5H <sub>2</sub> 0	15m	39
Magnesium fluoride (sellaite), $MgF_2$	4	33
Magnesium fluoride silicate	-	
(humite), $Mg_7F_2Si_3O_{12}$	TW	30
(norbergite) MgeFeSiO.	10	30
Magnesium gallium oxide. $MgGa_2O_4$	10	36
Magnesium germanium oxide,		• -
Mg <sub>2</sub> GeO <sub>4</sub> (cubic)	10	37
Magnesium germanium oxide,		
Mg <sub>2</sub> GeO <sub>4</sub> (orthorhombic)	10	38
Magnesium hydrogen phosphate	7	120
Magnesium hydroxide (hrucite)	/ш	139
Mg(OH) <sub>2</sub>	6	30
Magnesium iron hydroxide carbonate		
hydrate, pyroaurite,		
$Mg_6Fe_2(OH)_{16}CO_3 \cdot 4H_2O$ (rhomb.)	10m	104

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lagnesium iron hydroxide carbonate		
hydrate, sjögrenite,		
$Mg_6Fe_2(OH)_{16}CO_3 \cdot 4H_2O$ , (hexag.)	10m	103
lagnesium lanthanum nitrate		
hydrate, $Mg_3La_2(NO_3)_{12} \cdot 24H_2O$	lm	22
lagnesium manganese oxide, MgMn <sub>2</sub> 0 <sub>4</sub>	10m	35
lagnesium molybdenum oxide MaMoO	om 7m	04 28
lagnesium nickel oxide. MgNiO <sub>2</sub>	10m	36
lagnesium oxide (periclase), MgO	1	37
lagnesium phosphate, Mg(PO <sub>3</sub> ) <sub>2</sub>	13m	26
lagnesium phosphate, $\alpha$ -Mg <sub>2</sub> P <sub>2</sub> O <sub>7</sub>	9m	73
Magnesium selenide, MgSe	5m	70
lagnesium selenite hydrate,	0	11/
lagnesium silicate enstatite	om	110
MeSiO	6	32
lagnesium silicate (forsterite).	U	52
Mg <sub>2</sub> SiO <sub>4</sub>	1	83
lagnesium sulfate hydrate		
(epsomite), $MgSO_4 \cdot 7H_2O$	7	30
Magnesium sulfide, MgS	7	31
lagnesium sulfite hydrate,	0	00
MgSU <sub>3</sub> *OH <sub>2</sub> U	9m	26
lagnesium tin oxide Massno.	10m	41
lagnesium titanium oxide	rom	57
(geikielite), MgTiO <sub>3</sub>	5	43
Magnesium titanium oxide, Mg <sub>2</sub> TiO <sub>4</sub>	12m	25
lagnesium tungsten oxide, MgWO4	13m	27
1anganese, α-Mn	7m	142
fanganese aluminum oxide (galaxite),		
$MnAl_2O_4$	9	35
langanese bromide, MnBr <sub>2</sub>	4m	63
(rhodochrosite) MnCO	7	32
Manganese chloride (scacchite).	,	52
MnCl <sub>2</sub>	8m	43
langanese chloride hydrate,		
$MnCl_2 \cdot 2H_2O$	llm	38
Manganese chloride hydrate,		
$MnCl_2 \cdot 4H_2O$	9m 0	28
langanese cobalt oxide, $mco_2U_4$	9m 10m	105
langanese iodide MnIo	10111 4m	63
Manganese iron oxide (jacobsite).		00
MnFe <sub>2</sub> O <sub>4</sub>	9	36
Manganese(II) oxide (manganosite),		
Mn0	5	45
1anganese oxide (hausmannite),		
$\operatorname{Mn}_30_4$	10m	38
langanese oxide (DixDylte), $\alpha$ -Mn <sub>2</sub> O <sub>3</sub>	11m 10m	30
langanese oxide hydroxide groutite	100	59
$\alpha$ -MnOOH	11m	97
langanese phosphate, Mn(PO <sub>3</sub> ) <sub>2</sub>	14m	21
langanese phosphate, $Mn_2P_2O_7$	15m	41
1anganese selenide, MnSe	10	41
Manganese sulfide (alabandite),	,	
α-MnS	4	11
langanese titanium oxide	15-	1.0
(pyrophanice), Mn1103	T2W	42
(huebnerite), MnWO,	2m	24
langanese vanadium oxide. Mn <sub>2</sub> V <sub>2</sub> O <sub>7</sub>	9m	75
fercury amide chloride, HgNH <sub>2</sub> C1	10m	40
fercury ammine chloride,		
$Hg(NH_3)_2Cl_2$	11m	39
hercury bromate, $Hg(BrU_3)_2$	IUm	107

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Mercury bromide, HgBr <sub>2</sub>	10m	110
Mercury bromide, Hg <sub>2</sub> Br <sub>2</sub>	7	33
Mercury chloride, HgCl <sub>2</sub>	13m	29
Mercury chloride (calomel),	10	0.0
Hg <sub>2</sub> Cl <sub>2</sub>	13m	30
Mercury chloride sulfide,	0 m	110
$\alpha$ -Hg <sub>3</sub> U1 <sub>2</sub> S <sub>2</sub>	6	25
Mercury(II) cyanide, ng(CN) <sub>2</sub>	2m	25
Moreury(II) indide Hal	2.11	2.5 //Q
Mercury(II) iodide Holo (tetragonal)		32
Mercury(II) oxide (montroydite).	,	5-
Hg0	9	39
Mercury(II) selenide (tiemannite),		
HgSe	7	35
Mercury(II) sulfide (cinnabar),		
HgS (hexagonal)	4	17
Mercury(II) sulfide (metacinnabar),		
HgS (cubic)	4	21
Molybdenum, Mo	1	20
Molybdenum arsenide, Mo <sub>2</sub> As <sub>3</sub>	10m	115
Molybdenum osmium, Mo <sub>3</sub> Os	6m	28
Molybdenum oxide (molybdite), MoO <sub>3</sub>	3	30
Molybdenum sulfide (molybdenite),	-	17
MoS <sub>2</sub>	5	4/
Neodymium arsenate, NdAsU <sub>4</sub>	4m	28
Neodymium arsenide, NdAs	4m	04
Neodymium borate, NdBO3	1m	32
Neodymium chloride, NdCl <sub>3</sub>	101	22
Neodymium fluoride NdF	0	26
Neodymium avida Nd.O.	0	26
Neodymium phoephate NdPO	11m	40
Neodymium selepide NdSe	5m	71
Neodymium silver NdAg	5m	71
Neodymium vanadium oxide NdVO.	4m	30
Neptunium nitride. NpN	4m	64
Nickel, Ni	1	13
Nickel aluminum oxide, NiAl <sub>2</sub> O <sub>4</sub>	9	42
Nickel arsenide (rammelsbergite),		
NiAs <sub>2</sub>	10	42
Nickel arsenic sulfide		
(gersdorffite), NiAsS		35
Nickel bromide, NiBr <sub>2</sub>	IUm	119
(tricopal)	1-	26
Nickel chloride NiCle	Qm	81
Nickel chloride hydrate.	2.11	01
NiCl <sub>2</sub> •6H <sub>2</sub> O	llm	42
Nickel fluoride, NiF <sub>2</sub>	10m	121
Nickel fluoride hydrate, NiF2.4H20	11m	43
Nickel gallium oxide, NiGa <sub>2</sub> O <sub>4</sub>	10	45
Nickel germanium oxide, Ni <sub>2</sub> GeO <sub>4</sub>	9	43
Nickel iron oxide (trevorite),		
NiFe <sub>2</sub> 0 <sub>4</sub>	10	44
Nickel nitrate hydrate,		
$Ni(NO_3)_2 \cdot 6H_2O$	12m	26
Nickel(II) oxide (bunsenite), NiO	1	4/
Nickel phosphate, $Ni(PO_3)_2$	14m	22
Nickel silicon fluoride hydrate	90	0.5
NisiFa.6HaO	8	38
Nickel sulfate. NiSO4	2m	26
Nickel sulfate hydrate (retgersite).		
NiSO <sub>4</sub> ·6H <sub>2</sub> O	7	36
Nickel sulfide, millerite, NiS	lm	37
Nickel tungsten oxide, NiWO4	2m	27
Nickel yttrium, Ni <sub>3</sub> Y	10m	123
Niobium chloride oxide, NbOCl <sub>3</sub>	7 m	148

