NBS MONOGRAPH 25— SECTION 15

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

Standard X-ray Diffraction Powder Patterns

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[1]Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington,D.C. 20234.
[2]Some divisions within the center are located at Boulder, Colorado, 80303.

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Standard X-ray Diffraction Powder Patterns Section 15—Data for 112 Substances

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ERRATA

A book has been published containing card images of NBS Standard X-ray Diffraction Powder Patterns[1]. 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 2θ = 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 $\bar{3}01$.
p. 26, at d = 1.3085, hkℓ should be $\bar{6}32$.
Sec. 7, p. 60, in the paragraph "Structure," the space group should be $P4_2/mbc$.

[1]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.

NBS Publication	Number	NBS Publication	Number
Circular 539, Volume 1	PB 178 902	Monograph 25, Section 1	PB 178 429
Volume 2	PB 178 903	Section 2	PB 178 430
Volume 3	PB 178 904	Section 3	PB 178 431
Volume 4	PB 178 905	Section 4	
Volume 5	PB 178 906	Section 5	
Volume 6	PB 178 907	Section 6	
Volume 7	PB 178 908	Section 7	
Volume 8	PB 178 909	Section 8	PB 194 872
Volume 9	PB 178 910	Section 9	COM 72-50002
Volume 10	PB 178 911	Section 10	COM 72-51079
		Section 11	COM 74-50183
		Section 12	COM 75-50162
		Section 13	PB 254 073
		Section 14	PB 272 372

Also, until the present supply is exhausted, the following issues are for sale from the Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402. Order by given catalog number, and add 25% to the price, for other than U. S. mailing.

	Catalog Number	Price
Section 11	SN 003-003-01234-3	$1.55
Section 12	SN 003-003-01376-5	1.50
Section 13	SN 003-003-01629-2	1.80
Section 14	SN 003-003-01842-2	2.75

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 15. --- Data for 112 Substances

by

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Standard x-ray diffraction patterns are presented for 112 substances. Fifty-four 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,[1] 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]

EXPERIMENTAL POWDER PATTERNS

Sample. 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 2θ 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.

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[1] 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.

[2] 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 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Calculated 2θ Angles, $CuK\alpha_1$ λ = 1.540598Å

hkℓ	W a=3.16524Å ±.00004	Ag a=4.08651Å ±.00002	Si a=5.43088Å ±.00004
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.303
310	100.632		
311		77.390	56.123
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.131
331		110.499	76.377
420		114.914	
422		134.871	88.032
511/333		156.737	94.954
440			106.710
531			114.094
620			127.547
533			136.897
444			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 ± 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].

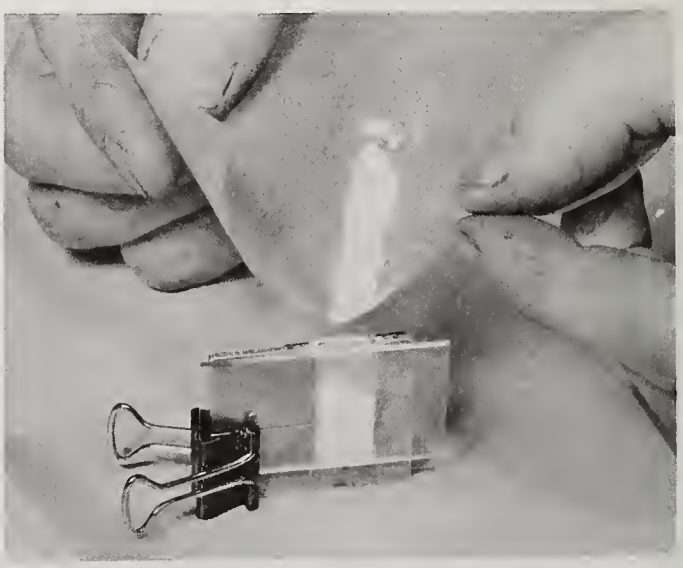
Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of *Crystal Data* [1973]. For primitive cells, the transformed cell axes are an alternate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

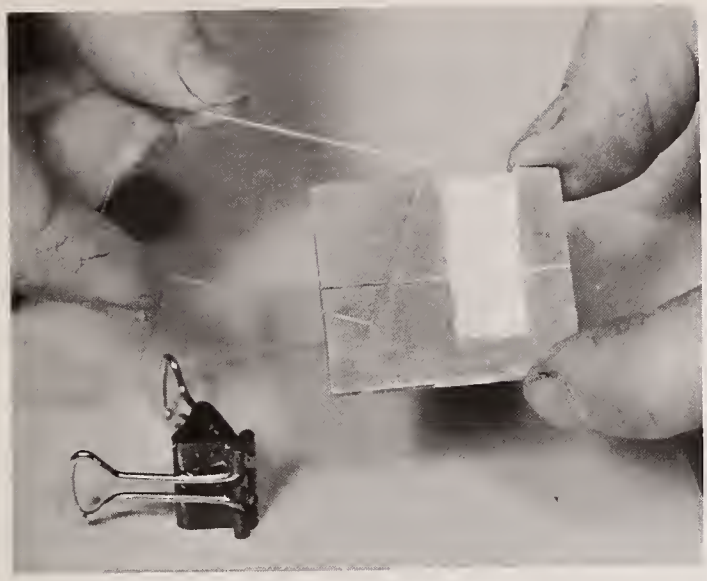
A computer program [Evans et al., 1963] assigned hkℓ's and refined the lattice constants. Cell refinement was based only upon $2\theta_{obs}$ values which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{obs}-\theta_{calc})^2$. The estimated standard deviations (e.s.d.'s) 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 h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943 x 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 μm, 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_c, 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 (α-Al_2O_3) [Visser and de Wolff, 1964]. The ratio is tabulated for copper K$\bar{\alpha}$ 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 $I(\underline{h})$ and $I(\underline{k})$ are measured for several sets of reflections $\underline{h}$ and $\underline{k}$, usually within the same region of 2θ, to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{I(\underline{h}_0)}{I_c(113)} = \frac{x_c}{x_s} \cdot \frac{I_c^{rel}(\underline{k})}{I^{rel}(\underline{h})} \cdot \frac{I(\underline{h})}{I(\underline{k})}$$

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 $\langle I/I_c \rangle$. From these data, the e.s.d., Δ, 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 d-spacing 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 Crystal Data 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.

Scattering factors. 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.

Thermal parameters. The computer program used thermal parameter data of only two forms, the isotropic B's(Å^2) or the anisotropic β_{ij}'s in the following expressions:

$$e^{(-B \sin^2\theta)/\lambda^2}$$

or

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

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:

$$B = 4\left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a^{*2}\ b^{*2}\ c^{*2}}\right]^{\frac{1}{3}}$$

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
μ 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.

Scale factor (integrated intensities). The scale factor, γ, was defined to convert the tabulated I^{rel} to the "absolute-relative" scale [Hubbard, Evans, and Smith, 1976]. That is:

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

and

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

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

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

From γ, 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 ρ is the density and the subscript c represents corundum (α-Al_2O_3).

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_c and γ 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 α_1 and the α_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 2θ. [The values of the FWHM vs 2θ 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 2θ angles and produce only one composite peak in the simulated pattern. The 2θ 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 α_2 lines were omitted. If an α_1 peak and an α_2 peak overlapped, the α_1 reflection was listed only when it contributed a significant intensity (>10%) at the peak 2θ.

The peak search routine located peaks only at 2θ angles which were a multiple of 0.02°.

2θ CuKα1	FWHM	2θ CuKα1	FWHM
0°	0.12°	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 Ångström unit (10Å=1nm) was selected for presentation of the d-spacings and lattice parameters to maintain consistence with (a) the earlier publications of Standard X-ray 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 Å of the three strongest lines. Consistent with the choice of the Å unit for length, the volume of the unit cell is expressed in $Å^3$ (=1 x 10^{-30} m^3). Other reported parameters and their units are density in g/cm^3 (1 gm/cm^3 = 10^{-3} kg/m^3) and the linear absorption coefficient in cm^{-1}.

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International Union of Pure and Applied Chemistry (1972). Pure Appl. Chem. *30*, Nos. 3-4, 639.

ISCC-NBS Centroid Color Charts, SRM 2106, or Color Kit, SRM 2107 which contains both SRM 2106 and *Color*, an NBS Special Publication #SP440. These can be obtained from the National Bureau of Standards, Office of Standard Reference Materials, Washington, D. C. 20234. Current prices will be quoted on request.

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Aluminum Iron Oxide, $AlFeO_3$

Sample
The sample was prepared by mixing solutions of $Al(NO_3)_3$, $Fe(NO_3)_3$, and NH_4OH. Hydroxides of aluminum and iron precipitated and were heated 1/2 hr. at 1350 °C.

Color
Gray brown.

Structure
Orthorhombic, $Pc2_1n(33)$ or Pcmn (62), Z = 8, isostructural with $GaFeO_3$ [Dayal et al., 1965].

Lattice constants of this sample:
a = 8.566(2) Å
b = 9.249(1)
c = 4.989(1)

a/b = 0.9262
c/b = 0.5394

Volume
395.2 $Å^3$

Density
(calculated) 4.397 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.04(8)

Additional patterns
1. PDF card 11-562 [Atlas and Sumida, 1958]
2. PDF card 18-633 [Dayal et al., 1965]

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$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ			2θ(°)
6.28	13	1	1	0	14.09
4.626	5	0	2	0	19.17
4.314	3	1	0	1	20.57
3.907	8	1	1	1	22.74
3.250	5	2	0	1	27.42
3.146	30	2	2	0	28.35
3.066	6	2	1	1	29.10
2.900	35	1	3	0	30.81
2.729	5	3	1	0	32.79
2.656	100	2	2	1	33.69
2.506	20	1	3	1	35.81
2.495	17	0	0	2	35.96
2.478	9	3	0	1	36.22
2.408	13	0	1	2	37.32
2.394M	25	1	0	2	37.54
2.394M		3	1	1	37.54
2.320	4	1	1	2	38.78
2.313	2	0	4	0	38.91
2.237	11	2	3	1	40.29
2.196	15	0	2	2	41.07
2.185	30	3	2	1	41.29
2.141	4	4	0	0	42.18
2.127	14	1	2	2	42.47
2.099	3	2	1	2	43.05
2.033	2	2	4	0	44.52
1.969	6	4	0	1	46.07
1.940	15	0	3	2	46.80
1.931	17	3	3	1	47.01
1.891	8	1	3	2	48.09
1.879	3	3	0	2	48.41
1.8085	6	1	5	0	50.42
1.7676	4	2	3	2	51.67
1.6959	12	0	4	2	54.03
1.6915	16	3	4	1	54.18
1.6243	2	4	0	2	56.62
1.5519	2	3	5	0	59.52
1.5390	8	1	2	3	60.07
1.5295M	4	5	2	1	60.48
1.5295M		2	1	3	60.48
1.4974	14	5	3	0	61.92
1.4861	18	0	5	2	62.44
1.4825	40	3	5	1	62.61
1.4581	1	3	4	2	63.78
1.4370M	30	4	3	2	64.83
1.4370M		3	0	3	64.83
1.4278	10	6	0	0	65.30
1.3923	5	2	6	1	67.18
1.3847	11	2	3	3	67.60
1.3724M	3	6	0	1	68.29
1.3724M		3	2	3	68.29
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	3	2	73.71
1.2628	4	1	7	1	75.18
1.2355	3	0	1	4	77.14

Aluminum Sulfate, $Al_2(SO_4)_3$

Sample
A sample of $Al_2(SO_4)_3 \cdot 18H_2O$ was obtained from Fisher Scientific Co., New York. It was heated at 600 °C for 6 hours to produce the anhydrous salt.

Color
Colorless

Structure
Hexagonal, $R\bar{3}$ (148), Z = 6, [Thiard, 1965].

Lattice constants of this sample:
a = 8.055(1) Å
c = 21.191(5)

c/a = 2.6307

Volume
1191.0 $Å^3$

Density
(calculated) 2.863 g/cm^3

Reference intensity
$I/I_{corundum}$ = 6.0

This material showed evidence of preferred orientation for the hkℓ 119.

Additional pattern
1. PDF card 22-21 [Perret & Rosso, 1968].

References
Perret, R. and Rosso, B. (1968). Bull. Soc. Chim. France, p. 2700.
Thiard, R. (1965). Thesis of 3rd Cycle in Physical Chemistry, Dijon, France.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ			2θ(°)
5.82	35	0	1	2	15.21
4.221	14	1	0	4	21.03
4.024	1L	1	1	0	22.07
3.502	100	1	1	3	25.41
3.317	1	2	0	2	26.86
2.915	17	0	2	4	30.65
2.654	16	1	1	6	33.74
2.618	10	2	1	1	34.22
2.560	1	1	2	2	35.02
2.361	3	2	1	4	38.08
2.327	20	3	0	0	38.66
2.285	1	0	2	7	39.40
2.209	5	3	0	3	40.82
2.033	40	1	1	9	44.53
1.989	2	2	1	7	45.57
1.942	3	3	0	6	46.75
1.903	1	3	1	2	47.76
1.8693	2	1	2	8	48.67
1.8169	2	1	3	4	50.17
1.7660	1	0	0	12	51.72
1.7494	3	2	2	6	52.25
1.7209	1	0	4	2	53.18
1.6522	3	2	1	10	55.58
1.6304	2	1	3	7	56.39
1.6172	1L	1	1	12	56.89
1.5957	1L	3	2	1	57.73
1.5624	1	3	1	8	59.08

Ammonium Cadmium Bromide, $(NH_4)_4CdBr_6$

Sample
The sample was obtained from The City Chemical Corporation of New York.

Color
Colorless

Structure
Hexagonal, $R\bar{3}c$ (167), Z = 6, isostructural with K_4CdCl_6. The structure of $(NH_4)_4\ CdBr_6$ was determined by Grabowski and Swaryczewski [1966].

Lattice constants of this sample:

a = 12.9313(5) Å
c = 16.206(1)
c/a = 1.2532

Volume
2436.8 $Å^3$

Density
(calculated) 2.819 g/cm^3

Reference intensity
$I/I_{corundum}$ = 3.43(10)

Additional pattern
1. PDF card 24-1455 [Hardt & Pazen, 1971].

References
Grabowski, M. and Swaryczewski, A. (1966). Soc. Sci. Lodz. Acta Chim. 11, 57.
Hardt, H. D. and Pazen, F. (1971). Z. Anorg. Allgem. Chem. 380, 16.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.57	100	012	13.47
6.47	60	110	13.67
4.605	30	202	19.26
4.145	20	113	21.42
4.096	30	211	21.68
3.810	10	104	23.33
3.751	3	122	23.70
3.283	8	024	27.14
3.235	4	220	27.55
3.051	40	131	29.25
2.928	85	214	30.51
2.901	30	312	30.80
2.774	90	223	32.24
2.702	12	006	33.13
2.573	< 1	125	34.84
2.538	1	321	35.34
2.493	4	116	36.00
2.465	11	134	36.42
2.444	20	410	36.75
2.303	6	404	39.08
2.243	3	315	40.18
2.227	2	413	40.47
2.189	14	306	41.21
2.170	14	324	41.58
2.158	7	502	41.82
2.099	3	241	43.07
2.072	16	226	43.64
2.031	10	217	44.57
2.013	2	235	45.00
1.996	11	511	45.40
1.994	13	018	45.46
1.960	4	054	46.29
1.952	12	152	46.48
1.876	4	244	48.48
1.866	14	600	48.76
1.856	10	137	49.03
1.830	7	431	49.80
1.828	9	128	49.85
1.8015	4	514	50.63
1.7952	8	342	50.82
1.7932	8	520	50.88
1.7724	4	425	51.52
1.7343	< 1	119	52.74
1.7197	2	327	53.22
1.7090	6	155	53.58
1.7017	8	523	53.83
1.6843	1	336	54.43
1.6767	1	434	54.70
1.6710	2	612	54.90
1.6413	3	048	55.98
1.6038	6	1·0·10	57.41
1.5906	1	238	57.93
1.5733	4	164,229	58.63
1.5694	3	532	58.79
1.5569	< 1	0·2·10	59.31
1.5483	2	443	59.67
1.5455	2	621	59.79
1.5350	1	606	60.24
1.5252	3	262	60.67
1.5179	2	517	60.99
1.5135	2	2·1·10	61.19
1.5112	2	615	61.29
1.5024	1	508	61.69
1.4939	3	526	62.08
1.4874	6	354	62.38
1.4632	2	428	63.53
1.4496	2	624,419	64.20
1.4412	3	437	64.62
1.4272	1	158	65.33
1.4115	2	452,630	66.15

Ammonium Cadmium Bromide, $(NH_4)_4CdBr_6$ (continued)

d(Å)	I	hkℓ	2θ(°)
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 Strontium Sulfate, $(NH_4)_2Sr(SO_4)_2$

Sample
The sample was precipitated by adding a strong solution of $SrCl_2$ to a hot solution of $(NH_4)_2SO_4$ following the method of Schwarz [1966].