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	,	20
Niobium osmium, Nb <sub>3</sub> OS	6m	30
Niobium platinum, ND <sub>3</sub> Pt	om	31
Niobium silicide, NDS12	0 15m	29
Nichium silicide B=Nh-Sic	15m	43
Osmium Os	4	8
Osmium titanium. OsTi	6m	85
Palladium. Pd	1	21
Palladium hydride, PdHo 706	5m	72
Palladium oxide, PdO	4	27
Palladium vanadium, PdV <sub>3</sub>	6m	32
Phosphorus bromide, PBr <sub>7</sub>	7m	150
Phosphorus oxide (stable form I),		
$P_2O_5$ (orthorhombic)	9m	86
Phosphorus oxide (stable form II),		
$P_2O_5$ (orthorhombic)	9m	88
Phosphorus oxide (metastable form),	0	01
$P_4 U_{10}$ (rnombonedral)	9m	91
Platinum, Pt	1 6m	22
Platinum vanadium PtV.	6m	34
Plutonium arsenide PuAs	4m	65
Plutonium phosphide PuP	4m	65
Plutonium telluride PuTe	4m	66
Potassium aluminum sulfate.		00
$KA1(SO_4)_2$	9m	31
Potassium aluminum sulfate hydrate		
(potash alum), $KAl(SO_4)_2 \cdot 12H_2O$	6	36
Potassium barium chromium oxide,		
$K_2Ba(CrO_4)_2$	14m	23
Potassium barium molybdenum oxide,		
$K_2Ba(MoO_4)_2$	14m	24
Potassium barium nickel nitrite,		
$K_2BaNi(NO_2)_6$	9m	32
Potassium borate hydroxide hydrate,	15	10
$K_2B_4U_5(UH)_4 \cdot 2H_2U$	mcT 0	40
Potassium bromato KPrO	9	28
Potassium bromide KBr	1	66
Potassium bromide, kbr	-	00
KBro sClo s	8m	46
Potassium bromide iodide,		
KBr 33I 67	11m	44
Potassium bromide iodide,		
KBr 67I 33	11m	45
Potassium cadmium fluoride, KCdF <sub>3</sub>	8m	47
Potassium cadmium sulfate,		
$K_2Cd_2(SO_4)_3$	7 m	34
Potassium calcium carbonate		10
(fairchildite), $K_2Ca(CO_3)_2$	8m 7	48
Potassium calcium chloride, KCaCl <sub>3</sub>	/m	36
Potassium calcium fluoride, KCaF <sub>3</sub>	Sm	49
Potassium calcium magnesium suffate,	7-	27
$R_2 Cang(SU_4)_3$	7ш	57
$K_{\rm r}$ (NO <sub>2</sub> ).	Qm	33
Potassium calcium sulfate	711	55
KoCao(SO <sub>4</sub> )	7m	39
Potassium calcium sulfate hydrate		0.5
(syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$	14m	25
Potassium cerium fluoride, β-KCeF <sub>4</sub>	12m	59
Potassium chlorate, KClO <sub>3</sub>	3m	42
Potassium chlorate, KClO <sub>4</sub>	6	43
Potassium chloride (sylvite), KCl	1	65
Potassium chromium oxide, K <sub>3</sub> CrO <sub>8</sub>	3m	44
Potassium chromium oxide (lopezite),		
$K_2 Cr_2 O_7$	15m	47
Potassium chromium oxide sulfate,	10	0.0
$K_2(Ur0_4)_{.33}(S0_4)_{.67}$	12m	28

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Potassium chromium oxide sulfate,	10	07
$R_2(Ur0_4)_{.67}(SU_4)_{.33}$	12m	27
$KCr(SO_4)_2 \cdot 12H_2O_1 \dots \dots \dots \dots \dots \dots$	6	39
Potassium cobalt(II) fluoride,		
KCoF <sub>3</sub>	6m	37
Potassium cobalt fluoride, K <sub>2</sub> CoF <sub>4</sub>	11m	. 46
Potassium cobalt nitrite,	0	
$R_3 UO(NU_2)_6$ Potassium cobalt(II) sulfate	9	45
$K_2Co_2(SO_4)_2$	6m	35
Potassium copper chloride, KCuCl <sub>3</sub>	7m	41
Potassium copper chloride hydrate		
(mitscherlichite), $K_2CuCl_4 \cdot 2H_2O$	9m	34
Potassium copper(11) fluoride,	6-	2.0
Potassium cyapate KCNO	om 7	38 20
Potassium cyanide KCN	1	29
Potassium fluoride. KF	ī	64
Potassium germanium fluoride,	-	
K <sub>2</sub> GeF <sub>6</sub>	6	41
Potassium hydrogen arsenate,		
KH <sub>2</sub> AsO <sub>4</sub>	lm	38
Reference in the second	2	60
Potassium hydroxide. KOH at 300 °C	5 4m	66
Potassium iodate. KIO <sub>2</sub>	15m	48
Potassium iodate, KIO <sub>4</sub>	7	41
Potassium iodide, KI	1	68
Potassium iron chloride hydrate		
(erythrosiderite), K <sub>2</sub> FeCl <sub>5</sub> ·H <sub>2</sub> O	14m	27
Potassium iron cyanide, $K_3Fe(CN)_6$	9m	35
Potassium iron fluoride, Kref <sub>3</sub>	0m 0m	39
Potassium lead chloride, K3Per6	Эш 13m	33
Potassium lead chromium oxide,	1.011	55
$K_2Pb(CrO_4)_2$	14m	28
Potassium lead molybdenum oxide,		
$K_2Pb(MoO_4)_2$	14m	29
K-Pb(PO.)	15m	50
Potassium lead selenate	TOW	50
$K_2Pb(SeO_4)_2$	15m	52
Potassium lead sulfate (palmierite),		
$K_2 Pb(SO_4)_2$	14m	30
Potassium magnesium chloride		5.0
hydrate (carnallite), KMgUl <sub>3</sub> ·6H <sub>2</sub> O	8m	50
KoMeo(CrO <sub>4</sub> )o	8m	52
Potassium magnesium fluoride. KMgF <sub>2</sub>	6m	42
Potassium magnesium fluoride,	•	
K <sub>2</sub> MgF <sub>4</sub>	10m	42
Potassium magnesium selenate		
hydrate, $K_2Mg(SeO_4)_2 \cdot 6H_2O$	10m	43
(langhoinite) K Mg (SO )	6-	40
Potassium magnesium sulfate hydrate	ош	40
(picromerite), K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	8m	54
Potassium manganese(II) fluoride,		-
KMnF <sub>3</sub>	бm	45
Potassium manganese oxide, KMnO <sub>4</sub>	7	42
Potassium manganese(II) sulfate	6.	10
(manganorangpernite), $K_2 m_2 (SU_4)_3$ Potassium molybdenum ovide K.Moo	om 15m	43
Potassium molybdenum oxide	1.5 m	55
phosphate hydrate,		
$K_3(MoO_3)_{12}PO_4 \cdot 4H_2O$	8	43
Potassium nickel fluoride, KNiF3	7m	42
Potassium nickel fluoride, $K_2NiF_4$	10m	45

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Potoggium pickol(II) gulfato		
KoNio(SO.)	6m	46
Potassium niobium fluoride, K <sub>2</sub> NbF <sub>7</sub>	8m	120
Potassium nitrate (niter), KNO3	3	58
Potassium nitrite, KNO <sub>2</sub>	9m	38
Potassium nitroso ruthenium		
chloride, K <sub>2</sub> (NO)RuCl <sub>5</sub>	2m	29
Potassium oxide, K <sub>2</sub> 0	10m	125
Potassium platinum bromide, K <sub>2</sub> PtBr <sub>6</sub>	8	40
rotassium platinum chloride,	12m	27
Potassium platinum fluoride	TOW	54
KoPtFo	6	42
Potassium rhenium chloride. KoReCle	2m	28
Potassium rhenium oxide, KReO4	8	41
Potassium rubidium chloride,		
K <sub>0.5</sub> Rb <sub>0.5</sub> Cl	8m	76
Potassium rubidium chromium oxide,		
KRbCrO <sub>4</sub>	12m	29
Potassium ruthenium chloride,	10	
K <sub>2</sub> KuCl <sub>6</sub>	10	46
bydroto K By OCl + H O	10	1.7
Potassium selenate $K_2 Selenate$	10 9m	47
Potassium selenide, K <sub>2</sub> Seo <sub>4</sub>	10m	126
Potassium selenium bromide. KoSeBro	8	41
Potassium silicon fluoride	Ū	
(hieratite), K <sub>2</sub> SiF <sub>6</sub>	5	50
Potassium silver cyanide, KAg(CN) <sub>2</sub>	8m	78
Potassium sodium aluminum fluoride		
(elpasolite), K <sub>2</sub> NaAlF <sub>6</sub>	9m	43
Potassium sodium bromide,		6.
K <sub>2</sub> Na <sub>8</sub> Br	12m	62
V No. Dr.	10-	60
R <sub>4</sub> Na <sub>6</sub> BI Potassium sodium bromide	120	02
K Na Br	12m	62
Potassium sodium bromide.	1.011	~-
K 8Na 2Br	12m	62
Potassium sodium chloride,		
K <sub>.2</sub> Na <sub>.8</sub> Cl	12m	63
Potassium sodium chloride,		
K <sub>4</sub> Na <sub>6</sub> C1	12m	63
Potassium sodium chloride,	10	()
R <sub>6</sub> Na <sub>4</sub> UI	12m	63
K Na cl	12m	63
Potassium sodium sulfate	120	05
$K_{67}Na_{1} a_{3}SO_{4} \dots \dots \dots \dots$	6m	48
Potassium sodium sulfate, KNaSO4	6m	50
Potassium sodium sulfate		
(aphthitalite), K <sub>3</sub> Na(SO <sub>4</sub> ) <sub>2</sub>	6m	52
Potassium strontium chromium oxide,		
$K_2$ Sr(CrO <sub>4</sub> ) <sub>2</sub>	15m	57
Potassium strontium selenate,	15-	5.0
$K_2Sr(SeU_4)_2$	15m	28
$(k_{a})$ $(k_{a})$ $(k_{a})$ $(k_{a})$ $(k_{a})$	1.4m	31
Potassium sulfate KoSoOr	9m	99
Potassium sulfate (arcanite). K <sub>2</sub> SO <sub>4</sub>	3	62
Potassium sulfide, K <sub>2</sub> S	10m	127
Potassium telluride, K2Te	10m	128
Potassium thiocyanate, KCNS	8	44
Potassium tin chloride, K <sub>2</sub> SnCl <sub>6</sub>	6	38
Potassium titanium fluoride, K2TiF6	7	40
Potassium tungsten oxide, K <sub>2</sub> WO <sub>4</sub>	llm	47
Potassium vanadium oxide, $KV_3O_8$	8m	56
K7pBr. 2H.O	11-	104
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Potassium zinc fluoride, KZnF <sub>3</sub>	5 10m	51
Potassium zinc iodide hydrate,	TOW	40
KZnI3•2H20	11m	107
Potassium zinc sulfate, K <sub>2</sub> Zn <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	6m	54
Potassium zinc sulfate hydrate,	7-	1.2
$K_2 \Delta n (50_4)_2 \circ 0 n_2 0 \dots \dots \dots \dots \dots \dots$ Potassium zinc vanadium oxide	/ш	45
hydrate, $K_2 Zn_2 V_{10} O_{28} \cdot 16 H_2 O$	3m	45
Potassium zirconium fluoride,		
K <sub>3</sub> ZrF <sub>7</sub>	,9	46
Praseodymium arsenate, PrAsO <sub>4</sub>	4m	32
Praseodymium arsenide, PrAs	4m	67
Praseodymium chloride, PrCl <sub>3</sub>	1m	39
Praseodymium chloride oxide, PrOC1	9	47
Praseodymium fluoride, PrF <sub>3</sub>	5	52
Praseodymium sulfide, PrS	4m	67
Praseodymium vanadium oxide, PrVO <sub>4</sub>	5m	40
Praseodymium zinc, PrZn	5m	72
Rhenium, Re	2	13
Rhodium, Rh	3	9
Rhodium vanadium, RhV <sub>3</sub>	6m	56
Rubidium aluminum sulfate		.,
hydrate, $RbA1(SO_4)_2 \cdot 12H_2O$	6	44
Rubidium amide, RbNH <sub>2</sub>	5m	73
Rubidium barium chromium oxide,	7/	~~
$Rb_2Ba(CrO_4)_2$	14m	32
Rubidium barium molybdenum oxide,	1.5	5.0
$Rb_2Ba(MoO_4)_2$	15m	59
Rubidium bromate, RbBrO <sub>3</sub>	8	45
Rubidium bromide, RbBr	7	43
Rubidium cadmium chloride, high	_	( )
form, RbCdCl <sub>3</sub> (tetragonal)	5m	43
Rubidium cadmium chloride,	-	/ 1
low form, RbCdCl <sub>3</sub> (orthorhombic)	5m	41
Rubidium cadmium sulfate,	7	
$\text{KD}_2(\text{C}_2(\text{SU}_4)_3 \dots \text{A}_3)$	/m 7	43
Rubidium calcium chloride, RbCall <sub>3</sub>	/m 0	4/
Rubidium calcium fluoride, RDCar <sub>3</sub>	Sm	57
Ph. Co. (SO.)	7m	/. 0
$RD_2Ca_2(SO_4)_3$ $PbClO$	/ III 0	40
Rubidium chlorate, RbClO <sub>3</sub>	2m	20
Pubidium chlorido PbCl	211	/1
Rubidium chronium swide Db CrO	3~	41
Rubidium chromium oxide, $Rb_2CrO_4$	15m	40
Rubidium chromium oxide, KD <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>	1.200	00
Phore(SO ) 124 O	6	1.7
Rubidium cobalt $(II)$ chloride	0	47
RhCoCl.	6m	57
Rubidium cobalt fluoride RhCoF.	8m	58
Rubidium cobalt sulfate	OIII	50
RbsCos(SO4)	8m	59
Rubidium copper chloride hydrate.	C III	
$Rb_2CuCl_4 \cdot 2H_2O$	10m	47
Rubidium copper sulfate hydrate,		
$Rb_2Cu(SO_4)_2 \cdot 6H_2O$	8m	61
Rubidium fluoride, RbF	8m	63
Rubidium iodate, RbIO <sub>3</sub>	15m	62
Rubidium iodate, RbIO <sub>4</sub>	2m	31
Rubidium iodide, RbI	4	43
Rubidium iron chloride hydrate,		
Rb <sub>2</sub> FeCl <sub>5</sub> •H <sub>2</sub> O	14m	33
Rubidium iron sulfate hydrate,		
$Rb_2Fe(SO_4)_2 \cdot 6H_2O$	8m	64
Rubidium lead chromium oxide,		
$Rb_2Pb(CrO_4)_2$	14m	34
Rubidium lead molybdenum oxide,	15	10
	nct	03

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Rubidium magnesium chromium oxide,		
$Rb_2Mg_2(CrO_4)_3$	8m	66
Rubidium magnesium chromium oxide	0	(0
hydrate, KD <sub>2</sub> Mg(UrU <sub>4</sub> ) <sub>2</sub> ·OH <sub>2</sub> U	om	68
$Rb_{Mg_{\alpha}}(SO_{4})_{\alpha}$	7m	50
Rubidium magnesium sulfate	7 11	50
hvdrate. $Rb_2Mg(SO_4)_2 \cdot 6H_2O$	8m	70
Rubidium manganese(II) fluoride,		
RbMnF <sub>3</sub>	5m	44
Rubidium manganese sulfate,	·	
$\operatorname{Rb}_{2}\operatorname{Mn}_{2}(\operatorname{SO}_{4})_{3}$	7m	52
Rubidium nickel(II) chloride,		5.0
RDN1Cl <sub>3</sub>	6m	58
Rubidium nickel sulfate,	8-	72
$RD_2NI_2(SU_4)_3$ Rubidium pickel sulfate hydrate	ош	12
RhoNi (SO4) a •6HoO	8m	74
Rubidium nitrate. RbNO <sub>2</sub> (trigonal)	5m	45
Rubidium platinum chloride,		_
Rb <sub>2</sub> PtCl <sub>6</sub>	5	53
Rubidium platinum fluoride, Rb <sub>2</sub> PtF <sub>6</sub>	6	48
Rubidium selenate, Rb <sub>2</sub> SeO <sub>4</sub>	9m	44
Rubidium silicon fluoride, Rb <sub>2</sub> SiF <sub>6</sub>	6	49
Rubidium strontium chloride,		- 1
RbSrCl <sub>3</sub>	/m	54
Rubidium strontium chromium oxide,	15-	61.
$RD_2Sr(UrU_4)_2$	120	04
$Rb_sr(SO_s)_s$	15m	65
Rubidium sulfate. Rb <sub>2</sub> SO <sub>4</sub>	8	48
Rubidium tellurium bromide.	-	
Rb <sub>2</sub> TeBr <sub>6</sub>	8	46
Rubidium tellurium chloride,		
Rb <sub>2</sub> TeCl <sub>6</sub>	8	48
Rubidium tin chloride, Rb <sub>2</sub> SnCl <sub>6</sub>	6	46
Rubidium zinc fluoride, RbZnF <sub>3</sub>	7 m	57
Rubidium zinc sulfate hydrate,	-	
$RD_2Zn(SO_4)_2 \circ 6H_2O$	/m	55
Ruthenium, Ru Puthenium PuTi	4 6m	86
Samarium arsenate SmAs0.	4m	33
Samarium arsenide. SmAs	4m	68
Samarium chloride, SmCl <sub>2</sub>	lm ·	40
Samarium chloride oxide, SmOCl	lm	43
Samarium fluoride, SmF <sub>3</sub>	lm	41
Samarium oxide, Sm <sub>2</sub> O <sub>3</sub> (cubic)	4m	34
Samarium silver, SmAg	5m	73
Samarium tin oxide, $Sm_2Sn_2O_7$	8m	77
Samarium vanadium oxide, SmVO <sub>4</sub>	5m	4/
Scandium arsenate, $ScAsO_4$	4m (/m	35
Scandium arsenide, SCAS	411	27
Scandium phosphate ScPO.	8	50
Scandium silicate (thortveitite).	0	50
Sc <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>	7 m	58
Selenium, Se	5	54
Selenium oxide (selenolite), SeO <sub>2</sub>	7m <sup>-</sup>	60
Silicon, Si	13m	35
Silicon, Si (reference standard)	12m	2
Silicon nitride, $\beta$ -Si <sub>3</sub> N <sub>4</sub>	14m	116
Silicon oxide ( $\alpha$ or low	10	1.0
Silicon ovide (v or lou	10	40
cristobalite) Sina (tetragonal)		
(calculated pattern)	15m	180
Silicon oxide ( $\alpha$ or low quartz).	2011	
SiO <sub>2</sub> (hexagonal)	3	24