Color
Colorless

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Sr_3(PO_4)_2$ and many other double chromates and sulfates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

Lattice constants of this sample:
a = 5.5321(3) Å
c = 21.964(2)

c/a = 3.9703

Volume
582.14 Å^3

Density
(calculated) 2.703 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.4(2)

Additional pattern
1. PDF card 19-71 [Schwarz, 1966]

References
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 41.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
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	2	1·1·18	87.25
1.1035	1	2·2·12	88.54
1.0978	1	048,321	89.12
1.0942	1	2·1·16,232	89.50
1.0792	2	3·0·15	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, $(NH_4)_3ZnCl_5$

Sample
The sample was prepared by slow evaporation at room temperature of a 3:1 molar aqueous solution of NH_4Cl and $ZnCl_2$.

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) Å
b = 12.638(4)
c = 8.722(3)

a/b = 0.7829
c/b = 0.6901

Volume
1090.6 $Å^3$

Density
(calculated) 1.807 g/cm^3

Reference intensity
$I/I_{corundum}$ = 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.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
7.78	45	1 1 0	11.37
7.17	13	0 1 1	12.33
6.32	8	0 2 0	14.00
5.805	75	1 1 1	15.25
5.116	65	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
2.903	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 3	33.89
2.632	15	3 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 0	36.28
2.393	6	0 3 3	37.55
2.358	20	1 5 1	38.14
2.339	6	4 1 1	38.45
2.273	8	2 4 2	39.62
2.228	6	4 2 1	40.45
2.208	6	3 4 1	40.83
2.181M	6	0 0 4	41.37
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	3 2 3	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
1.9702	8	2 1 4	46.03
1.9077M	20	5 1 1	47.63
1.9077M		0 5 3	47.63
1.8927	15	2 6 1	48.03

Antimony Bromide, α-$SbBr_3$

Sample
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 somewhat hygroscopic.

Color
Light gray

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. [Cushen and Hulme, 1964].

Lattice constants of this sample:
a = 10.162(3) Å
b = 12.388(2)
c = 4.459(1)

a/b = 0.8203
c/b = 0.3599

Volume
561.3 $Å^3$

Density
(calculated) 4.277 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.13(8)

Polymorphism
Antimony bromide, in some cases, crystallizes in a β-form which is also orthorhombic, but in space group Pbnm [Cushen and Hulme, 1962].

References

Cushen, D. W. and Hulme, R. (1962). J. Chem. Soc. 1962, 2218.
Cushen, D. W. and Hulme, R. (1964). J. Chem. Soc. 1964, 4162.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
7.88	4	1 1 0	11.22
6.20	55	0 2 0	14.28
5.289	3	1 2 0	16.75
5.087	30	2 0 0	17.42
4.701	19	2 1 0	18.86
4.199	50	0 1 1	21.14
4.085	9	1 0 1	21.74
3.931	25	2 2 0	22.60
3.879	40	1 1 1	22.91
3.829	16	1 3 0	23.21
3.622	14	0 2 1	24.56
3.413	18	1 2 1	26.09
3.352	14	2 0 1	26.57
3.269	25	3 1 0	27.26
3.235	70	2 1 1	27.55
3.204	18	2 3 0	27.82
3.098	35	0 4 0	28.79
3.031	25	0 3 1	29.45
2.970	70	3 2 0	30.06
2.966	65	1 4 0	30.11
2.949	100	2 2 1	30.28
2.904	65	1 3 1	30.76
2.698	12	3 0 1	33.18
2.646	9	2 4 0	33.85
2.603	30	2 3 1	34.43
2.539	3	4 0 0	35.32
2.488	25	4 1 0	36.07
2.468	25	1 4 1	36.37
2.409	14	1 5 0	37.30
2.287	6	3 4 0	39.37
2.258	6	3 3 1	39.89
2.227	4	2 5 0	40.47
2.165M	12	0 5 1	41.68
2.165M		4 3 0	41.68
2.118	7	1 5 1	42.65
2.097	7	0 2 2	43.11
2.064	3	0 6 0	43.82
2.033	13	3 4 1	44.52
1.999	15	3 5 0	45.32
1.993	13	2 5 1	45.48
1.873	4	0 6 1	48.57
1.842M	19	1 6 1	49.44
1.842M		3 1 2	49.44
1.824M	5	3 5 1	49.97
1.824M		5 3 0	49.97
1.808	20	0 4 2	50.42
1.782	20	1 4 2	51.23
1.7622	20	3 6 0	51.84
1.7575	19	2 6 1	51.99
1.7432	5	1 7 0	52.45
1.6967	9	3 3 2	54.00
1.6755	10	4 0 2	54.74
1.6230	7	1 7 1	56.67
1.5866	13	5 4 1	58.09
1.5677M	5	3 7 0	58.86
1.5677M		6 3 0	58.86
1.5483	7	0 8 0	59.67
1.4476	4	1 8 1	64.30

Barium Cadmium Chloride Hydrate, $BaCdCl_4 \cdot 4H_2O$

Sample
The sample was obtained from the City Chemical Corp., New York.

Color
Colorless

Structure
Triclinic. The structure of $BaCdCl_4 \cdot 4H_2O$ was studied by Brasseur and de Rossenfosse [1936]. Perloff [1977] determined the primitive triclinic cell by single crystal precession techniques.

Lattice constants of this sample:
a = 8.754(1) Å
b = 9.000(2)
c = 6.910(1)
α = 102.38(2)°
β = 98.68(2)
γ = 98.92(2)

a/b = 0.9727
c/b = .7678

Volume
515.7 $Å^3$

Density
(calculated) 2.986 g/cm^3 assuming Z = 2

References
Brasseur, H. and de Rossenfosse, A. (1936). Z. Kristallogr. Kristallgeomtrie. Kristallphys. Kristallchem. A95, 474.
Perloff, A. (1977). Private Communication.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
8.61	95	0 1 0	10.26
8.48	25	1 0 0	10.42
6.75	8	-1 1 0	13.10
6.63	4	0 0 1	13.35
6.01	14	0 -1 1	14.73
5.79	9	-1 0 1	15.29
5.53	100	1 1 0	16.01
4.996	8	-1 -1 1	17.74
4.815	35	1 -1 1	18.41
4.731	10	0 1 1	18.74
4.631	30	-1 1 1	19.15
4.312	3	0 2 0	20.58
4.184	12	-1 2 0	21.22
4.141	17	-2 1 0	21.44
4.100	4	0 -2 1	21.66
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
2.905M	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
2.865M		-1 -2 2	31.19
2.851	40	1 -3 1	31.35
2.830M	35	1 2 1	31.59
2.830M		3 0 0	31.59
2.797	40	1 -2 2	31.97
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
2.598	25	-3 -1 1	34.49
2.547M	35	3 1 0	35.21
2.547M		1 1 2	35.21
2.525	7	3 -1 1	35.53
2.495M	12	-2 -2 2	35.96
2.495M		-1 3 1	35.96
2.439	25	3 0 1	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	9	-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

d(Å)	I	hkℓ	2θ(°)
2.206+		3 1 1	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 -3 1	41.94
2.132	19	-2 0 3	42.37
2.127	25	-2 -3 2	42.47
2.121M	25	1 -1 3	42.59
2.121M		4 0 0	42.59
2.102	17	-3 3 1	42.99
2.096	14	-2 4 0	43.13
2.080M	40	1 -2 3	43.47
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	3	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
1.963M		-2 3 2	46.22
1.938	8	4 -2 1	46.84
1.932M	14	1 -3 3	47.00
1.932M		-4 1 2	47.00
1.918+	15	4 0 1	47.35
1.918+		0 4 1	47.35
1.915	10	-3 -1 3	47.44
1.902M	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
1.835	5	-4 -2 1	49.64
1.822	3	2 0 3	50.02
1.815+	2	-2 2 3	50.23
1.815+		4 -3 1	50.23
1.7958M	4	0 2 3	50.80
1.7958M		1 -5 1	50.80
1.7860M	8	2 -3 3	51.10
1.7860M		1 4 1	51.10
1.7821	6	4 1 1	51.22

Barium Chromium Oxide, $Ba_3(CrO_4)_2$

Sample
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 N_2.

Color
Blackish green

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Ba_3(PO_4)_2$ [Wilhelmi and Jonsson, 1965]. The structure of $Ba_3(PO_4)_2$ was studied by Zachariasen [1948].

Lattice constants of this sample:
a = 5.7406(5) Å
c = 21.389(3)

c/a = 3.7259

Volume
610.44 $Å^3$

Density
(calculated) 5.256 g/cm^3

Additional patterns
1. PDF card 19-120 [Banks and Jaunarajs, 1965]
2. PDF card 21-64 [Gordeev and Serdyukov, 1967]

References
Banks, E. and Jaunarajs, K. L. (1965). Inorg. Chem. 4, 78.
Gordeev, S. Ya. and Serdyukov, V. I. (1967). Inorg. Mater. USSR 3, 1440.
Wilhelmi, K.-A. and Jonsson, O. (1965). Acta Chem. Scand. 19, 177.
Zachariasen, W. H. (1948). Acta Crystallogr. 1, 263.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
7.12	1	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	0·0·15	65.39
1.4117	12	2·1·10	66.14
1.3759	1	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
Reddish purple

Structure
Orthorhombic, Fddd (70), Z = 8. The structure was determined by Hardy et al. [1971].

Lattice constants of this sample:
a = 11.915(1)Å
b = 14.778(1)
c = 7.4278(7)

a/b = 0.8063
c/b = 0.5026

Volume
1307.9 $Å^3$

Density
(calculated) 3.811 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.81(12)

Additional pattern
1. PDF card 14-697 [Hardy, 1962].

References
Hardy, A. (1962). Ann. Chim. Paris 7, 281.
Hardy, A., and Fourre, B. (1971). C. R. Acad. Sci. Paris Ser. C. 273, 1508.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.794	40	1 1 1	15.28
3.882	13	1 3 1	22.89
3.690	85	0 4 0	24.10
3.406	100	3 1 1	26.14
3.318	95	0 2 2	26.85
2.981	14	4 0 0	29.95
2.899	4	2 2 2	30.82
2.855	45	3 3 1	31.31
2.676	3	1 5 1	33.46
2.399	12	2 4 2	37.46
2.393	14	1 1 3	37.55
2.320	4	4 4 0	38.78
2.277	13	2 6 0	39.54
2.258	45	3 5 1	39.90
2.244	9	5 1 1	40.16
2.217	40	4 2 2	40.66
2.175	16	1 3 3	41.49
2.0797	9	3 1 3	43.48
2.0527	10	0 6 2	44.08
2.0015	5	1 7 1	45.27
1.9330	14	3 3 3	46.97
1.9183	7	6 2 0	47.35
1.8751	4	1 5 3	48.51
1.8572	8	0 0 4	49.01
1.8469	8	0 8 0	49.30
1.8078	11	3 7 1	50.44
1.7512	6	6 0 2	52.19
1.7236	2	2 2 4	53.09
1.7126	7	3 5 3	53.46
1.6901	6	4 6 2	54.23
1.6591	7	0 4 4	55.33
1.6484	5	7 1 1	55.72
1.5936	3	2 8 2	57.81
1.5891	4	1 9 1	57.99
1.5824	10	6 4 2	58.26
1.5755	9	4 0 4	58.54
1.5723	10	7 3 1	58.67
1.5457M	5	6 6 0	59.78
1.5457M		5 7 1	59.78
1.4893M	6	8 0 0	62.29
1.4893M		3 7 3	62.29
1.4868	8	3 9 1	62.41
1.4670	2	1 1 5	63.35
1.4498	6	4 4 4	64.19
1.4464M	8	7 5 1	64.36
1.4464M		4 8 2	64.36
1.3962	3	7 1 3	66.97
1.3852	5	3 1 5	67.57
1.3729	5	0 10 2	68.26
1.3595M	2	1 9 3	69.03
1.3595M		8 2 2	69.03
1.3487	4	7 3 3	69.66
1.3388	4	3 3 5	70.25
1.3340	5	6 2 4	70.54
1.3192	2	1 5 5	71.45
1.3140	2	1 11 1	71.78
1.3099	3	0 8 4	72.04
1.3046	4	7 7 1	72.38
1.2939	4	3 9 3	73.07
1.2709	1	6 8 2	74.62
1.2672	4	7 5 3	74.87
1.2588	3	3 5 5	75.46
1.2544	3	3 11 1	75.77
1.2473	3	4 10 2	76.28
1.2312	2	0 12 0	77.46

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

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) Å
c = 17.897 (1)

c/a = 2.5293

Volume
776.0 Å^3

Density
(calculated) 3.176 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.36(12)

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

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

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
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
2.316	14	210	38.85
2.296	45	211	39.20
2.280	7	116	39.49
2.241	55	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	3	221	51.91
1.736	9	222	52.69
1.717	15	1·0·10,217	53.31
1.700	16	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	3	2·0·10	59.81
1.5355	7	315	60.22
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

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

d(Å)	I	hkℓ	2θ(°)
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
1.3086	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
1.2516	6	1•0•14	75.97
1.2320	2	3•1•10,327	77.40
1.2228	3	501	78.09
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
1.1798	4	2•0•14,330	81.52
1.1754	5	3•1•11	81.89
1.1711	3	1•0•15	82.26
1.1593	2	505	83.28
1.1557	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
1.1117	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

Beryllium Sulfate, $BeSO_4$

Sample
Beryllium nitrate was treated with H_2SO_4 and evaporated. The process was repeated and the sample recrystallized from water. The tetrahydrate so formed was dehydrated at 44 °C for over an hour.

Color
Colorless

Structure
Tetragonal, $I\bar{4}(82)$, Z = 2. The structure was studied by powder and single crystal methods [Grund, 1955; Kokkoros, 1956].

Lattice constants of this sample:
a = 4.4927(4) Å
b = 6.8937(8)

c/a = 1.6059

Volume
139.14 $Å^3$

Density
(calculated) 2.507 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.9(2)

Additional patterns
1. PDF card 15-612 [Petersen, D. R., Rinn, H. W. and Sutton (1963. Dow Chemical Co., Midland, Michigan 48640].
2. Grund, A. [1955].

References
Grund, A. (1955). Tschermak's Mineral. Petrogr. Mitt. 5, 227.
Kokkoros, P. (1956). Tschermak's Mineral. Petrogr. Mitt. 6, 116.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ			2θ(°)
3.765	100	1	0	1	23.61
3.449	5	0	0	2	25.81
3.177	3	1	1	0	28.06
2.336	30	1	1	2	38.51
2.0457	2	1	0	3	44.24
1.9287	10	2	1	1	47.08
1.8817	6	2	0	2	48.33
1.7227	1L	0	0	4	53.12
1.5879	2	2	2	0	58.04
1.5126	10	2	1	3	61.23
1.4639	1L	3	0	1	63.50
1.4432	2	2	2	2	64.52
1.4203	2	3	1	0	65.69
1.3675	4	2	0	4	68.57
1.3134	2	3	1	2	71.82
1.2544	2	3	0	3	75.77
1.2261	4	3	2	1	77.84
1.1680	1L	2	2	4	82.52
1.1369	2	2	1	5	85.30
1.0956	2	3	2	3	89.35
1.0804	1	1	1	6	90.95
1.0764	2	4	1	1	91.39
1.0681	1	4	0	2	92.31
1.0590	1L	3	3	0	93.34
1.0229	1	2	0	6	97.71
1.0142	2	3	0	5	98.84
1.0123	1	3	3	2	99.10
1.0044	1	4	2	0	100.16
.9845	1L	4	1	3	102.96

Cadmium Titanium Oxide, $CdTiO_3$

Sample
The sample was prepared by heating a 1:1 mixture of TiO_2, anatase, and CdO in a torch, then heating in a furnace at 700 °C for approximately 65 hours.

Color
Colorless

Structure
Hexagonal, $R\bar{3}(148)$, Z = 6, isostructural with ilmenite, $FeTiO_3$. The structure of $FeTiO_3$ was determined by Barth and Posnjak [1934].

Lattice constants of this sample:
a = 5.2403(1) Å
c = 14.8380(6)

c/a = 2.8315

Volume
352.87 $Å^3$

Density
(calculated) 5.881 g/cm^3

Reference intensity
$I/I_{corundum}$ = 5.0(3)

Polymorphism
According to Posnjak and Barth [1934], a high temperature perovskite modification found by Zachariasen [1928] exists when $CdTiO_3$ is prepared at temperatures above 1050 °C.

Additional patterns
1. PDF card 3-818 [Megan, H. D., Philips Lamps Ltd.].
2. Posnjak and Barth [1934].

References

Barth, T. F. W. and Posnjak, E. (1934). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 88A, 265.

Posnjak, E. and Barth, T. F. W. (1934). Ibid. 271.

Zachariasen, W. H. (1928). Skr. Nor. Vidensk. Akad. Oslo, No. 4.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.946	7	0 0 3	17.92
4.344	18	1 0 1	20.43
3.870	14	0 1 2	22.96
2.873	100	1 0 4	31.11
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
1.9206	8	1 0 7	47.29
1.7985	25	1 1 6	50.72
1.7171	14	0 1 8	53.31
1.7040	5	2 1 1	53.75
1.6707	2	1 2 2	54.91
1.5569	30	2 1 4	59.31
1.5490	4	0 2 7	59.64
1.5130	20	3 0 0	61.21
1.4851	3	1 2 5	62.49
1.4466	2	3 0 3	64.35
1.4360	4	2 0 8	64.88
1.4102	6	1 0 10	66.22
1.3951	4	1 1 9	67.03
1.3335	4	2 1 7	70.57
1.3100	8	2 2 0	72.03
1.2930	3	0 1 11	73.13
1.2901	4	3 0 6	73.32
1.2664	2	2 2 3	74.93
1.2593	6	1 2 8	75.42
1.2540	2	1 3 1	75.80
1.2419	5	0 2 10	76.67
1.1918	10	1 3 4	80.53
1.1591M	5	2 0 11	83.30
1.1591M		3 1 5	83.30
1.1576	5	2 2 6	83.43
1.1312	1L	4 0 1	85.84
1.1220	5	2 1 10	86.71
1.1181	4	1 1 12	87.09
1.0849	5	4 0 4	90.47
1.0823	6	1 3 7	90.75
1.0604	4	1 2 11	93.18
1.0415	7	3 1 8	95.40
1.0385	5	3 2 1	95.76
1.0321	3	0 1 14	96.55
1.0257	1L	2 2 9	97.36
1.0024	9	3 2 4	100.43
.9903	11	4 1 0	102.13
.9824	1	2 3 5	103.27
.9711	3	4 1 3	104.97
.9680	3	0 4 8	105.46
.9602	8	2 0 14	106.69
.9345	1	3 2 7	111.03
.9256	4	1 1 15	112.66
.9194	8	4 1 6	113.83
.9079	4	2 3 8	116.09
.9016	7	1 2 14	117.38
.8817	5	0 5 4	121.78
.8734	5	3 3 0	123.76

Calcium Chromium Oxide, $Ca_3(CrO_4)_2$

Sample
The sample was prepared by heating a 3:1 molar mixture of $CaCO_3$ and Cr_2O_3 at 950 °C for 6 days, with intermittent grindings.

Color
Black

Structure
Hexagonal, $R\bar{3}c$ (167), Z = 21. The structure has been studied by Sinha and Srivastava [1973]. Earlier the formula was given as $Ca_9Cr_6O_{24}$ (or $9CaO \cdot 4CrO_3 \cdot Cr_2O_3$) to suggest that the chromium was present in two valences. Glasser and Osborn [1958] suggested the probability that all Cr ions were in a valence of 5 and that the structure is closely related to $Ca_3(PO_4)_2$ (whitlockite).

Lattice constants of this sample:
a = 10.779(1) Å
c = 38.099(8)

c/a = 3.5346

Volume
3833.6 $Å^3$

Density
(calculated) 3.204 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.00(7)

Additional patterns
1. PDF card 11-415 [Glasser & Osborn, 1958]
2. PDF card 25-130 [British Steel Corp., Rotherham, England]
3. Ford & Rees [1949]
4. Sinha and Srivastava [1973]

References
Ford, W. F. and Rees, W. J., (1949). Trans. Brit. Ceram. Soc. 48 291.
Glasser, F. P. and Osborn, E. F., (1958). J. Am. Ceram. Soc. 41 358.
Sinha, D. P. and Srivastava, B. C. (1973). Indian J. Phys. 47 746.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
8.39	9	0 1 2	10.54
6.66	9	1 0 4	13.29
5.391	25	1 1 0	16.43
4.962	2	1 1 3	17.86
4.535	14	2 0 2	19.56
4.237	8	0 1 8	20.95
4.193	20	0 2 4	21.17
4.115	4	1 1 6	21.58
3.524	40	1 0 10	25.25
3.469	3	1 2 2	25.66
3.308	50	2 1 4	26.93
3.176	4	0 0 12	28.07
3.109	10	3 0 0	28.69
2.951	100	0 2 10	30.26
2.834	25	1 2 8	31.54
2.795	6	3 0 6	32.00
2.736	10	1 1 12	32.71
2.694	75	2 2 0	33.23
2.636	6	2 2 3	33.98
2.612	4	0 1 14	34.30
2.588	16	2 1 10	34.63
2.480	10	2 2 6	36.19
2.453	5	3 1 5	36.60
2.351	2	2 0 14	38.26
2.315	6	0 4 2	38.87
2.308	10	1 0 16	38.99
2.273M	4	3 1 8	39.61
2.273M		2 2 9	39.61
2.269	5	4 0 4	39.70
2.222	5	3 0 12	40.57
2.139	4	3 2 1	42.22
2.129	5	2 3 2	42.43
2.122	3	0 2 16	42.57
2.096	8	0 4 8	43.12
2.091	7	3 2 4	43.24
2.054	2	2 2 12	44.06
2.011	3	4 1 3	45.05
1.990	30	4 0 10	45.54
1.953	6	2 3 8	46.45
1.940M	14	1 3 13	46.80
1.940M		4 1 6	46.80
1.876	4	3 1 14	48.48
1.868M	12	3 2 10	48.72
1.868M		0 1 20	48.72
1.8323	11	0 5 4	49.72
1.7972	2	3 3 0	50.76
1.7785	2	3 3 3	51.33
1.7638	35	2 0 20	51.79
1.7509	7	3 0 18	52.20
1.7382	7	5 0 8	52.61

Calcium Chromium Oxide, $Ca_3(CrO_4)_2$

d(Å)	I	hkℓ	2θ(°)
1.7352	8	2 4 4	52.71
1.7150	4	4 1 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 16	55.07
1.6525M	6	5 1 4	55.57
1.6525M		3 3 9	55.57
1.6007	12	2 4 10	57.53
1.5924	10	3 2 16	57.86
1.5819	5	1 5 8	58.28
1.5629	3	3 3 12	59.06
1.5557	8	6 0 0	59.36
1.5339M	3	3 1 20	60.29
1.5339M		4 3 1	60.29
1.5150	5	4 3 4	61.12
1.4943	2	5 2 0	62.06
1.4755	7	0 4 20	62.94
1.4672M	5	4 1 18	63.34
1.4672M		3 3 15	63.34
1.4604	4	3 4 8	63.67
1.4550M	8	5 1 13	63.93
1.4550M		5 2 6	63.93
1.4231+	6	4 3 10	65.54
1.4231+		2 3 20	65.54

Calcium Fluoride Phosphate Hydrate, $CaFPO_3 \cdot 2H_2O$

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 overnight. The crystallites were dried in a dessicator.

*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

Structure
Triclinic, $P\bar{1}(2)$, Z = 2. The structure was determined by Perloff [1972].

Optical data
Biaxial (+), N_α = 1.485, N_β = 1.495, N_γ = 1.512. 2V is large.

Lattice constants of this sample:
a = 6.225(2) Å
b = 8.378(2)
c = 5.738(1)
α = 93.31(2)°
β = 114.75(2)
γ = 109.07(2)

a/b = 0.7430
c/b = 0.6849

Volume
250.17 $Å^3$

Density
(calculated) 2.311 g/cm^3

Reference
Perloff, A.(1972). Acta Crystallogr. B28, 2183.

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

d(Å)	I*	hkℓ	2θ(°)
7.69	100	0 1 0	11.50
5.211	2	1 0 0	17.00
4.971	7	-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 0	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
2.849	30	-1 -2 1	31.37
2.820	4	-2 1 0	31.70
2.782M	7	0 2 1	32.15
2.782M		-2 2 1	32.15
2.697	13	-2 2 0	33.19
2.606	30	2 0 0	34.39
2.590	24	0 -1 2	34.60
2.569	1L	0 3 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
2.472	6	-2 1 2	36.32
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	39.79
2.157	1L	-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
2.017	3	1 3 0	44.91
1.952M	10	-2 4 0	46.48
1.952M		1 0 2	46.48
1.927	7	0 4 0	47.13
1.898	8	-3 3 1	47.90
1.8526	6	2 2 0	49.14
1.8282	2	-2 1 3	49.84
1.7863	5	-1 1 3	51.09
1.7750	4	-1 -2 3	51.44
1.7463M	5	-3 -1 2	52.35
1.7463M		-3 -1 1	52.35
1.7355	4	0 -4 2	52.70
1.7141	1	-1 -4 1	53.41
1.6915M	6	-3 4 1	54.18

d(Å)	I*	hkℓ	2θ(°)
1.6915M		0 0 3	54.18
1.6801M	2	0 4 1	54.58
1.6801M		1 3 1	54.58
1.6652M	4	-1 5 0	55.11
1.6652M		-2 -2 3	55.11
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	3 0 1	64.14
1.4443	2	0 -4 3	64.46
1.4321+	2	-4 0 1	65.08
1.4321+		-2 0 4	65.08
1.4255+	2	-4 1 3	65.42
1.4255+		-2 -4 2	65.42
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

Cesium Iodate, $CsIO_3$

Sample
The compound was made by reacting HIO_3 with Cs_2CO_3, filtering and drying.

Color
Colorless

Structure
Cubic, Pm3m (221), Z = 1. It is a perovskite type structure [Zachariasen, 1928].

Lattice constant of this sample:
a = 4.6736(2) Å

Volume
102.08 $Å^3$

Density
(calculated) 5.007 g/cm^3

Reference intensity
$I/I_{corundum}$ = 7.7(4)

Additional pattern
1. PDF card 20-279 [Bousquet et al., 1967].

References
Bousquet, J., Rivière, R. and Remy, J.-C. (1967). C. R. Acad. Sci. Ser. C 265, 712.
Zachariasen, F. W. H. (1928). Skr. Nor. Vidensk. Akad. Oslo 1, #4.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.665	2	1 0 0	19.01
3.303	100	1 1 0	26.97
2.697	3	1 1 1	33.19
2.336	30	2 0 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	3 0 0	59.24
1.4783	16	3 1 0	62.81
1.4092	1	3 1 1	66.27
1.3494	4	2 2 2	69.62
1.2967	1L	3 2 0	72.89
1.2491	15	3 2 1	76.15
1.1684	1	4 0 0	82.49
1.1336	1L	4 1 0	85.61
1.1013	5	3 3 0	88.76
1.0719	1	3 3 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 3 0	111.00
.9166	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

Chromium Phosphate Hydrate, $CrPO_4 \cdot 6H_2O$

Sample
The sample was prepared at the National Institutes of Health using a modified method of Joseph and 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, the material was recrystallized out of solution with $(NH_4)_2HPO_4$.

Color
Purplish gray

Optical data
Biaxial(-). N_α=1.568, N_β=1.592, N_γ=1.599, 2V≈15°.

Structure
Monoclinic, A2/a(15), Z = 8. This appears to be isostructural with $MgSO_4 \cdot 6H_2O$. The initial lattice constants were obtained by using a syntex $P2_1$ diffractometer.

Lattice constants of this sample:
a = 23.473(5) Å
b = 6.890(1)
c = 9.882(2)
β = 99.42(2)°

a/b = 3.4069
c/b = 1.4343

Volume
1576.76 $Å^3$

Density
(calculated) 2.149 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.21(8)

Additional pattern
1. PDF card 5-312 [Swanson and Fuyat, 1951] [Sullivan and McMurdie, 1952]

References
Joseph, A. F. and Rae, W. N. (1917). J. Chem. Soc. III, 196.
Ness, A.T., Smith, R. E., and Evans, R. L. (1952). J. Am. Chem. Soc. 74, 4685.
Swanson, H. E. and Fuyat, R. K., (1951). Joint Committee Fellowship Report, Nat'l. Bur. Stand., U.S., October.
Sullivan, B.M. and McMurdie, H. F. (1952). J. Res. Nat. Bur. Stand. 48No.2, 159.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.783	7	4 0 0	15.31
5.622	25	0 1 1	15.75
5.349	11	1 1 1	16.56
5.257	25	-2 1 1	16.85
4.876M	40	2 1 1	18.18
4.876M		0 0 2	18.18
4.779	18	-2 0 2	18.55
4.356	11	3 1 1	20.37
4.237	100	-4 1 1	20.95
4.066	25	-4 0 2	21.84
3.855M	45	6 0 0	23.05
3.855M		4 1 1	23.05
3.756	7	-5 1 1	23.67
3.460	30	4 0 2	25.73
3.446	25	0 2 0	25.83
3.408	3	1 2 0	26.13
3.334	6	-6 1 1	26.72
3.300M	6	2 2 0	27.00
3.300M		-6 0 2	27.00
3.050	6	6 1 1	29.26
2.970	6	-1 1 3	30.06
2.956	8	-2 1 3	30.21
2.939	6	0 1 3	30.39
2.893M	7	-3 1 3	30.88
2.893M		8 0 0	30.88
2.826	20	-1 2 2	31.64
2.812M	25	0 2 2	31.80
2.812M		6 0 2	31.80
2.795M	30	-2 2 2	32.00
2.795M		-4 1 3	32.00
2.762M	3	5 2 0	32.39
2.762M		1 2 2	32.39
2.728	5	-3 2 2	32.80
2.689	13	-8 0 2	33.29
2.677M	11	-8 1 1	33.45
2.677M		2 2 2	33.45
2.569M	10	6 2 0	34.90
2.569	10	3 2 2	34.90
2.525	2	-6 1 3	35.53
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			2θ(°)
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	3	40.35
2.233+		-1	3	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	7	2	3	1	41.42
2.178M		6	2	2	41.42
2.169	6	-3	3	1	41.61
2.121	5	-8	2	2	42.60
2.113	4	-4	3	1	42.76
2.097	1	-9	1	3	43.11
2.060	2	4	3	1	43.92
2.035M	4	-8	0	4	44.49
2.035M		-11	1	1	44.49
2.006M	2	-2	2	4	45.17
2.006M		-1	2	4	45.17
1.994	3	-9	2	2	45.44
1.992	3	-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	6	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		-6	2	4	48.57
1.8554	2	1	3	3	49.06
1.8431	1L	-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	0	2	53.83
1.7017+		-8	1	5	53.83
1.6832M	2	12	2	0	54.47
1.6832M		5	3	3	54.47
1.6668	2	-12	2	2	55.05

Cobalt Hydroxide, β-$Co(OH)_2$

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 H_2O and dried at 150 °C.