Silicon ovide (B or high		
cristobalite). SiO <sub>2</sub> (cubic)	1	42
Silver, Ag	ī	23
Silver, Ag (reference standard)	8m	2
Silver arsenate, Ag <sub>3</sub> AsO <sub>4</sub>	5	56
Silver arsenic sulfide,		
xanthoconite, Ag <sub>3</sub> AsS <sub>3</sub>	8m	126
Silver bromate, AgBrO <sub>3</sub>	5	57
Silver bromide (bromargyrite), AgBr	4	46
Silver carbonate, Ag <sub>2</sub> CO <sub>3</sub>	13m	36
Silver chlorate, AgClO <sub>3</sub>	7	44
Silver chloride (chlorargyrite),	,	
AgC1	4	44
Silver chromium oxide, $Ag_2CrO_4$	12m	30
Silver cyanide, Agun	9m 5	48
Silver fluoride, $Ag_2F$	Sm	53
Silver iodate, $AglO_4$	9	49
(hever lodide (lodargyrite), Agi	Q	51
(llexagonal)	0	/8
Silver mangapase oxide AgMnO.	7m	155
Silver molybdenum oxide AgoMoO.	7	45
Silver nitrate AoNO.	5	59
Silver nitrite AoNOo	5	60
Silver oxide Ago	lm	45
Silver(II) oxide nitrate Aga0oN0	4	61
Silver phosphate AgePO	5	62
Silver rhenium oxide. AgReO4	8	53
Silver selenate. Ag <sub>2</sub> SeO <sub>4</sub>	2m	32
Silver sodium chloride,		
$Ag_0 = 5Na_0 = 5C1$	8m	79
Silver sulfate, Ag <sub>2</sub> SO <sub>4</sub>	13m	37
Silver sulfide (acanthite), Ag <sub>2</sub> S	10	51
Silver terbium, AgTb	5m	74
Silver thulium, AgTm	5m	74
Silver yttrium, AgY	5m	75
Sodium, Na	9m	105
Sodium aluminum chloride silicate,		
<pre>sodalite, Na<sub>8</sub>Al<sub>6</sub>Cl<sub>2</sub>(SiO<sub>4</sub>)<sub>6</sub></pre>	7m	158
Sodium aluminum sulfate hydrate		
(soda alum), NaAl( $SO_4$ ) <sub>2</sub> ·12H <sub>2</sub> O	15m	68
Sodium azide, $\alpha$ -NaN <sub>3</sub> , at -90 to		100
	8m	129
Sodium azide, $\beta$ -NaN <sub>3</sub>	8m	130
fluoride oride gilioste meliphonite		
(Non $C_{2}$ (Non $C_{2}$ (Non $C_{2}$ ) $P_{O}(A) = S_{1}^{2}$ (Non $C_{2}$ ) $P_{O}(A) = S_{1}^{2}$	,	
$(Ra_{0.63}Ca_{1.37}) De(Ri_{0.13}Di_{1.87})$	8m	135
Sodium bervllium calcium fluoride	Uni	+55
silicate, leucophanite.		
NaBeCaFSioOc	8m	138
Sodium borate. Na <sub>2</sub> B <sub>2</sub> O <sub>12</sub>	7m	160
Sodium boron hydride, NaBH,	9	51
Sodium bromate, NaBrO3	5	65
Sodium bromide, NaBr	3	47
Sodium bromide chloride,		
NaBr <sub>33</sub> Cl <sub>67</sub>	11m	49
Sodium bromide chloride,		
NaBr <sub>.67</sub> Cl <sub>.33</sub>	11m	50
Sodium calcium aluminum fluoride		
hydrate, thomsenolite,		
$NaCaAlF_6 \cdot H_2O$	8m	132
Sodium calcium carbonate hydrate,		3.0.4
pirssonite, $Na_2Ca(CO_3)_2 \cdot 2H_2O$	9m	106
Sodium calcium phosphate, $\beta$ -NaCaPO <sub>4</sub>	15m	69
Sodium calcium silicate, $Na_2CaSiO_4$	TOW	48
Na. Ca(SO)	6-	50
Ma20a(004)2	OII	72

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Sodium carbonate hydrate (thermo-		
patrite) NacCo. +HaO	8	5/
Sodium carbonate sulfate Na.CO.SO.	11m	51
Sodium carbonate sulfate (burkeite)	TIM	51
Na $_{0}(0, (S_{0}))$	, 11m	52
Sodium carbonate sulfate	TIM	52
$N_{2} = (\Omega_{2} (S_{1}))_{2}$	11m	53
Sodium carbonate sulfate	11m	55
Na $(\Omega_{2})$ SO.	11m	5/
Sodium chlorate NaClO	3	51
Sodium chlorate NaClO	5	JI
(orthorhombic)	7	/.0
Sodium chloride (balite) NaCl	2	49
Sodium chromium oxide NacCrO.	Qm	41
Sodium chromium oxide hydrate	Jui	40
NaoCr0. • 4Ho0	9m	50
Sodium chromium oxide hydrate	7Ш	50
NacCro0. * 2Ho0	7m	62
Sodium chromium oxide sulfate	7 Ш	02
Na $(Cr0_{\star})(S0_{\star})$	11m	55
Sodium cobalt nitrite $Na_{co}(NO_{a})$	15m	70
Sodium cobalt(II) sulfate hydrate.	1911	10
Na $CO(SO_{\star})$ • 4HaO	6m	61
Sodium cyanate NaCNO	2m	33
Sodium cyanide NaCN (cubic)	20	78
Sodium cyanide, NaCN (orthorhombic)	-	/0
at 6 °C	1	79
Sodium fluoride (villiaumite) NaF	1	63
Sodium hydrogen carbonate hydrate	-	00
trona Na $H(CO_a) \circ 2H_0O$	15m	71
Sodium hydrogen fluoride NaHFo	5	63
Sodium hydrogen phosphate	5	05
Na-H(PO-).	10m	130
Sodium hydrogen silicate hydrate	Tom	150
Nachosio. •4Hoo	7m	163
Sodium hydrogen sulfate hydrate	710	105
NaHSO. •HoO	9m	52
Sodium bydroxide NaOH at 300 °C	4m	69
Sodium iodate NaIO	7	47
Sodium iodate NaIO.	7	48
Sodium iodide Nal	4	31
Sodium iron fluoride NasFeFs	9m	54
Sodium lanthanum fluoride silicate	2111	5.
(NacLac)Fo(SiO <sub>4</sub> )	7m	64
Sodium lanthanum molybdenum oxide	, m	
NaLa (MoO.)	10m	49
Sodium magnesium aluminum horon	Tom	
hydroxide silicate dravite		
NaMgaAlaBa(OH) SiaOaz	Зm	47
Sodium magnesium carbonate	511	• • •
(oitelite) No.Ma(CO.).	11m	56
Sodium magnesium sulfate	1111	50
(vanthoffite) Na-Ma(SO.).	15m	72
Sodium magnesium sulfate hydrate.	1011	, -
bloedite NacMa(SO.) a.4HaO	6m	63
Sodium magnesium sulfate hydrate	011	00
(loeweite) NatoMar(SO.) to 15Ho0	14m	35
Sodium manganese(II) fluoride	1 114	55
NaMnFa	6m	65
Sodium manganese sulfate hydrate	011	05
Na $M_{n=}(SO_{1}) = \cdot 15H_{-}O_{1}$	1.4m	37
Sodium mercury(II) chloride hydrate	T-410	57
NaHeCla+2HaO	, 6m	66
Sodium molybdenum oxide NacMoO.	lm	46
Sodium molybdenum oxide NacMocO-	9m	110
Sodium neodymium fluoride silicate	700	
(NaoNde)Fo(SiOa)	7m	66
Sodium nickel(II) sulfate hydrate	, 10	, J
NaoNi (SO4) 2.4Ho0	6m	68
Mazni (104) 2 mizo	- Cini	