Color
Reddish gray

Structure
Hexagonal, $P\bar{3}m1$ (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 $Å^3$

Density
(calculated) 3.781 g/cm^3

Reference intensity
$I/I_{corundum}$ 1.5(3)

Polymorphism
There is a less stable, blue-green form, called α [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. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 93, 368.
Weiser, H. B., and Milligan, W. O. (1932). J. Phys. Chem. 36, 729.

CuKα1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
4.653	60	0 0 1	19.06
2.755	45	1 0 0	32.47
2.371	100	1 0 1	37.92
2.327	7	0 0 2	38.67
1.7776	45	1 0 2	51.36
1.5911	35	1 1 0	57.91
1.5507	4	0 0 3	59.57
1.5059	25	1 1 1	61.53
1.3786	5	2 0 0	67.94
1.3512	13	1 0 3	69.51
1.3213	13	2 0 1	71.32
1.3138	6	1 1 2	71.79

Cobalt Tin Oxide, Co_2SnO_4

Sample
The sample was prepared by treating a mixture of the metals with HNO_3 and heating the resultant nitrates at 1000 °C for 35 hours. There were weak lines of SnO_2 and Co_3O_4 present.

Color
Black

Structure
Cubic, Fd3m (227), Z = 8, spinel structure [Natta and Passerini, 1929].

Lattice constants of this sample:
a = 8.6376(3) A

Volume
644.43 A^3

Density
(calculated) 6.196 g/cm^3[3]

Reference intensity
$I/I_{corundum}$ = 3.5(2)

Additional patterns
1. PDF card 1-1137 [Hanawalt et al., 1938]
2. PDF card 2-1391 [Natta and Passerini, 1929]

References
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Natta, G. and Passerini, L. (1929). Gazz, Chim. Ital. 59 640.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ			2θ(°)
4.987	25	1	1	1	17.77
3.056	15	2	2	0	29.20
2.605	100	3	1	1	34.40
2.493	20	2	2	2	35.99
2.1593	30	4	0	0	41.80
1.9820	4	3	3	1	45.74
1.7632	7	4	2	2	51.81
1.6621	30	5	1	1	55.22
1.5268	45	4	4	0	60.60
1.4599	5	5	3	1	63.69
1.3655	1	6	2	0	68.68
1.3172	9	5	3	3	71.58
1.3021	8	6	2	2	72.54
1.2466	5	4	4	4	76.33
1.2097	2	7	1	1	79.10
1.1542	1	6	4	2	83.73
1.1243	15	7	3	1	86.49
1.0796	4	8	0	0	91.04
1.0178	1	8	2	2	98.37
.9975	9	7	5	1	101.11
.9909	4	6	6	2	102.04
.9658	6	8	4	0	105.80

Creatinine, $C_4H_7N_3O$

Synonym
2-amino-1,5-dihydro-1-methyl-4H-imidazol-4-one

Sample
NBS standard reference material #914. The material seemed to deteriorate somewhat under exposure to x-rays, i.e. peak heights would decrease if the same sample were re-run.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure was determined by du Pré & Mendel [1955].

Lattice Constants of this sample:
a = 11.432(2) Å
b = 5.931(2)
c = 8.019(2)
β = 96.29(2)°

a/b = 1.9275
c/b = 1.3520

Volume
540.4 $Å^3$

Density
(calculated) 1.390 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.46(10)

Additional pattern
1. PDF card 7-724 [du Pré and Mendel, 1955]

Reference
du Pré, S. and Mendel, J. (1955). Acta Crystallogr. 8, 311.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.89	35	-1 0 1	12.84
6.21	25	1 0 1	14.24
5.690	1	2 0 0	15.56
5.257	30	1 1 0	16.85
4.754	1	0 1 1	18.65
4.496	40	-1 1 1	19.73
4.103	5	2 1 0	21.64
3.775	12	-2 1 1	23.55
3.537	2	2 1 1	25.16
3.445	100	-2 0 2	25.84
3.308	8	0 1 2	26.93
3.257	75	-1 1 2	27.36
3.191	1	3 1 0	27.94
3.108	1	2 0 2	28.70
3.061	8	-3 1 1	29.15
2.980	20	-2 1 2	29.96
2.868	2	1 2 0	31.16
2.842	1	4 0 0	31.45
2.779	2	0 2 1	32.18
2.723	3	-1 2 1	32.86
2.676	2	1 2 1	33.46
2.630	2	2 2 0	34.06
2.562	2	4 1 0	34.99
2.512	4	-4 1 1	35.71
2.442	1	-4 0 2	36.78
2.423M	2	0 1 3	37.07
2.423M		-1 1 3	37.07
2.385	2	3 1 2	37.68
2.332	1	3 2 0	38.57
2.317	1	-2 1 3	38.84
2.297M	1	-3 0 3	39.19
2.297M		1 2 2	39.19
2.247	3	-2 2 2	40.09
2.202M	1	3 2 1	40.96
2.202M		4 0 2	40.96
2.122	1	5 1 0	42.56
2.071	1	3 0 3	43.68
2.051	1L	4 2 0	44.13
2.000	2	5 1 1	45.30
1.979	1	0 2 3	45.82
1.957M	2	3 2 2	46.36
1.957M		-5 1 2	46.36
1.944	1	-4 1 3	46.69
1.9179M	2	-2 2 3	47.36
1.9179M		0 3 1	47.36
1.8857	1	-4 2 2	48.22
1.8278	2	-5 0 3	49.85
1.8156	2	-3 2 3	50.21
1.8008	1	-6 1 1	50.65
1.7644	4	-3 1 4	51.77

Iron Carbonate, Siderite, $FeCO_3$

Sample
The sample was a natural mineral from Ivigtut, Greenland, U. S. Nat. Museum #132849. X-ray spectrographic analysis indicated that it contained from 1 to 2% of Mn.

Color
Light yellowish brown

Structure
Hexagonal, $R\bar{3}c(167)$, Z = 6, isostructural with calcite ($CaCO_3$) and other bivalent carbonates. The structure was determined by Erenburg and Samilov [1963].

Lattice constants of this sample:
a = 4.6935(2) Å
c = 15.3860(8)

c/a = 3.2782

Volume
293.53 $Å^3$

Density
(calculated) 3.932 g/cm^3

Additional pattern
1. PDF card 8-133 [Andrews, United Steel Co., Ltd.]

Reference
Erenburg, B. G. and Samilov, O. Ya. (1963). Zh. Strukt. Khim. 4, 868.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
3.593	25	0 1 2	24.76
2.795	100	1 0 4	32.00
2.564	1L	0 0 6	34.97
2.346	20	1 1 0	38.34
2.134	20	1 1 3	42.32
1.9650	20	2 0 2	46.16
1.7968	12	0 2 4	50.77
1.7382	30	0 1 8	52.61
1.7315	35	1 1 6	52.83
1.5291	3	2 1 1	60.50
1.5063	14	1 2 2	61.51
1.4390	3	1 0 10	64.73
1.4266	11	2 1 4	65.36
1.3969	6	2 0 8	66.93
1.3818	3	1 1 9	67.76
1.3548	11	3 0 0	69.30
1.2823	5	0 0 12	73.84
1.2593	1	2 1 7	75.42
1.2269	3	0 2 10	77.78
1.2002	5	1 2 8	79.85
1.1977	4	3 0 6	80.05
1.1737	2	2 2 0	82.04
1.1254	4	1 1 12	86.39
1.1154	1	3 1 2	87.36
1.0872	3	2 1 10	90.23
1.0820	5	1 3 4	90.78
1.0671	4	2 2 6	92.42
.9825	5	4 0 4	103.26
.9724	5	3 1 8	104.78
.9666	2	2 0 14	105.68
.9358	2	1 0 16	110.80
.9309	6	3 2 1	111.68
.9256	3	2 3 2	112.66

Iron Phosphate, $FePO_4$

Sample
It was prepared by treating Na_2HPO_4 with $FeCl_3$, in solution. The resulting precipitate was dried at 100°C, then heated about 5 minutes at 1100°C.

Color
Yellowish white

Structure
Hexagonal, $P3_12_1$ (152), Z = 3, analogous to the structure of low quartz [Cagliotti, 1935]. Because of the ordering of the cations, the lattice parameter "c" is double the size of the "c" of the analogous quartz phase.

Lattice constants of this sample:
a = 5.0347(4)Å
c = 11.245(1)

c/a = 2.2335

Volume
246.86 $Å^3$

Density
(calculated) 3.044 g/cm^3

Polymorphism
PDF card 3-379 is labelled $FePO_4$ [Hanawalt et al., 1938]. It appears to be a mixture, or an entirely different phase.

An inversion from low to high temperature phase takes place at 707±5°C, analogous to the similar inversion from α- to β-quartz. No inversions to other forms were found.

Additional patterns
1. PDF card 17-837 [Schafer et al., 1956]
2. PDF card 18-649 [Kleber et al., 1965] (composition uncertain)

References

Cagliotti, V. (1935). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. 22, 146.

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Kleber, W., Wilde, W., and Frenzel, M. (1965). Chem. Erde 24, 77.

Schafer, E. C., Schafer, M. W., and Roy, R. (1956). Z. Kristallogr. Kristallgeometrie, Kristallphys. Kristallchem. 108, 263.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
4.360	19	1 0 0	20.35
4.066	2	1 0 1	21.84
3.750	2	0 0 3	23.71
3.445	100	1 0 2	25.84
2.843	1L	1 0 3	31.44
2.518	7	1 1 0	35.63
2.458	1	1 1 1	36.53
2.362	14	1 0 4	38.07
2.298	7	1 1 2	39.17
2.180	10	2 0 0	41.38
2.142	1L	2 0 1	42.16
2.090	1L	1 1 3	43.25
2.0335	3	2 0 2	44.52
1.9986	2	1 0 5	45.34
1.8846	12	2 0 3	48.25
1.7221M	6	2 0 4	53.14
1.7221M		1 0 6	53.14
1.6772	1	1 1 5	54.68
1.6304	1	2 1 1	56.39
1.5814	8	2 1 2	58.30
1.5081M	3	2 1 3	61.43
1.5081M		1 0 7	61.43
1.5035	2	1 1 6	61.64
1.4214M	10	2 1 4	65.63
1.4214M		2 0 6	65.63
1.4068	4	3 0 2	66.40
1.3376	3	1 0 8	70.32
1.2912	2	3 0 4	73.25
1.2588	1L	2 2 0	75.46
1.2375	2	2 1 6	76.99
1.2273	2	1 1 8	77.75
1.2093	2	3 1 0	79.13
1.0889	1	1 0 10	90.05
1.0699	2	4 0 2	92.11
1.0449	1L	2 2 6	94.99
1.0268	1L	1 1 10	97.21
1.0160M	2	4 0 4	98.60
1.0160M		3 1 6	98.60

Iron Titanium Oxide (Ilmenite), $FeTiO_3$

Sample

The sample was prepared at NBS by W. S. Brower. High purity α-Fe_2O_3 and TiO_2 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_2 and 5% H_2. The middle pellet was ground and leached in dilute HCl to remove faint trace of Fe.

Color

Gray, metallic

Structure

Hexagonal, $R\bar{3}(148)$, 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 $Å^3$

Density

(calculated) 4.784 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.77(11)

Additional patterns

1. 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. 88A, 265.

Michel, A. and Pouillard, E. (1948). Bull. Soc. Chim. Fr. 15, 962.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
3.737	30	0 1 2	23.79
2.754	100	1 0 4	32.49
2.544	70	1 1 0	35.25
2.349	2	0 0 6	38.29
2.237	30	1 1 3	40.28
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

Lanthanum Titanium Oxide, $La_2Ti_2O_7$

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, $P2_1(4)$ or $P2_1/m(11)$, Z = 4. The structure was determined by Gasperin [1975] and the compound was shown to be isostructural with monoclinic $Ca_2Nb_2O_7$. $La_2Ti_2O_7$ could be indexed on a pseudo-orthorhombic cell $a_o=4a_m\sin\beta$, $b_o=b_m$, $c_o=c_m$ like the $Ca_2Nb_2O_7$ 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 $Ca_2Nb_2O_7$: $a_o\approx 2a_m\sin\beta$, $b_o=b_m$, $c_o=c_m/2$, $\beta\approx 90°8'$ which would index the data when weak $\ell=2n+1$ 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

Volume
557.80 $Å^3$

Density
(calculated) 5.782 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.7(1)

Additional patterns
1. PDF card 27-1182 [Nanot et al., 1974]
2. MacChesney and Sauer [1962]
3. Roth [1956]

References

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

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
12.84	7	1 0 0	6.88
6.426	10	2 0 0	13.77
5.095	8	1 1 0	17.39
4.201	40	2 1 0	21.13
4.014	4	-3 0 1	22.13
3.864M	11	0 0 2	23.00
3.864M		-1 0 2	23.00
3.546	2	2 1 1	25.09
3.392	11	3 1 0	26.25
3.251	9	-3 1 1	27.41
3.217	50	4 0 0	27.71
3.172M	30	0 1 2	28.11
3.172M		-1 1 2	28.11
3.112M	13	2 0 2	28.66
3.112M		-3 0 2	28.66
2.995M	100	1 1 2	29.81
2.995M		-2 1 2	29.81
2.782	50	4 1 0	32.15
2.774	50	0 2 0	32.25
2.713M	55	2 1 2	32.99
2.713M		-3 1 2	32.99
2.677M	25	3 0 2	33.44
2.677M		-4 0 2	33.44
2.573M	3	0 0 3	34.84
2.573M		5 0 0	34.84
2.560	2	-5 0 1	35.03
2.516	2	4 1 1	35.66
2.411M	3	3 1 2	37.27
2.411M		-4 1 2	37.27
2.376	2	2 2 1	37.84
2.355	4	-1 1 3	38.18
2.336M	5	0 1 3	38.51
2.336M		5 1 0	38.51
2.329	6	3 2 0	38.62
2.307M	5	4 0 2	39.01
2.307M		-5 0 2	39.01
2.282	3	-3 2 1	39.46
2.277	4	2 0 3	39.54
2.253M	20	0 2 2	39.99
2.253M		-1 2 2	39.99
2.187M	6	1 2 2	41.24
2.187M		-2 2 2	41.24
2.181M	5	3 2 1	41.36
2.181M		-3 1 3	41.36
2.144	11	6 0 0	42.11
2.131M	17	4 1 2	42.39
2.131M		-5 1 2	42.39
2.1008	25	4 2 0	43.02
2.0711M	17	2 2 2	43.67
2.0711M		-3 2 2	43.67

d(Å)	I	hkℓ			2θ(°)
2.0261	2	-4	1	3	44.69
2.0078M	8	5	0	2	45.12
2.0078M		-6	0	2	45.12
2.0007	8	6	1	0	45.29
1.9783	2	4	2	1	45.83
1.9542	30	-1	0	4	46.43
1.9264M	20	3	2	2	47.14
1.9264M		-4	2	2	47.14
1.8865+	30	5	2	0	48.20
1.8865+		0	2	3	48.20
1.8385M	2	1	2	3	49.54
1.8385M		7	0	0	49.54
1.8302	2	1	3	0	49.78
1.8240M	2	0	1	4	49.96
1.8240M		-2	1	4	49.96
1.8018	2	-3	2	3	50.62
1.7873	3	5	2	1	51.06
1.7772	8	2	3	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	3	1	53.36
1.6967+	8	3	3	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	6	1	2	54.51
1.6821M		-7	1	2	54.51
1.6691+	20	3	0	4	54.97
1.6691+		-5	0	4	54.97
1.6522	3	7	1	1	55.58
1.6402M	11	1	3	2	56.02
1.6402M		-2	3	2	56.02
1.6256M	3	5	2	2	56.57
1.6256M		-6	2	2	56.57
1.6025	13	4	3	0	57.46
1.5977	25	-1	2	4	57.65
1.5889M	16	2	3	2	58.00
1.5889M		-3	3	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	3	4	2	3	59.37
1.5446	6	8	1	0	59.83
1.5211M	3	3	3	2	60.85
1.5211M		-4	3	2	60.85
1.5110M	8	7	1	2	61.30
1.5110M		-8	1	2	61.30
1.4984M	3	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, $PbHPO_4$

Sample
The sample was prepared by adding acidified Pb acetate solution to a cold solution of $NaHPO_4$. The precipitate was then washed with distilled water and dried in the air.