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Sodium nitrate (soda niter), NaNO3	6	50	Stront
Sodium nitrite, NaNO <sub>2</sub>	4	62	Stront
Sodium oxide, Na <sub>2</sub> O	10m	134	Stront
Sodium phosphate, Na <sub>3</sub> P <sub>3</sub> O <sub>9</sub>	3m	49	Stront
Sodium phosphate hydrate,			Stront
$Na_3P_3O_9 \cdot H_2O$	Зm	50	Sr <sub>3</sub> Sc
Sodium phosphate hydrate,			Stront
$\alpha$ -Na <sub>4</sub> P <sub>4</sub> O <sub>12</sub> ·4H <sub>2</sub> O (monoclinic)	13m	39	Stront
Sodium phosphate hydrate,			SrS04
$\beta$ -Na <sub>4</sub> P <sub>4</sub> O <sub>12</sub> ·4H <sub>2</sub> O (triclinic)	2m	35	Stront
Sodium phosphate hydrate,			Stront
$Na_6P_6O_{18} \cdot 6H_2O$	5m	54	Stront
Sodium praseodymium fluoride			Stront
silicate, (Na <sub>2</sub> Pr <sub>8</sub> )F <sub>2</sub> (SiO <sub>4</sub> ) <sub>6</sub>	7m	68	Stront
Sodium selenate, Na <sub>2</sub> SeO <sub>4</sub>	9m	55	Stront
Sodium selenide, Na <sub>2</sub> Se	10m	135	Stront
Sodium silicate, $\alpha(III)$ , Na <sub>2</sub> Si <sub>2</sub> O <sub>5</sub>	8m	141	Stront
Sodium silicate, β-Na <sub>2</sub> Si <sub>2</sub> O <sub>5</sub>	10m	136	Sulfam
Sodium sulfate, Na <sub>2</sub> SO <sub>4</sub>	11m	57	Sulfur
Sodium sulfate (thenardite), Na <sub>2</sub> SO <sub>4</sub>	2	59	Tantal
Sodium sulfide, Na <sub>2</sub> S	10m	140	Tantal
Sodium sulfite, Na <sub>2</sub> SO <sub>3</sub>	3	60	Tellur
Sodium telluride, Na2Te	10m	141	Tellur
Sodium tin fluoride, NaSn <sub>2</sub> F <sub>5</sub>	7 m	166	Te02
Sodium tungsten oxide, Na <sub>2</sub> WO <sub>4</sub>	lm	47	Tellur
Sodium tungsten(VI) oxide hydrate,			TeO <sub>2</sub>
$Na_2WO_4 \cdot 2H_2O$	2m	33	Tellur
Sodium zinc fluoride, NaZnF3	6m	74	TeO <sub>2</sub>
Sodium zinc sulfate hydrate,			Terbiu
$Na_2Zn(SO_4)_2 \cdot 4H_2O$	6m	72	Terbiu
Sodium zirconium fluoride,			Terbiu
Na <sub>7</sub> Zr <sub>6</sub> F <sub>31</sub>	8m	144	Terbiu
Strontium aluminum hydroxide,			Terbiu
$Sr_3Al_2(OH)_{12}$	10m	50	Terbiu
Strontium aluminum oxide, Sr <sub>3</sub> Al <sub>2</sub> O <sub>6</sub>	10m	52	Terbiu
Strontium arsenate, $Sr_3(AsO_4)_2$	2m	36	Terbiu
Strontium azide, $Sr(N_3)_2$	8 m	146	Thalli
Strontium borate, SrB <sub>2</sub> O <sub>4</sub>	3m	53	T1A1(
Strontium borate, SrB <sub>4</sub> 07	4m	36	Thalli
Strontium bromide fluoride, SrBrF	10m	54	Thalli
Strontium bromide hydrate,			Thalli
SrBr <sub>2</sub> ·6H <sub>2</sub> 0	4	60	Thalli
Strontium carbonate (strontianite),			Thalli
SrCO <sub>3</sub>	3	56	Tl <sub>2</sub> Cd
Strontium chloride, SrCl <sub>2</sub>	4	40	Thalli
Strontium chloride fluoride, SrClF	10m	55	Thalli
Strontium chloride hydrate,			Thalli
$SrCl_2 \cdot 2H_2O$	11m	58	Thalli
Strontium chloride hydrate,			Thalli
SrCl <sub>2</sub> ·6H <sub>2</sub> 0	4	58	TlCr(
Strontium chloride hydroxide			Thalli
phosphate, Sr <sub>5</sub> Cl <sub>.65</sub> (OH) <sub>.35</sub> (PO <sub>4</sub> ) <sub>3</sub>	11m	60	Tl <sub>2</sub> Co
Strontium fluoride, SrF <sub>2</sub>	5	67	Thalli
Strontium hydroxide, Sr(OH) <sub>2</sub>	13m	41	Tl <sub>2</sub> Co
Strontium hydroxide hydrate,			Thalli
$Sr(OH)_2 \cdot H_2O$	13m	42	Tl <sub>2</sub> Cu
Strontium hydroxide hydrate,			Thalli
$Sr(OH)_2 \cdot 8H_2O$	13m	43	TlGa(
Strontium indium hydroxide,			Thalli
$Sr_3In_2(OH)_{12}$	6m	76	Thalli
Strontium iodide hydrate,			(orth
SrI <sub>2</sub> •6H <sub>2</sub> 0	8	58	Thalli
Strontium manganese oxide,			Tl <sub>2</sub> Fe
SrMnO <sub>3</sub> (cubic)	10m	56	Thalli
Strontium manganese oxide,			Tl <sub>2</sub> Pb
SrMnO <sub>3</sub> (hexagonal)	10m	58	Thalli
Strontium molybdenum oxide, SrMoO <sub>4</sub>	7	50	Tl <sub>2</sub> Mg
Strontium nitrate, Sr(NO <sub>3</sub> ) <sub>2</sub>	12m	31	Thalli
Strontium oxide, SrO	5	68	Tl <sub>2</sub> Mg
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Strontium oxide, SrO <sub>2</sub>	6	52
Strontium oxide hydrate, SrO <sub>2</sub> ·8H <sub>2</sub> O	11m	61
Strontium phosphate, $\alpha$ -Sr <sub>2</sub> P <sub>2</sub> O <sub>7</sub>	11m	62
Strontium phosphate, $\alpha$ -Sr <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>	11m	64
Strontium scandium oxide nydrate,	6	78
Stroptium silicate SraSi0-	13m	10
Strontium sulfate (celestite)	1.Jui	
SrS04	2	61
Strontium sulfide, SrS	7	52
Strontium telluride, SrTe	4m	69
Strontium tin oxide, SrSnO3	8m	80
Strontium titanium oxide, SrTiO3	3	44
Strontium tungsten oxide, SrWO <sub>4</sub>	7	53
Strontium tungsten oxide, $Sr_2WO_5$	12m	32
Strontium vanadium oxide, $Sr_3(VO_4)_2$	15m	73
Strontium zirconium oxide, SrZrO <sub>3</sub>	9	51
Sulfamic acid, H <sub>2</sub> NSO <sub>3</sub> H	7	54
Sulfur, S (orthorhombic)	9	54
Tantalum, la		29
Tallumium To	0	29
Tollurium(IV) ovide (paratollurite)	T	20
Tella (tetragonal)	7	56
Tellurium(IV) oxide, paratellurite.	'	50
TeO <sub>2</sub> (tetragonal)	10	55
Tellurium(IV) oxide, tellurite.	10	55
TeO <sub>2</sub> (orthorhombic)	9	57
Terbium arsenate, TbAsO <sub>4</sub>	3m	54
Terbium arsenide, TbAs	5m	75
Terbium nitride, TbN	4m	70
Terbium phosphide, TbP	5m	76
Terbium selenide, TbSe	5m	76
Terbium sulfide, TbS	5m	77
Terbium telluride, TbTe	5m	77
Terbium vanadium oxide, TbVO <sub>4</sub>	5m	56
Thallium aluminum sulfate hydrate,		5.0
$TIAI(SU_4)_2 \cdot I2H_2U$	6	53
Thallium (1) arsenate, $II_3ASU_4$	2m	3/
Thallium (I) bromato TIPro	011	60
Thallium bromide TIBr	7	57
Thallium cadmium sulfate	1	57
$Tl_{o}Cd_{o}(SO_{4})_{2}$	8m	83
Thallium(I) chlorate. TlClO <sub>4</sub>	2m	38
Thallium(I) chlorate, TlC103	8	61
Thallium(I) chloride, TlCl	4	51
Thallium chromium oxide, Tl <sub>2</sub> CrO <sub>4</sub>	Зm	54
Thallium chromium sulfate hydrate,		
$T1Cr(SO_4)_2 \cdot 12H_2O$	6	55
Thallium cobalt sulfate,		
$T1_2Co_2(SO_4)_3$	8m	85
Thallium cobalt sulfate hydrate,	~	70
$\Pi_2 \text{Lo}(\text{SU}_4)_2 \cdot \text{bH}_2 \text{U}$	/ m	/0
There is a set of the	7m	70
Thallium callium culfate hydrate	7 111	12
TlGa(SQ4)a·12HoQ	6	57
Thallium(I) iodate. $TIIO_2$	8	62
Thallium(I) iodide, TII		
(orthorhombic)	4	53
Thallium iron sulfate hydrate,		
$T1_2Fe(S0_4)_2 \cdot 6H_20$	8m	87
Thallium lead sulfate,		
$T1_2Pb(S0_4)_2$	15m	74
Thallium magnesium chromium oxide,		
$T1_2Mg_2(CrO_4)_3$	8m	89
Thallium magnesium sulfate hydrate,	_	7 /
$11_2$ Mg(SU <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	7m	74

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Thallium manganese sulfate,			Yttrium chloride oxide, YClO	lm	51
$Tl_2Mn_2(SO_4)_3$	7m	76	Yttrium oxide, Y <sub>2</sub> O <sub>3</sub>	3	28
Thallium nickel sulfate hydrate.			Yttrium phosphate (xenotime), YPO	8	67
$Tl_{o}Ni(SO_{4})_{o}:6H_{o}O$	7m	78	Vttrium sulfide VS	5m	80
Thallium $(I)$ nitrate TINO.	6	5.8	Vttrium telluride VTe	//m	75
(1) $(1)$	0	00		4111	110
Inallium(III) oxide, $II_2U_3$	2	28	ittrium titanium oxide, 121105	TTW	113
Thallium(I) phosphate, Tl <sub>3</sub> PO <sub>4</sub>	7	58	Yttrium vanadium oxide, YVO <sub>4</sub>	5m	59
Thallium(III) phosphate, T1PO <sub>4</sub>	7	59	Zinc, Zn	1	16
Thallium platinum chloride.			Zinc aluminum oxide (gahnite).		
TloPtClo	5	70	ZnAloO	2	38
Thellium cilicon flueride Tl SiF	6	56	7 inc. amming hyperide $7n(MU)$ Pr	11m	60
mailium silicon liuolide, li251r6	0	20	Zinc annine bromide, Zn(Mr3)2br2	110	00
Thallium strontium sulfate,			Zinc ammine chloride, $Zn(NH_3)_2Cl_2$	TOW	59
$\mathrm{Tl}_{2}\mathrm{Sr}(\mathrm{SO}_{4})_{2}$	15m	75	Zinc antimony oxide, ZnSb <sub>2</sub> O <sub>4</sub>	4m	39
Thallium(I) sulfate, Tl <sub>2</sub> SO <sub>4</sub>	6	59	Zinc borate, $Zn_4B_6O_{13}$	13m	48
Thallium(I) thiocvanate, TICNS	8	63	Zinc carbonate, smithsonite, ZnCO <sub>2</sub>	8	69
Thallium tin chloride TloSnClo	6	54	Zinc chromium oxide ZnCroO	Qm	59
Thallium (I) tungatan avida Tl 10	1-	1.0	Zine coholt avide 7nCo 0	10m	60
mailium(1) tungsten oxide, 112w04	TIII	40	Zine cobalt oxide, $2nco_20_4$	TOU	00
Thallium zinc sulfate hydrate,			Zinc cyanide, $Zn(CN)_2$	5	/3
$Tl_2Zn(SO_4)_2 \cdot 6H_2O$	7 m	80	Zinc fluoride, ZnF <sub>2</sub>	6	60
Thorium arsenide, ThAs	4m	70	Zinc fluoride hydrate, ZnF <sub>2</sub> ·4H <sub>2</sub> O	11m	69
Thorium oxide (thorianite), ThO <sub>2</sub>	1	57	Zinc germanium oxide, Zn <sub>2</sub> GeO <sub>4</sub>	10	56
Thulium arsenate . TmAs().	Зm	56	Zinc hydroxide silicate hydrate		• •
Thulium ansender, Thusson Thulium ansender	/m	71	beningershite 7 (OII) Si O all O	2	60
Inulium arsenide, ImAs	4m	/1	nemimorphite, $2n_4(0H)_2S1_20_7 H_20$ .	2	02
Thulium nitride, TmN	4m	71	Zinc iodide, Znl <sub>2</sub>	9	60
Thulium oxide, $Tm_2O_3$	9	58	Zinc iron oxide (franklinite),		
Thulium telluride, TmTe	4m	72	ZnFe <sub>2</sub> O <sub>4</sub>	9m	60
Thulium vanadium oxide TmVO	5 m	57	Zinc manganese oxide (hetaerolite)		
Tip W-Sp (cubic)	2	12	ZnMn.O.	10m	61
	2	12		1011	170
lin, p-Sn (tetragonal)	1	24	Zinc molybdenum oxide, $2n_2Mo_3U_8$	/m	1/3
Tin arsenide, SnAs	4m	37	Zinc nitrate hydrate,		
Tin arsenide, Sn <sub>3,8</sub> As <sub>3</sub>	15m	76	$\alpha$ -Zn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	12m	- 36
Tin(II) fluoride, SnF <sub>2</sub>	3m	51	Zinc oxide (zincite), ZnO	2	25
Tin hydrogen phosphate SnHPO.	13m	46	Zinc selenide ZnSe	3	23
Tin (IV) iodido Spl	5	71	Zine silicate (willowite) Zn SiO	7	62
$\operatorname{TII}(1V)$ founde, $\operatorname{SIII}_4$	5	/1	21 $11$ $21$ $21$ $21$ $21$ $210$ $4$	/	02
lin(11) oxide (romarchite), SnU	4	28	Zinc silicon fluoride hydrate,		
Tin(IV) oxide (cassiterite), $SnO_2$	1	54	$ZnSiF_6 \cdot 6H_2O$	8	70
Tin sulfide (berndtite), $\beta$ -SnS <sub>2</sub>	9m	57	Zinc sulfate (zinkosite), ZnSO <sub>4</sub>	7	64
Tin(II) telluride, SnTe	7	61	Zinc sulfate hydrate (goslarite),		
Titanium. Ti	3	4	$ZnSO_4 \cdot 7H_2O$	8	71
Titanium ovide (anatase) Tilo	7m	82	Zinc sulfide (wurtzite) N-7nS		
Titopium oxide brookite Tio	7 44	02	(hereareal)	2	17
ficalitum oxide, brookice, filo2	2			۷.	14
(orthorhombic)	3m	57	Zinc sulfide (sphaelerite), B-ZnS		
Titanium oxide (rutile), TiO <sub>2</sub>	7m	83	(cubic)	2	16
Titanium(III) oxide, TiO <sub>1,515</sub>	9	59	Zinc telluride, ZnTe	3m	58
Titanium silicide. TisSia	8	64	Zinc tin oxide. Zn <sub>2</sub> SnO <sub>4</sub>	10m	62
Titanium sulfide TiSo	4m	72	Zinc titanium oxide ZnTiO	13m	49
Titanium culfido Ti-S	9m	1/0	Zine titanium oxide, Zhilog	12m	37
		149	Zinc treation oxide, $2n_2n_4$	1211	57
lungsten, w	1	20	Zinc tungsten oxide (sanmartinite),		
Tungsten, W (reference standard)	8m	2	ZnWO <sub>4</sub>	2m	40
Tungsten sulfide (tungstenite), WS <sub>2</sub>	8	65	Zirconium, α-Zr	2	11
Uranium oxide. UO	5 m	78	Zirconium hydride, ZrH <sub>2</sub>	5m	60
Uranium oxide (uraninite) 100	2	33	$7irconium iodate 7r(10_{o})$	lm	51
Uranium colorido USo	5 -	70	Zinconium nitrido ZrN	5 m	80
	5111	70		511	00
Uranium telluride, Ule	4m	/3	Zirconium oxide, ZrU	Sm	81
Vanadium, V	9m	58	Zirconium phosphide, ZrP	4m	75
Vanadium(V) oxide (shcherbinaite),			Zirconium silicate, zírcon, ZrSiO <sub>4</sub>	4	68
V <sub>2</sub> O <sub>5</sub>	8	66	Zirconium sulfate hydrate		
Vanadium sulfide <i>α</i> -V <sub>o</sub> S	1.4m	118	$(zircosulfate) Zr(SO_4) \circ 4H_0O_1$	7	66
Vanadium sulfide, a V35	1/m	120	(211003011000), 21(004)2 220 200		
Variautum surrive, $p^{-1}v_{3}$	1411	20			
itterbium arsenate, iDASU4	4m	38			
Itterbium arsenide, YbAs	4m	/3			
Ytterbium nitride, YbN	4m	74			
Ytterbium oxide, Yb <sub>2</sub> O <sub>3</sub>	6m	80			
Ytterbium selenide. YbSe	5m	79			
Ytterbium telluride VbTe	5 m	79			
Vtterhium(III) varadium ovide	511	, ,			
VEVO	5	FO			
1DVU4	5m	58			
Yttrium arsenate, YAsO <sub>4</sub>	2m	39			
Yttrium arsenide, YAs	4m	74			