Color
Colorless

Structure
Monoclinic, P2/a (13), Z = 2. The structure of $PbHPO_4$ was studied by Bengtsson [1941].

Lattice constants of this sample:
a = 5.7822(5)Å
b = 6.6454(5)
c = 4.6843(4)
β = 97.14(1)°

a/b = 0.8701
c/b = 0.7049

Volume
178.6 $Å^3$

Density
(calculated) 5.638 g/cm^3

Reference intensity
$I/I_{corundum}$ = 5.2(2)

Additional pattern
1. PDF card 6-274 [X-ray Diffraction Patterns of Lead Compounds, 1954].

References
Bengtsson, E. (1941). Ark. Kemi Mineral. Geol. 15B, No. 7.
X-ray Diffraction Patterns of Lead Compounds (1954). (Thornton Research Center, The Shell Petroleum Co., Ltd.) p. 54.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ			2θ(°)
6.64	25	0	1	0	13.33
4.650	30	0	0	1	19.07
4.341	50	1	1	0	20.44
3.808	11	0	1	1	23.34
3.332	90	-1	1	1	26.73
3.325	100	0	2	0	26.79
3.032	80	1	1	1	29.44
2.876	30	1	2	0	31.07
2.868	35	2	0	0	31.16
2.702	15	0	2	1	33.13
2.632	7	2	1	0	34.03
2.589	13	-2	0	1	34.62
2.516	20	-1	2	1	35.65
2.380	5	1	2	1	37.77
2.324	15	0	0	2	38.71
2.316	20	2	0	1	38.86
2.216	7	0	3	0	40.69
2.186	6	2	1	1	41.26
2.171	18	2	2	0	41.57
2.133	17	-1	1	2	42.34
2.066	7	1	3	0	43.79
2.042	12	-2	2	1	44.32
1.9994	10	0	3	1	45.32
1.9726	9	1	1	2	45.97
1.9271	10	-2	0	2	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	0	4	1	59.02
1.5495	3	0	0	3	59.62
1.5339	3	-3	1	2	60.29
1.5252	7	-1	4	1	60.67
1.5170	7	2	2	2	61.03
1.5106M	7	1	3	2	61.32
1.5106M		3	2	1	61.32
1.5044	7	-1	1	3	61.60
1.4932	7	1	4	1	62.11
1.4536	5	-2	3	2	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	6	-4	0	1	65.68
1.4204M		-3	3	1	65.68
1.4174	8	1	1	3	65.84
1.4045	3	0	2	3	66.52
1.4010	5	-1	2	3	66.71
1.3645	2	3	1	2	68.74
1.3509M	3	0	4	2	69.53
1.3509M		2	3	2	69.53
1.3467	4	3	3	1	69.78
1.3371	2	-1	4	2	70.35

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å					
d(Å)	I	h	k	ℓ	2θ(°)
1.3291M	4	1	2	3	70.84
1.3291M		0	5	0	70.84
1.3215	3	-2	2	3	71.31
1.3167	4	4	2	0	71.61
1.3071	1	-4	2	1	72.22
1.2947+	5	1	4	2	73.02
1.2947+		-4	0	2	73.02
1.2947+		1	5	0	73.02
1.2841	1	-3	3	2	73.72
1.2780	3	0	5	1	74.13
1.2697	3	0	3	3	74.70
1.2672	3	-1	3	3	74.87
1.2611	4	-3	1	3	75.30
1.2582	3	-2	4	2	75.50
1.2541	2	3	4	0	75.79
1.2367	3	-3	4	1	77.05
1.2305	2	4	2	1	77.51
1.2138	1	1	3	3	78.78
1.2062M	7	2	5	0	79.38
1.2062M		-4	2	2	79.38
1.2043	6	4	3	0	79.53
1.1965	2	-4	3	1	80.15
1.1900	1	2	4	2	80.68
1.1869	4	3	4	1	80.93
1.1826	3	-2	5	1	81.29
1.1620	1	0	0	4	83.04
1.1581	2	4	0	2	83.39
1.1531	5	2	5	1	83.83
1.1435	2	-3	4	2	84.70
1.1408	2	4	1	2	84.94
1.1373	1	4	3	1	85.27
1.1312+	6	-5	1	1	85.84
1.1312+		-1	4	3	85.84
1.1312+		5	1	0	85.84

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

Sample
The sample was prepared at NBS from an aqueous solution of $MgCrO_4$ by slow evaporation at room temperature.

Color
Vivid orange yellow

Structure
Triclinic, $P\bar{1}(2)$, 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) Å
b = 10.787 (2)
c = 6.1592(9)
α = 98.60 (1)°
β = 108.80 (1)
γ = 75.58 (2)

a/b = 0.5950
c/b = 0.5710

Volume
389.87 $Å^3$

Density
(calculated) 1.962 g/cm^3

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 $7H_2O$ 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.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
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 1	23.77
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 3 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 3 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	3	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	40.69

d(Å)	I	hkℓ	2θ(°)
2.207	18	2 4 0	40.86
2.122	12	1 -2 2	42.57
2.113+	16	-1 -5 1	42.76
2.113+		1 5 0	42.76
2.084	9	0 5 0	43.39
2.062	18	-2 -4 2	43.87
2.052+	30	-2 2 2	44.10
2.052+		2 -2 1	44.10
2.024	7	3 1 0	44.75
2.015M	5	0 -4 2	44.94
2.015M		-3 -3 1	44.94
1.997M	20	3 2 0	45.38
1.997M		-1 -2 3	45.38
1.978M	6	3 0 0	45.84
1.978M		-3 -2 2	45.84
1.973	6	-2 -5 1	45.97
1.945	13	-2 -1 3	46.66
1.938M	18	0 0 3	46.85
1.938M		-1 1 3	46.85
1.923+	16	-3 0 2	47.22
1.923+		-2 -2 3	47.22
1.917	16	0 5 1	47.38
1.904+	30	-3 -3 2	47.74
1.904+		3 3 0	47.74
1.881+	12	-1 -3 3	48.35
1.881+		-1 -5 2	48.35
1.871M	15	-3 1 0	48.62
1.871M		0 4 2	48.62
1.865	11	-3 -4 1	48.78
1.841M	4	2 -3 1	49.46
1.841M		-2 -3 3	49.46
1.8220M	10	2 0 2	50.02
1.8220M		2 1 2	50.02
1.8045M	6	-2 1 3	50.54
1.8045M		-1 4 2	50.54
1.8008	6	-1 2 3	50.65
1.7785M	17	-1 -6 1	51.33
1.7785M		-2 4 0	51.33
1.7718M	17	-1 5 1	51.54
1.7718M		1 6 0	51.54
1.7491	5	0 -3 3	52.26
1.7466M	6	3 1 1	52.34
1.7466M		1 -5 1	52.34
1.7343	8	-1 -4 3	52.74
1.7249	6	1 -4 2	53.05
1.7197	8	-2 -4 3	53.22
1.6979M	25	-3 -2 3	53.96
1.6979M		-3 -5 1	53.96
1.6738	2	2 3 2	54.80
1.6566+	16	3 -1 1	55.42
1.6566+		-3 -3 3	55.42
1.6454	18	-1 3 3	55.83
1.6196M	12	-2 -6 2	56.80
1.6196M		3 5 0	56.80
1.6092M	8	-2 4 2	57.20
1.6092M		-3 3 1	57.20
1.5992	7	-4 -2 1	57.59
1.5821	10	-2 -5 3	58.27
1.5792+	15	-3 3 0	58.39
1.5792+		-1 -5 3	58.39
1.5770+	12	1 5 2	58.48
1.5770+		-1 5 2	58.48
1.5672	3	-4 -3 1	58.88
1.5597M	7	3 4 1	59.19
1.5597M		-4 -1 2	59.19
1.5559M	7	2 4 2	59.35
1.5559M		-2 5 0	59.35
1.5443	6	-4 -3 2	59.84
1.5420M	6	0 -6 2	59.94
1.5420M		-2 5 1	59.94
1.5334M	5	-1 -1 4	60.31
1.5334M		-3 -6 1	60.31
1.5222	6	1 7 0	60.80
1.5182M	8	1 -6 1	60.98
1.5182M		-2 -1 4	60.98
1.5164M	6	-4 0 2	61.06
1.5164M		4 2 0	61.06
1.5061M	5	2 6 1	61.52
1.5061M		-4 -4 1	61.52
1.4976	4	-2 -7 1	61.91
1.4881	4	0 7 0	62.35
1.4842+	6	4 3 0	62.53
1.4842+		4 0 0	62.53
1.4736M	4	-3 2 3	63.03
1.4736M		-2 -3 4	63.03
1.4620	6	2 7 0	63.59
1.4575	7	3 1 2	63.81
1.4532	6	0 0 4	64.02
1.4512	5	3 -3 1	64.12
1.4490	4	-4 1 2	64.23
1.4443	1L	-2 -6 3	64.46
1.4400+	7	-2 -7 2	64.68
1.4400+		3 2 2	64.68
1.4384	7	2 0 3	64.76
1.4274+	14	4 4 0	65.32
1.4274+		-4 -3 3	65.32
1.4096	3	-1 2 4	66.25
1.3967+	3	-1 -4 4	66.94
1.3967+		3 3 2	66.94

Manganese Phosphate, $Mn_2P_2O_7$

Sample
It was prepared from a stoichiometric mixture of MnO_2 and P_2O_5.

Color
Pinkish white

Structure
Monoclinic, C2/m (12), Z = 2, isostructural with $Sc_2Si_2O_7$ (thortveitite). The structure of $Mn_2P_2O_7$ was determined by Lukaszewicz and Smajkiewicz [1961].

Lattice constants of this sample:
a = 6.636(1) Å
b = 8.584(1)
c = 4.5457(9)
β = 102.78(1)°

a/b = 0.7731
c/b = 0.6850

Volume
252.55 $Å^3$

Density
(calculated) 3.733 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.50(6)

Additional pattern
1. PDF card 3-555 [Dow Chemical Co.].

Reference
Lukaszewicz, K. and Smajkiewicz, R. (1961). Rocz. Chem. 35, 741.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ			2θ(°)
5.166	8	1	1	0	17.15
4.432	7	0	0	1	20.02
4.294	3	0	2	0	20.67
3.107	60	1	1	1	28.71
3.086	100	0	2	1	28.91
2.944	60	-2	0	1	30.34
2.618	18	1	3	0	34.22
2.585	20	2	2	0	34.67
2.376	4	2	0	1	37.83
2.348	2	-1	3	1	38.30
2.217	3	0	0	2	40.66
2.181	6	-1	1	2	41.37
2.171	20	1	3	1	41.56
2.147	4	0	4	0	42.06
2.093	6	3	1	0	43.19
2.078	15	2	2	1	43.52
2.070	15	-3	1	1	43.69
2.053	8	-2	0	2	44.08
1.971	3	0	2	2	46.02
1.932	4	0	4	1	46.99
1.851	14	-2	2	2	49.18
1.7708	4	-1	3	2	51.57
1.7519	1	3	1	1	52.17
1.7333	4	-2	4	1	52.77
1.7227	7	3	3	0	53.12
1.7108	7	-3	3	1	53.52
1.6649	9	2	0	2	55.12
1.6591	8	1	5	0	55.33
1.6209	18	1	3	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	3	3	1	61.01
1.4937	4	-3	3	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	3	4	0	1	65.58
1.3921	2	-4	2	2	67.19
1.3659	3	-1	5	2	68.66
1.3390	9	-1	3	3	70.24

Manganese Titanium Oxide (Pyrophanite), $MnTiO_3$

Sample
The sample was prepared by grinding together equimolar amounts of $MnCO_3$ and K_2TiO_3. The mixture was heated in a silver boat which was placed in a tube with N_2 current. The sample was then heated about 5 min. with a torch until the sample was red hot (≈900 °C).

Color
Gray yellowish brown

Structure
Hexagonal, $R\bar{3}$ (148), Z = 6, isostructural with $FeTiO_3$. The structure of $FeTiO_3$, ilmenite, was determined by Barth and Posnjak [1934]. Shirane, Pickart and Ishikawa [1959] confirmed the structure of $MnTiO_3$ by neutron diffraction.

Lattice constants of this sample:
a = 5.1396(1) Å
c = 14.2902(6)

c/a = 2.7804

Volume
326.91 $Å^3$

Density
(calculated) 4.596 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.5(1)

Polymorphism
Syono et al. [1969] report the existence of a high pressure magnetic phase of $MnTiO_3$.

Additional patterns
1. PDF card 12-435 [Lee, 1955]
2. Portnov [1963]
3. Posnjak and Barth [1934]

References
Barth, T. F. W. and Posnjak, E. (1934). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 88A, 265.
Lee, D. E. (1955). Stanford Univ. Publ, Univ. Ser. Geol. Sci. 5, 44.
Portnov, A. M. (1963). Dokl. Akad. Nauk. SSSR 153, 187.
Posnjak, E. and Barth, T. F. W. (1934). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 88A, 271.
Shirane, G., Pickart, S. J., and Ishikawa, Y. (1959). J. Phys. Soc. Jap. 14, No. 10.
Syono, Y., Akimoto, S., Ishikawa, Y., and Endoh, Y. (1969). J. Phys. Chem. Solids 30, 1665.

CuKα1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.253	2	1 0 1	20.87
3.776	25	0 1 2	23.54
2.785	100	1 0 4	32.11
2.569	70	1 1 0	34.89
2.3811	4	0 0 6	37.75
2.2620	30	1 1 3	39.82
2.1985	4	0 2 1	41.02
2.1244	2	2 0 2	42.52
1.8887	40	0 2 4	48.14
1.7469	40	1 1 6	52.33
1.6710	5	2 1 1	54.90
1.6577	10	0 1 8	55.38
1.6378	3	1 2 2	56.11
1.5220	35	2 1 4	60.81
1.4838	30	3 0 0	62.55
1.4496	2	1 2 5	64.20
1.3929	3	2 0 8	67.15
1.3605	11	1 0 10	68.97
1.3507	4	1 1 9	69.54
1.2849	8	2 2 0	73.67
1.2593	3	3 0 6	75.42
1.2403	2	2 2 3	76.79
1.2247	4	1 2 8	77.95
1.2164	3	3 1 2	78.58
1.2023	6	0 2 10	79.69
1.1668	10	1 3 4	82.63
1.1307	6	2 2 6	85.88
1.0996	1	0 4 2	88.94
1.0892	7	2 1 10	90.02
1.0804	2	1 1 12	90.95
1.0673	1	1 0 13	92.40
1.0625	3	4 0 4	92.93
1.0157	3	3 1 8	98.65
.9989	1	2 2 9	100.91
.9949	3	0 1 14	101.47
.9818	7	3 2 4	103.36
.9714	5	4 1 0	104.93
.9615	1	2 3 5	106.48
.9526	2	0 0 15	107.92
.9517	1	4 1 3	108.07
.9444	3	0 4 8	109.30
.9342	5	1 3 10	111.09
.9279	4	2 0 14	112.23
.8994	7	4 1 6	117.85

Niobium Silicide, α-Nb_5Si_3

Sample
The sample was prepared by R. M. Waterstrat at NBS by arc melting in vacuo four times and annealing at 1600 °C in vacuo for 4 hours.

Color
Gray metallic

Structure
Tetragonal, I4/mcm(140), Z=4, isostructural with Cr_5B_3. The structure of α-Nb_5Si_3 was determined by Parthé et al. [1955].

Lattice constants of this sample:
a = 6.5698(3) Å
c = 11.8877(8)

c/a = 1.8094

Volume
513.10 $Å^3$

Density
(calculated) 7.104 g/cm^3

Reference intensity
$I/I_{corundum}$ = 3.9(3)

Polymorphism
Three modifications of Nb_5Si_3 have been reported by Knapton [1955]. The α-Nb_5Si_3, stable at low temperature is tetragonal, Cr_5B_3 type, and the β-Nb_5Si_3, high temperature form is also tetragonal, W_5Si_3 type. The transition occurs between 1900°C and 2100°C. The third modification reported by Knapton [1955] and found to exist when 1-2% carbon is present is hexagonal, Mn_5Si_3 type.

In some literature the composition is given as "Nb_3Si_2."

Additional pattern
1. PDF card 9-222 [Parthé, 1955].

References

Knapton, A. G. (1955). Nature 175, 730.
Parthé, E., Lux, B., and Nowotny, H. (1955). Monatsh. Chem. 86, 859.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
3.660	8	112	24.30
3.283	2	200	27.14
2.971	3	004	30.05
2.875	17	202	31.08
2.854	25	211	31.32
2.504	25	114	35.84
2.360	100	213	38.10
2.325	13	220	38.70
2.204	30	204	40.92
2.963	<1	222	41.72
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

Niobium Silicide, β-Nb_5Si_3

Sample
The sample was prepared by R. M. Waterstrat at NBS. Niobium and silicon placed in a copper crucible were arc melted under argon. The product was then rapidly cooled.

Color
Gray metallic

Structure
Tetragonal, I4/mcm (140), Z=4 [Parthé, Schachner, and Nowotny, 1955], isostructural with W_5Si_3. The structure of W_5Si_3 was determined by Aronsson [1955].

Lattice constants of this sample:
a = 10.0289(4) Å
c = 5.0698(4)

c/a = 0.5058

Volume
509.91 $Å^3$

Density
(calculated) 7.149 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.22(15)

Polymorphism
Three modifications of Nb_5Si_3 have been reported by Knapton [1955]. The α-Nb_5Si_3, stable at low temperatures, is tetragonal Cr_5B_3-type and the β-Nb_5Si_3 high temperature phase is reported here. The α-β transformation occurs between 1,900 and 2100 °C. The third modification reported by many authors and found by Knapton [1955] to exist when 1-2% carbon is present is hexagonal Mn_5Si_3-type.

In some of the literature, M_5Si_3 compounds have been labelled "M_3Si_2."

Additional pattern
1. PDF card 9-272 [Parthé, Nowotny, and Schmid, 1955].

References
Aronsson, B. (1955). Acta Chem. Scand. 9, 1107.
Knapton, A. G. (1955). Nature London 175, 730.
Parthé, E., Nowotny, H., and Schmid, H. (1955). Monatsh. Chem. 86, 385.
Parthé, E., Schachner, H., and Nowotny, H. (1955). Monatsh. Chem. 86, 182.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ			2θ(°)
7.10	3	1	1	0	12.46
5.021	2	2	0	0	17.65
3.546	6	2	2	0	25.09
3.361	25	2	1	1	26.50
3.172	30	3	1	0	28.11
2.536	30	0	0	2	35.37
2.507	14	4	0	0	35.79
2.440	80	3	2	1	36.81
2.387	14	1	1	2	37.66
2.365	11	3	3	0	38.02
2.263	40	2	0	2	39.80
2.243	55	4	2	0	40.18
2.193	100	4	1	1	41.12
2.0625	60	2	2	2	43.86
1.7824	3	4	0	2	51.21
1.7481	6	5	2	1	52.29
1.7200	1	5	3	0	53.21
1.6801	1L	4	2	2	54.58
1.6721	1	6	0	0	54.86
1.5854	14	6	2	0	58.14
1.5809	10	2	1	3	58.32
1.5674	1	6	1	1	58.87
1.5538	13	5	1	2	59.44
1.4961	10	5	4	1	61.98
1.4526	9	4	4	2	64.05
1.4437	18	3	2	3	64.49
1.4336	17	6	3	1	65.00
1.4229	14	5	3	2	65.55
1.4183	20	5	5	0	65.79
1.3953	18	6	0	2	67.02
1.3878	30	4	1	3	67.43
1.3443	1L	6	2	2	69.92
1.3293	1	7	2	1	70.83
1.3165	1	7	3	0	71.62
1.2672	8	0	0	4	74.87
1.2513	2	5	2	3	75.99
1.2446	2	6	5	1	76.47
1.2378	10	5	5	2	76.97
1.2196	15	6	4	2	78.34
1.2162	15	8	2	0	78.60
1.2082	1	7	4	1	79.22
1.1820	5	6	6	0	81.34
1.1772	5	3	1	4	81.74
1.1684	6	7	3	2	82.49
1.1656	4	7	5	0	82.73
1.1489	4	5	4	3	84.21
1.1435	14	8	3	1	84.70
1.1313	3	4	0	4	85.83
1.1237	7	8	0	2	86.55
1.1197	8	6	3	3	86.94

Niobium Silicide, β-Nb_5Si_3 - (continued)

d(Å)	I	hkℓ			2θ(°)
1.1169	5	3	3	4	87.21
1.1076	2	9	1	0	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
1.0150	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
.9982	3	9	4	1	101.01

Potassium Borate Hydroxide Hydrate, $K_2B_4O_5(OH)_4 \cdot 2H_2O$

Sample
The sample was made by slow evaporation from aqueous solution at room temperature.

Color
Colorless

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure was studied by Marezio et al. [1963].

Lattice constants of this sample:
a = 11.785(3) Å
b = 12.917(3)
c = 6.865(1)

a/b = 0.9124
c/b = 0.5315

Volume
1045.0 $Å^3$

Density
(calculated) 1.942 g/cm^3

Reference intensity
$I/I_{corundum}$ = 0.20(1)

Additional patterns
1. PDF card 19-950 [Toledano, 1966]

References

Marezio, M., Plettinger, H. A., and Zachariasen, W. H. (1963). Acta Crystallogr. 16, 975.
Tolédano, P. (1966). Bull. Soc. Chim. France 1966, 2302.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.46	18	0 2 0	13.70
6.05	55	0 1 1	14.62
5.94	90	1 0 1	14.91
5.388	95	1 1 1	16.44
4.471	40	2 0 1	19.84
4.367	16	1 2 1	20.32
4.223	20	2 1 1	21.02
4.042	6	1 3 0	21.97
3.759	35	3 1 0	23.65
3.673	35	2 2 1	24.21
3.648	45	0 3 1	24.38
3.480M	25	1 3 1	25.58
3.480M		2 3 0	25.58
3.428	20	0 0 2	25.97
3.409	75	3 0 1	26.12
3.317	65	0 1 2	26.86
3.227	45	0 4 0	27.62
3.194	100	1 1 2	27.91
3.112	50	1 4 0	28.66
3.102	50	2 3 1	28.76
3.030	45	0 2 2	29.46
3.019	45	3 2 1	29.57
2.964	40	2 0 2	30.13
2.945	60	4 0 0	30.33
2.922	45	0 4 1	30.57
2.891	50	2 1 2	30.91
2.872	35	4 1 0	31.12
2.833M	40	1 4 1	31.55
2.833M		2 4 0	31.55
2.706	50	4 0 1	33.08
2.698	40	2 2 2	33.18
2.683M	70	0 3 2	33.37
2.683M		4 2 0	33.37
2.650	20	4 1 1	33.80
2.617M	45	2 4 1	34.23
2.617M		1 3 2	34.23
2.585	7	3 0 2	34.68
2.524	11	1 5 0	35.54
2.495M	55	4 2 1	35.96
2.495M		3 4 0	35.96
2.431	15	4 3 0	36.95
2.399	6	3 2 2	37.46
2.368M	18	1 5 1	37.97
2.368M		2 5 0	37.97
2.344	12	3 4 1	38.37
2.305	50	1 4 2	39.04
2.292	25	4 3 1	39.27
2.253	13	0 1 3	39.98
2.248	12	1 0 3	40.08
2.236M	10	2 5 1	40.31
2.236M		4 0 2	40.31
2.202	40	4 1 2	40.95
2.196	35	5 1 1	41.06
2.157M	30	3 5 0	41.84
2.157M		0 2 3	41.84
2.132	20	2 0 3	42.36
2.115	30	4 2 2	42.72
2.105	35	2 1 3	42.94
2.075	40	4 4 1	43.59
2.068	30	5 3 0	43.74
2.055	12	0 6 1	44.03
2.033	12	1 5 2	44.52
2.022+	35	1 6 1	44.78
2.022+		2 6 0	44.78
1.991	40	1 3 3	45.52
1.985	35	4 3 2	45.66
1.978	20	3 0 3	45.84
1.948	17	2 5 2	46.58
1.942+	17	4 5 0	46.73
1.942+		6 1 0	46.73
1.922	11	5 1 2	47.26
1.891	14	3 2 3	48.08
1.887M	14	6 0 1	48.18
1.887M		3 6 0	48.18
1.869M	13	4 5 1	48.68
1.869M		6 1 1	48.68
1.8392	7	4 4 2	49.52

Potassium Chromium Oxide (Lopezite), $K_2Cr_2O_7$

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) Å
b = 13.419(5)
c = 7.391(3)
α = 98.13(3)°
β = 90.86(3)
γ = 96.23(3)

a/b = .5565
c/b = .5508

Volume
728.5 $Å^3$

Density
(calculated) 2.682 g/cm^3

Polymorphism
$K_2Cr_2O_7$ 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.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.79	10	$\bar{1}10$	13.02
6.59	12	020	13.42
6.04	10	011	14.65
5.30	8	$0\bar{2}1,\bar{1}01$	16.70
5.13	14	101	17.27
5.09	14	$1\bar{1}1$	17.40
4.949	17	$\bar{1}\bar{1}1$	17.91
4.873	30	$\bar{1}11$	18.19
4.682	6	120	18.94
4.516	20	111	19.64
4.454	15	$1\bar{2}1$	19.92
4.182	6	$\bar{1}\bar{2}1$	21.23
3.711	30	200	23.96
3.657	55	$0\bar{1}2,002$	24.32
3.553	5	031	25.04
3.473	85	210	25.63
3.428	20	$\bar{1}31$	25.97
3.401	20	$\bar{2}20,012$	26.18
3.347	40	$\bar{2}01,\bar{1}31$	26.61
3.300	100	$040,2\bar{1}1$	27.00
3.242	16	102	27.49
3.222	16	$\bar{2}\bar{1}1$	27.66
3.183	7	$0\bar{4}1$	28.01
3.141	6	$2\bar{2}1,1\bar{2}2$	28.39
3.087	12	220	28.90
3.065	30	$\bar{1}\bar{2}2$	29.11
3.024	40	$11\bar{2},022$	29.52
3.009	35	$\bar{2}30$	29.67
2.946	9	$\bar{2}\bar{2}1$	30.31
2.874	35	$\bar{1}22$	31.09
2.856	25	$041,2\bar{3}1$	31.29
2.757	8	$\bar{1}3\bar{2},221$	32.45
2.711	6	$\bar{2}31$	33.01
2.692	7	230	33.25
2.640	16	050	33.93
2.609	13	$2\bar{1}2,\bar{2}\bar{1}2$	34.35
2.575	13	$\bar{1}41$	34.81
2.547	16	$2\bar{2}2,1\bar{4}2$	35.21
2.540	18	$1\bar{5}1,2\bar{4}1$	35.31
2.475	10	$\bar{2}\bar{2}2,300$	36.26
2.438	11	$212,003$	36.84
2.404	10	$\bar{3}20,150$	37.38
2.385	15	$\bar{1}5\bar{1},310$	37.68
2.338	9	$013,\bar{1}03$	38.47
2.301	11	$3\bar{2}1$	39.12
2.293	12	$\bar{2}\bar{3}2,1\bar{2}3$	39.25
2.273	8	$0\bar{3}3,\bar{2}50$	39.62
2.252	10	$\bar{1}42,1\bar{5}2$	40.00
2.193	12	$151,1\bar{3}3$	41.12
2.151	8	$241,\bar{1}5\bar{2}$	41.96
2.132	10	142	42.37
2.089	12	$\bar{2}42$	43.27
2.061	18	$\bar{2}1\bar{3},330$	43.90
2.055	20	$1\bar{4}3$	44.02
2.047	20	$160,250$	44.21
1.990	7	$\bar{1}52,\bar{3}22$	45.55
1.905	8	$\bar{1}\bar{6}2,133$	47.69

Potassium Iodate, KIO_3

Sample
The sample was reagent material from Fisher Scientific Co., Bloomfield, N.J.

Color
Colorless

Structure
Triclinic, Pl(1), Z = 4, pseudo-monoclinic and a distorted perovskite-type. The structure was refined by Hamid [1973]. Much work has been done on the symmetry problems of KIO_3 and a summary was given by Crane [1972].

Lattice constants of this sample:
a = 7.708(1) Å
b = 7.722(2)
c = 7.689(2)
α = 109.25(2)°
β = 108.96(2)
γ = 109.37(2)

a/b = 0.9982
c/b = 0.9975

The NBS data could be indexed only with this triclinic cell, refined from the one derived by Hamid [1973].

Volume
355.9 Å^3

Density
(calculated) 3.994 g/cm^3

Polymorphism
Between -200 °C and +250 °C there are at least 5 phase changes. The room temperature triclinic symmetry becomes monoclinic at 72.5 °C and rhombohedral at 212 °C [Hamid, 1973; Salje, 1973].

Additional pattern
1. PDF card 1-776 [Hanawalt et al., 1938].

References
Crane, G.R. (1972). J. Appl. Crystallogr. 5, 360.
Hamid, S.A. (1973). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 137, 412.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Salje, E. (1973). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 137, 1.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.27M	1	0 -1 1	14.11
6.27M		-1 0 1	14.11
4.467+	45	1 -1 1	19.86
4.467+		-1 1 1	19.86
3.676+	1	1 1 0	24.19
3.676+		0 1 1	24.19
3.645+	1	-1 2 0	24.40
3.645+		-2 1 0	24.40
3.170	100	0 0 2	28.13
3.142	80	0 -2 2	28.38
2.831+	1	-1 -2 1	31.58
2.831+		-2 -1 1	31.58
2.812+	1	-1 -2 2	31.80
2.812+		-2 1 2	31.80
2.604	4	1 1 1	34.41
2.572M	6	1 -3 1	34.86
2.572M		-3 1 1	34.86
2.406+	1	2 1 0	37.35
2.406+		1 2 0	37.35
2.384+	1	-1 0 3	37.71
2.384+		-2 3 0	37.71
2.377+	1	0 -2 3	37.82
2.377+		-3 2 1	37.82
2.237	35	2 -2 2	40.29
2.232	30	-2 2 2	40.37
2.005+	15	-1 3 1	45.18
2.005+		-1 -3 1	45.18
1.994	11	3 -3 1	45.46
1.991	12	1 -3 3	45.52
1.989	13	-3 3 1	45.57
1.897M	1L	-1 -1 4	47.92
1.897M		-4 2 1	47.92
1.892	1L	-1 -2 4	48.05
1.839M	16	2 2 0	49.52
1.839M		2 0 2	49.52
1.822+	30	-4 2 0	50.02
1.822+		-2 4 0	50.02
1.819+	35	2 -4 2	50.12
1.819+		0 -2 4	50.12
1.815	18	-2 0 4	50.23
1.765+	1L	1 3 0	51.75
1.765+		3 0 1	51.75
1.755+	1L	-4 0 1	52.08
1.755+		-2 3 2	52.08
1.743M	1L	-4 3 1	52.45
1.743M		0 -3 4	52.45
1.6309+	1L	4 -3 1	56.37
1.6309+		-4 -1 2	56.37
1.6219M	1L	-3 1 4	56.71
1.6219M		-4 2 3	56.71

d(Å)	I	hkℓ	2θ(°)
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	9	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	3	-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	80.39
1.1910+	8	-6 4 0	80.60
1.1910+		-4 6 0	80.60
1.1884M	7	-6 4 2	80.81
1.1884M		0 -4 6	80.81
1.1851M	4	-4 0 6	81.08
1.1851M		-2 -4 6	81.08

Potassium Lead Phosphate, $K_2Pb(PO_3)_4$

Sample
The sample was prepared by heating a 1:1:4 molar mixture of $PbCO_3$, K_2CO_3 and $(NH_4)_2HPO_4$ at 350°C, followed by regrinding, melting at about 500 °C. The ground glass was then heated at 325 °C for a weekend.