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Acetanilide, CeHeNHCOCH,	14m	38	Nickel acetate hydrate.	
4-Acetyl-2'-fluorodiphenyl,			$Ni(C_2H_3O_2)_2 \cdot 4H_2O$	13m
C <sub>14</sub> H <sub>11</sub> FO	8m	91	Nickel hexaimidazole nitrate,	
Alanine, L-, CH <sub>3</sub> CHNH <sub>2</sub> CO <sub>2</sub> H	8m	93	$Ni(C_3H_4N_2)_6(NO_3)_2$	7m
Allobarbital, $C_{10}H_{12}N_2O_3$	14m	41	Nickel tetrapyrazole chloride,	•
Amobarbital, form I, $C_{11}H_{18}N_2O_3$	15m	114	$Ni(C_3H_4N_2)_4Cl_2$	8m
Amodardital, form II, C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> U <sub>3</sub>	1.5m	11/	$1.3.5.7$ -tetrazonipe ( $\alpha$ -HMY)	
Ammonium formate NH.HCO.	11m	9.J	$C_{\rm HeNeOe}$	11m
Ammonium oxalate hydrate	T TIW	,	Octahydro-1.3.5.7-tetranitro-	TTI
$(\text{oxammite}), (\text{NH}_{4})_{2}C_{2}O_{4} \cdot H_{2}O \dots$	7	5	1,3,5,7-tetrazocine (B-HMX),	
Ammonium yttrium oxalate			$C_4H_8N_8O_8$	llm
hydrate, $NH_4Y(C_2O_4)_2 \cdot H_2O$	8m	97	Palladium bis-(N-isopropyl-3-	
Amphetamine sulfate, (+)-,			ethylsalicylaldiminate),	
$C_{18}H_{28}N_2O_4S$	15m	119	$Pd(C_{12}H_{16}NO)_2$	7 m
Ascorbic acid, L-, C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>	8m	99	Pimelic acid, $(CH_2)_5(CO_2H)_2$	7 m
Azobenzene, $C_6H_5NNC_6H_5$	7m	86	Potassium formate-formic acid	
Barbital, form I, $C_8H_{12}N_2O_3$	15m	126	complex, $KO_2CH \cdot HO_2CH$	9m
Barbital, form II, L <sub>8</sub> H <sub>12</sub> N <sub>2</sub> U <sub>3</sub>	15m 15-	128	c u (coou)(cook)	1
Barbital, form IV, $C_8H_{12}N_2O_3$	15m	130	$C_{6n_4}(COOR)(COOR)$	411
Cadmium hevaimidazole nitrate	LOIN	133	KaCaO. HaO	Qm
Cd(CoH, No)o(NOo)o	8m	23	Potassium ovalate perhydrate	911
Calcium formate. $Ca(HCO_0)_0$	8	16	KoCoQ4 HoQo	9m
Calcium malate hydrate.	U	10	Potassium sodium tartrate hydrate.	211
$Ca(0_2C)_2(CH_2CHOH)\cdot 2H_2O$	10m	76	$C_4 H_4 KNa O_6 \cdot 4 H_2 O \ldots$	15m
Chlorpromazine, C17H19ClN2S	14m	60	Reservine, $C_{33}H_{40}N_2O_9$	8m
Cobalt acetate hydrate,			Rubidium oxalate perhydrate,	
$Co(C_2H_3O_2)_2 \cdot 4H_2O$	12m	19	$Rb_2C_2O_4 \cdot H_2O_2$	9m
Copper glutamate hydrate,			Silver oxalate, Ag <sub>2</sub> C <sub>2</sub> O <sub>4</sub>	9m
$Cu(O_2C)_2(H_2NCHCH_2CH_2)\cdot 2H_2O$	7m	110	Sodium acetate hydrate, C <sub>2</sub> H <sub>3</sub> NaO <sub>2</sub> ·3H <sub>2</sub> C	) 15m
Copper tetraimidazole nitrate,			Sodium D-tartrate hydrate,	
$Cu(C_{3}H_{4}N_{2})_{4}(NO_{3})_{2}$	13m	24	$(CHOH-CO_2Na)_2 \cdot 2H_2O$	llm
Copper tetrapyrazole chloride,		0.1	Sodium oxalate, $Na_2C_2O_4$	6m
$Cu(C_3H_4N_2)_4CL_2$	8m 35	31	Strontium formate, $Sr(CHO_2)_2$	8
Custoine $I = HSCH_*CH(NH_*)*COOH$	1.1m	21 86	$Sr(CHO_{2})$ , $2H_{2}O_{1}$ (orthorhombic)	8
Diazenam, CicHioClNoO	14m	106	Sucrose CroHooOrd	11m
Dibenzovlmethane. (CcHcCO) 2CH	7m	115	Tartaric acid. D (CHOHCO <sub>2</sub> H) <sub>2</sub>	7m
(N,N)-Dimethyltryptamine, C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>	14m	109	Trimethylammonium chloride,	
bis-(o-Dodecacarborane), C <sub>4</sub> B <sub>20</sub> H <sub>22</sub>	6m	7	(CH <sub>3</sub> ) <sub>3</sub> NHC1	9m
Glucose, D-, $\alpha$ , (dextrose), $C_6H_{12}O_6$	llm	28	2,4,6-Trinitrophenetole,	
Glyoxime, $H_2C_2(NOH)_2$	8m	102	$C_2H_5OC_6H_2(NO_2)_3$	8m
Hexamethylenediammonium adipate,	_		Urea, $CO(NH_2)_2$	7
$(CH_2)_4(CU_2H_3N)_2(CH_2)_6$	7m	121	Uric acid, $C_5H_4N_4O_3$	8m
Holmium ethylsulfate hydrate,	1	10	Zinc diimidazole chloride,	7
Hydroquinone $y=HOC_{-}U$ OU	1m Qm	107	$\frac{2\pi(\log_{4}N_{2})}{2\log_{4}N_{2}} + \frac{1}{2} + \frac$	/ m
Iron ovalate hydrate	om	107	$2\pi(0.0CHNH_0CH_0CH_0CO_0) \cdot 2H_00$	7m
(humboldtine), FeCoO <sub>4</sub> ·2HoO	1 Om	24		7 111
Lead formate. $Pb(HCO_2)_2$	8	30		
Lithium oxalate. Li <sub>2</sub> C <sub>2</sub> O <sub>4</sub>	10m	34		
Mercury o-phthalate, CeH4(CO2Hg)2	10m	113		
Methapyrilene hydrochloride,				
C <sub>14</sub> H <sub>20</sub> ClN <sub>3</sub> S	14m	112		
Metharbital, $C_9H_{14}N_2O_3$	15m	177		
Methyl sulfonanilide, C <sub>6</sub> H <sub>5</sub> NHSO <sub>2</sub> CH <sub>3</sub>	9m	78		
N-Methylphenazinium-7,7,8,8-tetra-				
cyanoquinodimethanide, $C_{25}H_{15}N_6$	7m	146		
2-Maphinylamine, N-phenyl-,	6-	20		
Neodymium ethylsulfate hydrate	om	29		
Nd((CoHr)SO() +9Ho0	Q	41		
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	bec.	Tage		Dec.	Tage
Acanthite, Ag <sub>2</sub> S	10	51	Cristobalite (α or low) SiO <sub>2</sub>		
Aeschynite CeNbTiO <sub>6</sub>	Зm	24	(tetragonal, calculated pattern)	15m	180
Alabandite, MnS	4	11	Cristobalite ( $\beta$ or high) SiO <sub>2</sub> (cubic)	1	42
Anatase, TiO <sub>2</sub>	7m	82	Cryolithionite, $Li_3Na_3Al_2F_{12}$	9m	23
Andradite, Ca <sub>3</sub> Fe <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>	9	22	Cryptohalite, (NH <sub>4</sub> ) <sub>2</sub> SiF <sub>6</sub>	5	5
Anglesite, PbSO <sub>4</sub>	3	67	Cuprite, $Cu_2O$	2	23
Anhydrite, $CaSO_4$	4	65	*Diamond, C	2	5
Antarcticite, CaCl <sub>2</sub> ·6H <sub>2</sub> O	12m	16	*Diaspore, $AI_2O_3 \cdot H_2O$	- 3	41
Antimony, Sb	3	14	Diopside, $Camg(SiU_3)_2$	5m 2	1/
Aphthitalite, $K_3Na(SO_4)_2$	om	52	$horder Mang_{3A1_6B_3S1_6U_27}(UH)_4 \dots$	3m	4/
Aragonite, $CaCO_3$ (coloulated pattern)	3	53	Ellerite, $Ma_2ng(UU_3)_2$	0.00	/2
Aragonite, LaCO <sub>3</sub> (calculated pattern)	) 14m 2	44 62	Elpasofile, K2NAAIr6	911	43
Arcanice, $\kappa_2 SO_4$	2	6	$\frac{\text{Mastalle, Mastal, Mastal, 70.0}}{\text{Fragmita}}$	7	30
Arsonalita As 0	1	51	Frythrosiderite K-FeCl-+H-O	1/m	27
Aurostibite AuSh.	1	18	Estolaite Crolo	5	22
$\dot{A}$ arusite $Cu_{0}(OH)_{0}(CO_{0})_{0}$	10	30	Ettringite CacaloSoOre:31HoO	8	3
Barvte BaSO	10m	12	Fairchildite. $K_0Ca(CO_2)_0$	8m	48
Berlinite AlPO	10	3	Fluorapatite, $Ca_FF(PO_4)_2$	3m	22
Berndtite SnSo	9m	57	Fluorite. CaF2	1	69
*Bervl. BealloSicOis	9	13	Forsterite, Mg_SiO4	ī	83
Bischofite. MgClo.6HoO	]]m	37	Franklinite. ZnFe <sub>2</sub> O <sub>4</sub>	9m	60
Bismite. $\alpha$ -Bi <sub>2</sub> O <sub>2</sub>	3m	17	Fresnoite, Ba <sub>2</sub> TiSi <sub>2</sub> O <sub>8</sub>	9m	14
Bismoclite. BiOCl	4	54	Gahnite, ZnAl <sub>2</sub> O <sub>4</sub>	2	38
Bismuth, Bi	3	20	Galaxite, MnAl204	9	35
Bismuthinite, Bi <sub>2</sub> S <sub>3</sub>	5m	13	Galena, PbS	2	18
Bixbyite, $\alpha$ -Mn <sub>2</sub> O <sub>3</sub>	llm	95	Gaspeite, NiCO3	lm	36
*Bloedite, $Na_2Mg(SO_4)_2 \cdot 4H_2O$	6m	63	Geikielite, MgTiO <sub>3</sub>	5	43
Boehmite, $Al_2O_3 \cdot H_2O$	3	38	Gersdorffite, NiAsS	lm	35
Bromargyrite, AgBr	4	46	Glauberite, Na <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub>	6m	59
Bromellite, BeO	1	36	Gold, Au	1	33
*Brookite, TiO <sub>2</sub>	3m	57	Goslarite, ZnSO <sub>4</sub> ·7H <sub>2</sub> O	8	71
Brucite, Mg(OH) <sub>2</sub>	6	30	Greenockite, CdS	4	15
Bunsenite, NiO	1	47	*Groutite, Mn0(OH)	llm	97
Burkeite, $Na_6CO_3(SO_4)_2$	11m	52	Halite, NaCl	2	41
*Butlerite, $Fe(0H)SO_4 \cdot 2H_2O$	10m	95	Hausmannite, Mn <sub>3</sub> 0 <sub>4</sub>	10m	38
Cadmoselite, CdSe	7	12	*Hemimorphite, $Zn_4(OH)_2Si_2O_7 \cdot H_2O$	2	62
Calcite, CaCO <sub>3</sub>	2	51	Hetaerolite, $2nMn_2O_4$	10m	61
Calomel, $Hg_2Cl_2$	13m	30	Hieratite, $K_2SiF_6$	5	50
Carnallite, $\text{KMgCl}_3 \cdot 6\text{H}_20$	8m	50	Huebnerite, $MnWO_4$	2m	24
Carobbilte, Kr	1	04 E/	Humboldtine, $FeC_2O_4 \cdot 2H_2O$	TOW	24
Calestite $Silon$	1	54 61	Humite, $\operatorname{Hg}_{7}\operatorname{F}_{2}\operatorname{S1}_{3}\operatorname{O}_{12}$	1m	10
Corionite $Colorianite Colorianite Colori$	2	56	Ilmonite Forio	15m	10
Corussite PbCO.	2	56	Indialite MacAl Si-O.	1.5m	29
Cervantite Sh-0.	10	8	Indiarrec, ng2A14015018	8	51
Chalcokvanite CuSO.	3m	20	Iron «-Fe	4	31
Chernovite $VAsO$ .	2m	30	Jacobsite MnFeoO.	9	36
Chloraluminite, AlCla.6Ho0	7	3	*Julgoldite.	í	50
Chlorargyrite. AgCl	4	44	$Ca_{2}Fe_{2}Si_{2}O_{1}O(OH_{2}O_{2}OH)$	10m	72
Chloromagnesite. MgCl <sub>2</sub>	llm	94	Kalistrontite, $K_0Sr(SO_4)_2$	14m	31
Chromatite, CaCrO <sub>4</sub>	7	13	Kremersite, (NH4,K) <sub>2</sub> FeCl <sub>5</sub> ·H <sub>2</sub> O	14m	8
Chrysoberyl, BeAl <sub>2</sub> 0 <sub>4</sub>	9	10	Langbeinite, $K_2Mg_2(SO_4)_3$	6m	40
Cinnabar, HgS	4	17	Lautarite, $Ca(IO_3)_2$	14m	12
Claudetite, As <sub>2</sub> O <sub>3</sub>	3m	9	Lead, Pb	1	34
Clausthalite, PbSe	5	38	*Leucophanite, NaCaBeFSi <sub>2</sub> 0 <sub>6</sub>	8m	138
Clinobisvanite, BiVO <sub>4</sub>	Зm	14	Lime, CaO	1	43
Copper, Cu	1	15	Lime, CaO (calculated pattern)	14m	49
Cordierite, Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub>	lm	28	Litharge, PbO (red)	2	30
Corundum, Al <sub>2</sub> O <sub>3</sub>	9	3	Lithiophosphate, Li <sub>3</sub> PO <sub>4</sub>	4m	21
Cotunnite, PbCl <sub>2</sub>	12m	23	Loellingite, FeAs <sub>2</sub>	10	34