Color
Colorless

Structure
Orthorhombic, Pcab (61), Z = 8. This agrees with Mahama et al. [1977] but is a different form of the space group than reported by Brunel-Laügt [1977].

Lattice constants of this sample:
a = 15.416(4) Å
b = 15.465(5)
c = 9.225(3)

a/b = 0.9968
c/b = 0.5965

Volume
2199.1 $Å^3$

Density
(calculated) 3.632 g/cm^3

Polymorphism
There is a second phase which is tetragonal referred to as $K_2PbP_4O_{12}$, stable below 537° [Mahama et al., 1977].

Additional pattern
1. Mahama et al. [1977]

References
Brunel-Laügt, M. and Guitel, J.-C. (1977). Acta Crystallogr. B33, 937.
Mahama, I., Brunel-Laügt, M., and Averbuch-Pouchot, M.-T. (1977). C. R. Acad. Sci. Ser. C 284, 681.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ			2θ(°)
7.70	10	2	0	0	11.49
7.03	55	1	1	1	12.58
6.89	45	1	2	0	12.83
5.91	30	2	0	1	14.98
5.53M	50	1	2	1	16.02
5.53M		2	1	1	16.02
4.609	6	0	0	2	19.24
4.416	20	0	1	2	20.09
4.308	25	3	1	1	20.60
4.277	45	3	2	0	20.75
4.247	19	1	1	2	20.90
3.962M	9	0	2	2	22.42
3.962M		2	0	2	22.42
3.877	55	3	2	1	22.92
3.850	80	4	0	0	23.08
3.748	4	1	4	0	23.72
3.552	25	4	0	1	25.05
3.520	25	2	2	2	25.28
3.456	35	2	4	0	25.76
3.437	100	0	3	2	25.90
3.388	9	3	3	1	26.28
3.348	30	3	1	2	26.60
3.235M	60	2	4	1	27.55
3.235M		4	2	1	27.55
3.139M	7	2	3	2	28.41
3.139M		3	2	2	28.41
3.088	4	3	4	0	28.89
2.963M	25	0	4	2	30.14
2.963M		1	1	3	30.14
2.928M	60	3	4	1	30.51
2.928M		4	3	1	30.51
2.906	30	4	1	2	30.74
2.875	35	5	1	1	31.08
2.859	30	3	3	2	31.26
2.810M	45	1	2	3	31.82
2.810M		2	1	3	31.82
2.766	9	2	4	2	32.34
2.731	25	4	4	0	32.77
2.680	6	2	2	3	33.41
2.618	5	4	4	1	34.22
2.602M	7	1	3	3	34.44
2.602M		3	1	3	34.44
2.567+	50	0	5	2	34.92
2.567+		3	4	2	34.92
2.543M	8	5	3	1	35.26
2.543M		1	6	0	35.26
2.499M	30	2	3	3	35.90
2.499M		3	2	3	35.90
2.475	8	6	0	1	36.26
2.445M	5	2	6	0	36.73
2.445M		6	1	1	36.73
2.403	4	4	0	3	37.39
2.363	12	2	6	1	38.05
2.306M	16	0	0	4	39.03
2.306M		3	6	0	39.03
2.299M	25	3	5	2	39.16
2.299M		2	4	3	39.16
2.258	4	1	1	4	39.90
2.231	10	6	3	1	40.40
2.222	12	6	1	2	40.56
2.189M	12	1	2	4	41.21
2.189M		2	1	4	41.21
2.182	10	3	4	3	41.35
2.158M	13	2	6	2	41.82
2.158M		1	5	3	41.82

d(Å)	I	hkℓ			2θ(°)
2.142	13	4	6	0	42.15
2.125M	12	5	5	1	42.51
2.125M		2	2	4	42.51
2.120	12	7	2	0	42.62
2.096	12	5	2	3	43.13
2.088M	13	4	6	1	43.30
2.088M		1	3	4	43.30
2.070	12	2	7	1	43.70
2.064	11	7	2	1	43.83
2.059	13	6	3	2	43.94
2.042	6	4	4	3	44.33
2.031M	10	2	3	4	44.58
2.031M		3	2	4	44.58
1.993	8	0	7	2	45.47
1.981+	19	3	7	1	45.76
1.981+		0	4	4	45.76
1.974	15	5	5	2	45.94
1.934+	9	5	6	1	46.95
1.934+		0	8	0	46.95
1.915M	12	7	4	0	47.45
1.915M		2	6	3	47.45
1.886	4	8	0	1	48.22
1.876M	9	4	7	1	48.49
1.876M		2	8	0	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+		3	4	4	49.26
1.843	8	3	6	3	49.41
1.820M	3	6	6	0	50.09
1.820M		1	1	5	50.09
1.796M	8	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	2	5	52.28

Potassium Lead Selenate, $K_2Pb(SeO_4)_2$

Sample
The sample was prepared by adding H_2SeO_4 to a solution of K_2CO_3 and $PbCO_3$, thus co-precipitating K_2SeO_4 and $PbSeO_4$. The solution was dried and the solids were heated for 17 hrs. at 600°C.

Color
Vivid pale yellow

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Ba_3(PO_4)_3$ and many double sulfates, chromates, and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ 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 $Å^3$

Density
(calculated) 4.776 g/cm^3

Additional patterns
1. PDF card 19-972 [Schwarz, 1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 214.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
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	0·0·15	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

Potassium Molybdenum Oxide, K_2MoO_4

Sample
The sample was prepared from stoichiometric amounts of KOH and MoO_3 ground together and heated for 15 minutes at 450 °C. The material was heated at 900 °C for a few minutes then allowed to cool.

Color
Yellowish white

Structure
Monoclinic, I2/m (12), Z = 4, isostructural with K_2WO_4. The structure was determined concurrently by Gatehouse and Leverett [1969] and by Koster, Kools and Rieck [1969].

Lattice constants of this sample:
a = 11.3406(9) Å
b = 6.0814(5)
c = 7.5393(7)
β = 101.07(1)°

a/b = 1.8648
c/b = 1.2397

Volume
510.28 $Å^3$

Density
(calculated) 3.100 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.5(1)

Polymorphism
Van den Akker et al. [1969] report two other polymorphic phases of K_2MoO_4 with transition points above 305° and above 440°.

Additional patterns
1. PDF card 24-880 [Kools et al., 1970]
2. Gatehouse and Leverett [1969]

References

Gatehouse, B. M. and Leverett, P. (1969). J. Chem. Soc. A, 849.
Kools, F. X. N. M., Koster, A.S., and Rieck, G.D. (1970). Acta Crystallogr. B26, 1974.
Koster, A.S., Kools, F. X. N. M., and Rieck, G.D. (1969). Acta Crystallogr. B25, 1704.
Van den Akker, A. W. M., Koster, A. S., and Rieck, G. D. (1970). J. Appl. Cryst. 3, 389.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ			2θ(°)
6.789	5	-1	0	1	13.03
5.676	19	1	0	1	15.60
5.566	12	2	0	0	15.91
5.336	14	1	1	0	16.60
4.699	40	0	1	1	18.87
3.828	30	-2	1	1	23.22
3.700	18	0	0	2	24.03
3.609	14	-3	0	1	24.65
3.396	70	-2	0	2	26.22
3.169	100	3	1	0	28.14
3.087	6	3	0	1	28.90
3.042	55	0	2	0	29.34
2.918	65	1	1	2	30.61
2.840	6	2	0	2	31.48
2.780	9	4	0	0	32.17
2.776	6	-1	2	1	32.22
2.680	4	1	2	1	33.41
2.669	3	2	2	0	33.55
2.627	3	-3	1	2	34.10
2.534	1	-4	1	1	35.40
2.464	2	-4	0	2	36.44
2.349	3	0	2	2	38.28
2.325	2	-3	2	1	38.70
2.316	2	1	0	3	38.85
2.286	13	0	1	3	39.38
2.2663	50	-2	2	2	39.74
2.2314	4	3	1	2	40.39
2.0911	2	5	1	0	43.23
2.0431	12	4	0	2	44.30
2.0274	4	5	0	1	44.66
1.9932	2	2	1	3	45.47
1.9796	25	-5	1	2	45.80
1.9546	3	0	3	1	46.42
1.9365	3	-1	2	3	46.88
1.9134	2	-4	2	2	47.48
1.8931	6	3	0	3	48.02
1.8744	4	-2	3	1	48.53
1.8547	12	6	0	0	49.08
1.8427	4	1	2	3	49.42
1.8156	3	2	3	1	50.21
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
1.6296	1	4	1	3	56.42
1.6071	3	3	2	3	57.28

Potassium Molybdenum Oxide, K_2MoO_4 - (continued)

d(Å)	I	hkℓ			2θ(°)
1.5901	4	-2	2	4	57.95
1.5834	7	6	2	0	58.22
1.5723	4	-5	2	3	58.67
1.5662	3	0	3	3	58.92
1.5502	2	-6	2	2	59.59
1.5481	2	3	3	2	59.68
1.5434	3	6	0	2	59.88
1.5286	2	-5	1	4	60.52
1.5202	7	0	4	0	60.89
1.4827	6	-4	2	4	62.60
1.4711	2	-7	0	3	63.15
1.4678	2	1	4	1	63.31
1.4591	10	-2	1	5	63.73
1.4563	11	-5	3	2	63.87
1.3878	5	-2	4	2	67.43
1.3804	6	-8	1	1	67.84

Potassium Sodium Tartrate Hydrate, $C_4H_4KNaO_6 \cdot 4H_2O$

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 sample was reagent material from J. T. Baker Chemical Company, Phillipsburg, N.J.

Color
Colorless

Structure
Orthorhombic, $P2_12_12$ (18), Z = 4. The structure of Rochelle salt was studied by Beevers and Hughes, [1941].

Lattice constants of this sample:
a = 11.899(3) Å
b = 14.279(3)
c = 6.229(2)

a/b = 0.8333
c/b = 0.4362

Volume
1058.3 $Å^3$

Density
(calculated) 1.771 g/cm^3

Additional pattern
1. PDF card 11-851 [Amendola, A., Polytechnic Inst. of Brooklyn, 1959]

Reference
Beevers, C. A. and Hughes, D. J. (1941). Proc. Roy. Soc. Ser. A, 177, 251.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ			2θ(°)
7.14	5	0	2	0	12.39
6.22	13	0	0	1	14.23
6.11	16	1	2	0	14.48
5.95	25	2	0	0	14.88
5.70	7	0	1	1	15.53
5.48	95	2	1	0	16.15
5.16	4	1	1	1	17.18
4.694	8	0	2	1	18.89
4.567	25	2	2	0	19.42
4.371	17	1	2	1	20.30
4.306	40	2	0	1	20.61
4.120	9	2	1	1	21.55
3.828	9	3	1	0	23.22
3.784	30	0	3	1	23.49
3.687	40	2	2	1	24.12
3.573	7	0	4	0	24.90
3.469	7	3	2	0	25.66
3.419	3	1	4	0	26.04
3.343	9	3	0	1	26.64
3.258	17	3	1	1	27.35
3.193	20	2	3	1	27.92
3.118	5	0	0	2	28.61
3.102	7	0	4	1	28.76
3.060	12	2	4	0	29.16
3.030	55	3	2	1	29.46
2.998	16	1	4	1	29.78
2.976	12	4	0	0	30.00
2.949	18	1	1	2	30.28
2.912	35	4	1	0	30.68
2.855	10	0	2	2	31.31
2.776M	40	1	2	2	32.22
2.776M		1	2	2	32.22
2.737	100	3	3	1	32.69
2.709	30	2	1	2	33.04
2.683	40	4	0	1	33.37
2.652	14	3	4	0	33.77
2.639	12	4	1	1	33.94
2.606	14	0	3	2	34.38
2.575	16	2	5	0	34.81
2.545	60	1	3	2	35.24
2.535	30	1	5	1	35.38
2.512	7	4	2	1	35.71
2.448	18	3	0	2	36.68
2.443	14	3	4	1	36.76
2.413	20	3	1	2	37.24
2.386	10	2	3	2	37.67
2.347M	16	0	4	2	38.32
2.347M		5	1	0	38.32
2.339	20	4	3	1	38.46
2.316M	16	3	5	0	38.86

d(Å)	I	hkℓ	2 (°)
2.316M		3 2 2	38.86
2.302	35	1 4 2	39.10
2.287	35	4 4 0	39.37
2.258	8	5 2 0	39.90
2.222M	19	0 6 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
2.126	2	4 1 2	42.48
2.081	15	2 6 1	43.44
2.058M	7	4 5 0	43.96
2.058M		4 2 2	43.96
2.040	6	3 6 0	44.38
2.026	18	1 1 3	44.70
2.014	7	5 3 1	44.97
1.994	11	0 2 3	45.46
1.955	6	4 5 1	46.40
1.940	8	3 6 1	46.78
1.938	7	0 7 1	46.84
1.915	4	1 7 1	47.45
1.889M	10	6 0 1	48.14
1.889M		5 4 1	48.14
1.875M	17	5 1 2	48.52
1.875M		6 1 1	48.52
1.858M	8	3 5 2	49.00
1.858M		4 6 0	49.00
1.843M	5	2 7 1	49.42
1.843M		4 4 2	49.42
1.829M	18	5 5 0	49.82
1.829M		5 2 2	49.82
1.825M	20	6 2 1	49.92
1.825M		3 1 3	49.92
1.812	7	2 3 3	50.32
1.785	7	0 8 0	51.12
1.781M	8	3 2 3	51.24
1.781M		4 6 1	51.24
1.757M	4	5 3 2	52.00
1.757M		6 3 1	52.00

Potassium Strontium Chromium Oxide, $K_2Sr(CrO_4)_2$

Sample
The sample was prepared by heating a 1:1 molar mixture of $SrCrO_4$ and K_2CrO_4 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, $R\bar{3}m$ (166), Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was determined by Møller [1954].

Lattice constants of this sample:
a = 5.6782(3) A
c = 21.027(2)

c/a = 3.7031

Volume
587.13 A^3

Density
(calculated) 3.375 g/cm^3

Reference Intensity
$I/I_{corundum}$ = 2.97 (16)

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

References
Møller, C. K. (1954). Acta Chem. Scand. 8, 6.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 345, 230.

$CuK\alpha_1$ λ = 1.540598 A; temp. 25±1 °C
Internal standard Ag, a = 4.08651 A

d(A)	I	hkℓ	2Θ(°)
7.02	6	003	12.60
4.458	13	012	19.90
3.591	1	104	24.77
3.508	2	006	25.37
3.198	100	015	27.88
2.840	90	110	31.48
2.632	11	113	34.03
2.564	5	107	34.96
2.396	5	202	37.51
2.338	5	009	38.47
2.227	6	024	40.47
2.207	6	116	40.86
2.122	35	205	42.56
1.933	25	1·0·10	46.97
1.830	2	122	49.78
1.804	2	119	50.54
1.796	2	208	50.78
1.753	2	214,0·0·12	52.13
1.7002	20	125	53.88
1.6392	10	300	56.06
1.5977	7	0·2·10	57.65
1.5802	1	217	58.35
1.5088	1	2·0·11	61.40
1.4911	1	1·1·12	62.21
1.4848	1	306	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	6	315	72.85
1.2568	9	1·1·15	75.60
1.2416	1	137	76.69
1.2133	1	229	78.82
1.1969	1	404,3·0·12	80.12
1.1800	2	045	81.51
1.1443	5	1·3·10	84.62
1.1050	<1	2·0·17	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
.9463	1	330,1·3·16	108.98
.9381	1	1·0·22,333	110.40
.9150	3	4·1·12,1·2·20+	114.67

Potassium Strontium Selenate, $K_2Sr(SeO_4)_2$

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.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Sr_3(PO_4)_2$ and many other double sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

Lattice constants of this sample:
a = 5.6846(6) Å
c = 21.105(3)

c/a = 3.7127

Volume
590.64 $Å^3$

Density
(calculated) 3.810 g/cm^3

Additional patterns
1. PDF card 19-995 [Schwarz, 1966].