Covellite, CuS .....

(tetragonal) .....

Cristobalite ( $\alpha$  or low) SiO<sub>2</sub>

4

10

13

48

Loeweite, Na<sub>12</sub>Mg<sub>7</sub>(SO<sub>4</sub>)<sub>13</sub>·15H<sub>2</sub>O ....

Lopezite, K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> .....

Macedonite, PbTiO<sub>3</sub>.....

	Vol. or	Daga		Vol. or	Page
	sec.	rage		Sec.	rage
Magnesiochromite, MgCr <sub>2</sub> O <sub>4</sub>	9	34	Sellaite, MgF <sub>2</sub>	4	33
Magnesite, MgCO <sub>3</sub>	7	28	Senarmontite, $Sb_2O_3$	3	31
$\begin{array}{cccc} \text{Magnetite, } \text{Fe}_{3} \cup_{4} & \dots & \dots & \dots \\ \text{Malachite, } & \text{Cua}(\text{OH}) \circ \text{COa} \end{array}$	10	31	Siderite FeCO	0 15m	32
Manganolangbeinite, $K_2Mn_2(SO_4)_2$	6m	43	Silver. Ag	1	23
Manganosite, Mn0	5	45	Silver, Ag (reference standard)	8m	2
Marshite, CuI	4	38	<pre>*Sjögrenite, Mg<sub>6</sub>Fe<sub>2</sub>CO<sub>3</sub>(OH)<sub>16</sub>·4H<sub>2</sub>O</pre>	10m	103
Mascagnite, (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	9	8	Skutterudite, CoAs <sub>3</sub>	10	21
Massicot, PbO (yellow)	12	32	*Smithsonite, $ZnCO_3$	15-	69
Matlockite, PDFUL	1.5m Qm	25 52	Soda alum, NaAl $(SU_4)_2 \cdot 12H_2U \dots$	15m 7m	158
Mayenite $CatoAltaOaa$	9	20	Soda niter. $NaNO_2$	6	50
Melanterite, $FeSO_4 \cdot 7H_2O$	8m	38	Sphaerocobaltite, CoCO <sub>3</sub>	10	24
*Meliphanite,			Sphalerite, ZnS	2	16
Na.63Ca1.37BeAl.13Si1.8706.25F.75	8m	135	Spinel, MgAl <sub>2</sub> 0 <sub>4</sub>	9m	25
Metaborite, HBU <sub>2</sub>	4m	27	Stibnite, $Sb_2S_3$	, 5	0 22
Miargyrite AgShS	-+ 5m	49	Stolzite PhWO.	5m	34
*Millerite, NiS	lm	37	Strontianite, $SrCO_3$	3	56
Minium, Pb <sub>3</sub> 0 <sub>4</sub>	8	32	Struvite, MgNH <sub>4</sub> PO <sub>4</sub> ·6H <sub>2</sub> O	3m	41
Mitscherlichite, K <sub>2</sub> CuCl <sub>4</sub> ·2H <sub>2</sub> O	9m	34	Sulfur, S (orthorhombic)	9	54
Molybdenite, MoS <sub>2</sub>	5	47	Sylvite, KCl	1	65
Molyddite, $MoU_3$	3	30	Syngenite, $K_2Ca(SO_4)_2 \cdot H_2O$	14m 2m	25
Montrovdite He0	9	39	Tellurite Tello	шс 9	57
Mullite, $Al_6Si_2O_{13}$	3m	3	Tellurium, Te	í	26
Nantokite, CuCl	4	35	Tellurobismuthite, Bi <sub>2</sub> Te <sub>3</sub>	3m	16
*Newberyite, MgHPO <sub>4</sub> ·3H <sub>2</sub> O	7m	139	Tenorite, CuO	1	49
Niter, KNO <sub>3</sub>	3	58	Teschemacherite, NH <sub>4</sub> HCO <sub>3</sub>	9	5
Nitrammite, $NH_4NU_3$	/ 11m	14	Thenardite, $Na_2SO_4$	2	54
Norbergite, $Mg_F_2SiO_4$	10	39	Thomsenolite, NaCaAlFa.HaO	8m	132
Oldhamite, CaS	7	15	Thorianite, ThO <sub>2</sub>	1	57
Otavite, CdCO <sub>3</sub>	7	11	Thortveitite, Sc <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>	7m	58
Oxammite, $(NH_4)_2C_2O_4 \cdot H_2O$	7	5	Tiemannite, HgSe	7	35
Palladium, Pd	1 1/m	21	Tin, $\alpha$ -Sn (cubic)	2	12
$^{*}$ Paratellurite TeO <sub>2</sub>	10	55	$\dot{T}$ (Letragonal)	I Im	4
Paratellurite, TeO <sub>2</sub>	7	56	Trevorite, NiFe $_2O_4$	10	44
Periclase, MgO	1	37	*Trona, Na <sub>3</sub> H(CO <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O	15m	71
Perovskite, CaTiO <sub>3</sub>	9m	17	Tschermigite, $NH_4A1(SO_4)_2 \cdot 12H_2O \dots$	6	3
*Phenakite, $Be_2SiO_4$	8		Tungstenite, WS <sub>2</sub>	8	65
*Pirssonite NacCa(CO <sub>2</sub> ) $\circ$ ·2HoO	0m 9m	106	Uvarovite $Ca_{1}Cr_{2}(SiO_{1})$	10	33 17
Platinum, Pt	1	31	*Valentinite, Sb <sub>2</sub> O <sub>3</sub>	10	6
Portlandite, Ca(OH) <sub>2</sub>	1	58	Vanthoffite, Na <sub>6</sub> Mg(SO <sub>4</sub> ) <sub>4</sub>	15m	72
Potash alum, $KAl(SO_4)_2 \cdot 12H_2O$	6	36	Villiaumite, NaF	1	63
Powellite, $Camoo_4$	6 5 m	22	Wakefieldite, $YVO_4$	5m 7	59
Pyrite FeSo	5	29	Willemite, $2\pi_2 510_4$	2	54
*Pyroaurite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$	10m	104	Wulfenite, PbMoO <sub>4</sub>	7	23
Pyrolusite, $\beta$ -MnO <sub>2</sub>	10m	39	Wurtzite, ZnS	2	14
Pyrope, $Mg_3Al_2(SiO_4)_3$	4m	24	*Xanthoconite, Ag <sub>3</sub> AsS <sub>3</sub>	8m	126
Pyrophanite, MnTiO <sub>3</sub>	15m	42	Xenotime, YPO <sub>4</sub>	8	67
Aquartz, S10 <sub>2</sub> (d or low)	10	24 42	Zinc, Zn	$\frac{1}{2}$	10 25
Retgersite, NiSO <sub>4</sub> ·6H <sub>2</sub> O	7	36	Zinkosite $ZnSO_4$	7	64
Rhodochrosite, MnCO <sub>3</sub>	7	32	*Zircon, ZrSiO <sub>4</sub>	4	68
Romarchite, SnO	4	28	Zircosulfate, Zr(SO <sub>4</sub> ) <sub>2</sub> ·4H <sub>2</sub> O	7	66
Rutile, TiO <sub>2</sub>	7m	83			
Salammoniae MU Cl	10	28			
Sanbornite, 8-BaSiaOr	1 ] 3m	59 10			
Sanmartinite, ZnWO <sub>4</sub>	2m	40			
Scacchite, MnCl <sub>2</sub>	8m	43			
*Scheelite, CaWO <sub>4</sub>	6	23			
Schultenite, PbHAsO <sub>4</sub>	14m	18			
Selenalite Sol	5	54			
berenorite, 5602 ······	710	00	100		

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