References
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 214.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
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
1.703	17	125	53.80
1.640	8	300	56.02
1.6023	7	0·2·10	57.47
1.5831	1	217	58.23
1.5128	1	2·0·11	61.22
1.4956	2	1·1·12	62.00
1.4214	8	220	65.63
1.4073	3	0·0·15	66.37
1.3958	9	2·1·10	66.99
1.3548	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	1	137	76.55
1.2002	<1	3·0·12	79.85
1.1816	2	045	81.37
1.1462	4	1·3·10	84.45

Rubidium Barium Molybdenum Oxide, $Rb_2Ba(MoO_4)_2$

Sample
The sample was prepared by grinding together stiochiometric amounts of Rb_2CO_3, $BaCO_3$ and MoO_3 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, $R\bar{3}m$ (166), Z = 3. The similarity of the cell size, powder pattern, and chemistry of $Rb_2Ba(MoO_4)_2$, $Sr_3(PO_4)_2$, $K_2Pb(SO_4)_2$ (palmierite) and $(NH_4)_2Pb(SO_4)_2$ strongly suggests an isostructural relationship. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

Lattice constants of this sample:
a = 6.0851 (4) Å
c = 22.017 (2)

c/a = 3.6182

Volume
706.01 Å^3

Density
(calculated) 4.432 g/cm^3

References
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
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, $Rb_2Cr_2O_7$

Sample
The sample was precipitated by adding solid CrO_3 to a solution of Rb_2CO_3 to which a drop of HCl had been added. The precipitate was then washed with ethanol.

Color
Vivid yellow

Optical data
Biaxial (+), N_α = 1.688, N_γ = 1.790, 2V is medium.

Structure
Monoclinic, $P2_1/n(14)$, Z = 4. The structure was determined by Löfgren [1971].

Lattice constants of this sample:
a = 13.711(2) A
b = 7.599(2)
c = 7.700(2)
β = 93.36(2)°

a/b = 1.8043
c/b = 1.0133

Volume
800.85 $Å^3$

Density
(calculated) 3.209 g/cm^3

Polymorphism
The existence of at least four modifications of $Rb_2Cr_2O_7$ was reported by Löfgren and Waltersson, [1971]. Three forms exist at room temperature and are obtainable from aqueous solution: a triclinic form isostructural with one form of $K_2Cr_2O_7$, a monoclinic form isostructural with a second form of $K_2Cr_2O_7$, and a monoclinic form isostructural with $(NH_4)_2Cr_2O_7$. The fourth is a quenchable high temperature form of unknown structure.

Additional patterns
1. PDF card 26-1363 [Löfgren, 1971]

References
Löfgren, P. (1971). Acta Chem. Scand. 25, 44.
Löfgren, P. and Waltersson, K. (1971). Acta Chem. Scand. 25, 35.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.847	3	200	12.92
5.404	6	011	16.39
5.098	3	$\bar{1}11$	17.38
4.954	3	111	17.89
4.331	1	$\bar{2}11$	20.49
4.164	6	211	21.32
3.917	11	310	22.68
3.847	20	002	23.10
3.800	30	020	23.39
3.666	20	120	24.26
3.559	10	$\bar{3}11$	25.00
3.432	90	$\bar{2}02$,012	25.94
3.419	100	400,311 +	26.04
3.371	3	$\bar{1}12$	26.42
3.326	30	$\bar{1}21$,220	26.78
3.271	40	202	27.24
3.133	25	$\bar{2}12$	28.47
3.124	11	410	28.55
3.083	9	$\bar{2}21$	28.94
3.020	18	221	29.55
2.949	4	$\bar{4}11$	30.28
2.923	4	320	30.56
2.840	3	411	31.47
2.814	3	$\bar{3}12$	31.77
2.763	2	$\bar{3}21$	32.38
2.698	13	321	33.18
2.676	12	$\bar{3}12$	33.46
2.633	6	$\bar{4}02$,122	34.02
2.629	5	$\bar{5}01$	34.08
2.576	2	510	34.80
2.544	18	$\bar{1}03$,420	35.25
2.484	17	402,$\bar{5}11$	36.13
2.446	2	$\bar{4}21$	36.72
2.414	7	$\bar{1}13$	37.22
2.407	8	031	37.33
2.383	16	$\bar{4}21$	37.72
2.377	17	$\bar{1}31$,230	37.81
2.369	15	$\bar{3}22$,113	37.95
2.328	3	$\bar{2}13$	38.64
2.282	5	$\bar{2}31$,600	39.46
2.220	3	520	40.60
2.214	7	330	40.72
2.196	5	$\bar{5}12$,$\bar{3}13$	41.07
2.164	9	$\bar{4}22$	41.70
2.161	15	$\bar{5}21$	41.77
2.144	3	$\bar{3}31$	42.12
2.134	4	$\bar{6}11$	42.31
2.116	5	032,$\bar{1}23$	42.70
2.111	3	331	42.80
2.083	3	123	43.41

Rubidium Chromium Oxide, $Rb_2Cr_2O_7$ (continued)

d(Å)	I	hkℓ	2θ(°)
2.058	6	$\bar{2}23$	43.97
2.037	4	430	44.45
2.014	6	$\bar{6}02$	44.98
2.002	13	232,223	45.27
1.985	3	$\bar{4}31$	45.66
1.963	4	$\bar{5}22,\bar{3}23$	46.22
1.957	3	620	46.37
1.948	6	$\bar{6}12$	46.59
1.929	3	413,$\bar{5}03$	47.08
1.922	5	$\bar{7}01$,004	47.25
1.894	6	710	48.00
1.879	4	$\bar{2}04$	48.41
1.869	5	701,$\bar{5}13$	48.67
1.864	5	$\bar{7}11$,014	48.83
1.844	4	$\bar{4}23$,041	49.38
1.830	8	240	49.79
1.824	10	$\bar{2}14,\bar{5}31$ +	49.97
1.815	6	711	50.24
1.795	2	$\bar{1}33$	50.82
1.779	5	$\bar{6}22$	51.32
1.768	8	513,423	51.66
1.738	1	720,$\bar{7}12$	52.62
1.710	4	$\bar{6}13$,622	53.56
1.7005	8	$\bar{5}32,\bar{3}33$ +	53.87
1.6767	5	721,$\bar{4}14$	54.70
1.6624	3	$\bar{2}42$,712	55.21
1.6505	3	$\bar{8}11$	55.64
1.6397	3	631,523	56.04
1.6338	3	$\bar{3}24,\bar{4}41$	56.26
1.6177	2	613	56.87
1.6118	2	$\bar{8}11$	57.10
1.6000	1	$\bar{7}03$	57.56
1.5600	2	820	59.18
1.5472	3	730	59.72

Rubidium Iodate, $RbIO_3$

Sample
The sample was prepared by adding HIO_3 to a solution of Rb_2CO_3.

Color
Colorless

Structure
Hexagonal, R3m (160), Z=3, distorted perovskite structure [Bousquet et al., 1967]. The structure of $RbIO_3$ has been determined by Alcock [1972].

Lattice constants of this sample:
a = 6.413(4) Å
c = 7.8920(8)

c/a = 1.2306

Volume
260.37 $Å^3$

Density
(calculated) 4.614 g/cm^3

Reference intensity
$I/I_{corundum}$ = 6.6(8)

Additional pattern
1. PDF card 20-997 [Bousquet et al., 1967]

References
Alcock, N. W. (1972). Acta Crystallogr. B28, 2783.
Bousquet, J., Rivière, R., and Remy, J. C. (1967). C. R. Acad. Sci. Ser. C 265, 712.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.539	17	1 0 1	19.54
3.212	100	0 1 2	27.75
3.205	95	1 1 0	27.81
2.631	2	0 0 3	34.05
2.271	35	2 0 2	39.65
2.033	3	1 1 3	44.53
2.029	3	2 1 1	44.63
1.860	13	1 0 4	48.93
1.853M	30	1 2 2	49.14
1.853M		3 0 0	49.14
1.6079	7	0 2 4	57.25
1.6035	9	2 2 0	57.42
1.5186	2	0 1 5	60.96
1.5135	2	3 0 3	61.19
1.4372	10	2 1 4	64.82
1.4346	13	3 1 2	64.95
1.3726	1	2 0 5	68.28
1.3692	1	2 2 3	68.47
1.3156	1	0 0 6	71.68
1.3094	2	0 4 2	72.07
1.2615	1	1 2 5	75.27
1.2575	1	3 2 1	75.55
1.2171	3	1 1 6	78.53
1.2138	7	1 3 4	78.78
1.2122M	9	2 3 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

Rubidium Lead Molybdenum Oxide, $Rb_2Pb(MoO_4)_2$

Sample
The sample was prepared by heating MoO_3 and combining it with $PbCO_3$ and Rb_2CO_3. The mixture was heated to 700 °C, then ground and heated at 700 PC for 15 hours.

Color
Colorless

Structure
Monoclinic, C-centered [Hubbard and Sadowski, 1977]. It has a rhombohedral sub-cell very similar to that of palmierite, $K_2Pb(SO_4)_2$.

Lattice constants of this sample:
a = 14.905(5) Å
b = 6.070(3)
c = 10.477(3)
β = 103.55(3)°

a/b = 2.4555
c/b = 1.7260

Volume
921.52 $Å^3$

Density
(calculated) 5.031 g/cm^3, assuming Z = 4

Reference
Hubbard, C. R. and Sadowski, L. (1977). Private communication.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
7.23	11	2 0 0	12.24
6.67	1L	-2 0 1	13.26
5.342	1	2 0 1	16.58
5.090	2	0 0 2	17.41
4.719M	13	1 1 1	18.79
4.719M		-2 0 2	18.79
3.778+	2	3 1 0	23.53
3.778+		-3 1 1	23.53
3.697	1	-4 0 1	24.05
3.607	1	1 1 2	24.66
3.346+	100	3 1 1	26.62
3.346+		-4 0 2	26.62
3.184	1	4 0 1	28.00
3.029	85	-1 1 3	29.47
2.794M	7	-3 1 3	32.01
2.794M		1 1 3	32.01
2.671M	2	-5 1 1	33.52
2.671M		4 0 2	33.52
2.617	2	5 1 0	34.24
2.606	2	0 2 2	34.38
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
2.199	1	4 2 1	41.02
2.149	1	5 1 2	42.00
2.009M	18	-7 1 1	45.10
2.009M		6 0 2	45.10
1.975	1	-2 2 4	45.91
1.951M	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		5 1 5	63.47
1.4492	2	10 0 0	64.22
1.4088M	1	-10 0 4	66.29
1.4088M		7 1 4	66.29
1.3798	7	-5 3 5	67.87

Rubidium Strontium Chromium Oxide, $Rb_2Sr(CrO_4)_2$

Sample
Stoichiometric amounts of Rb_2CrO_4, $SrCO_3$ and CrO_3 were dissolved in water and evaporated to dryness. The product was heated to 750 °C for 4 hours, reground and briefly heated to 850 °C where it had melted.

Color
Vivid yellow

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3. It is isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

Lattice constants of this sample:
a = 5.7455(5)Å
c = 21.854(2)

c/a = 3.8037

Volume
624.75 Å^3

Density
(calculated) 3.911 g/cm^3

Reference intensity
$I/I_{corundum}$ = 3.7(3)

Additional pattern
1. PDF card 19-1093 [Schwarz, 1966].

References
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 41.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
7.28	1	0 0 3	12.14
4.852	2	1 0 1	18.27
3.676	2	1 0 4	24.19
3.283	100	0 1 5	27.14
2.674	70	1 1 0	31.09
2.473	1L	0 2 1	36.30
2.426M	8	0 0 9	37.02
2.426M		2 0 2	37.02
2.395	2	0 1 8	37.53
2.263	8	0 2 4	39.80
2.255	10	1 1 6	39.94
2.161	35	2 0 5	41.76
2.0007	25	1 0 10	45.29
1.8547M	1	1 1 9	49.08
1.8547M		1 2 2	49.08
1.8445	1	0 1 11	49.37
1.8203	1L	0 0 12	50.07
1.7279	17	1 2 5	52.95
1.6585	10	3 0 0	55.35
1.6421	6	0 2 10	55.95
1.6107	1L	2 1 7	57.14
1.5094	2	3 0 6	61.37
1.4569	2	0 0 15	63.84
1.4366	8	2 2 0	64.85
1.4253	11	2 1 10	65.43
1.3160	6	3 1 5	71.65
1.2996	8	1 1 15	72.70
1.1974	3	0 2 16	80.08
1.1671	4	1 3 10	82.60
1.1052	3	2 1 16	88.37
1.0946	2	3 0 15	89.45
1.0856	2	4 1 0	90.40
1.0666	2	1 3 13	92.47

Rubidium Strontium Sulfate, $Rb_2Sr(SO_4)_2$

Sample
Prepared by dissolving 4.5 g Rb_2SO_4 in 10 ml water, adding 0.5 g $SrCl_2 \cdot 2H_2O$ dropwise with stirring, and then stirring for 8 days at room temperature. The product was suction-filtered and dried thoroughly on blotting paper. [According to Schwarz, 1966].

Color
Colorless

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

Lattice constants of this sample:
a = 5.5543(1)A
c = 21.572(1)

c/a = 3.8838

Volume
576.34 $Å^3$

Density
(calculated) 3.895 g/cm^3

Reference intensity
$I/I_{corundum}$ = 5.1(2)

Additional pattern
1. PDF card 19-1095 [Schwarz, 1966].

References
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 41.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.699	4	1 0 1	18.87
3.594M	1	0 0 6	24.75
3.594M		1 0 4	24.75
3.212	100	0 1 5	27.75
2.779	65	1 1 0	32.19
2.594	1L	1 0 7	34.55
2.398	4	0 0 9	37.48
2.352	8	0 1 8	38.24
2.348	9	2 0 2	38.31
2.197M	20	1 1 6	41.04
2.197M		0 2 4	41.04
2.1013	25	2 0 5	43.01
1.9682	25	1 0 10	46.08
1.8965	1	0 2 7	47.93
1.8145	5	1 1 9	50.24
1.8118	5	2 1 1	50.32
1.7972	1	0 0 12	50.76
1.7949	1	2 0 8	50.83
1.7230	1L	2 1 4	53.11
1.6755	15	1 2 5	54.74
1.6056	10	0 2 10	57.34
1.6030	10	3 0 0	57.44
1.5660M	1	2 1 7	58.93
1.5660M		3 0 3	58.93
1.5195	1L	2 0 11	60.92
1.5097	1L	1 1 12	61.36
1.5075	1L	1 2 8	61.46
1.4674	1	0 1 14	63.33
1.4645	2	3 0 6	63.47
1.4382	2	0 0 15	64.77
1.3901	15	2 1 10	67.30
1.3330M	2	1 2 11	70.60
1.3330M		3 0 9	70.60
1.2985	1L	1 0 16	72.77
1.2955M	1L	2 2 6	72.97
1.2955M		1 3 4	72.97
1.2772	10	1 1 15	74.19
1.2748	10	3 1 5	74.35
1.2015	1	2 2 9	79.75
1.1759M	1	0 2 16	81.85
1.1759M		1 2 14	81.85
1.1582	2	0 4 5	83.38
1.1346	4	1 3 10	85.52
1.1049	1	1 0 19	88.40
1.0705	5	3 0 15	92.03
1.0691	4	2 3 5	92.19
1.0525	2	0 1 20	94.09
1.0498	4	4 1 0	94.41
1.0405	1	1 2 17	95.52
1.0076	1	4 1 6	99.72
.9989	3	2 2 15	100.91
.9841	2	2 0 20	103.02
.9824	3	3 2 10	103.28
.9634	1	1 1 21	106.17
.9612	1	0 5 1	106.52
.9483	1	1 3 16	108.64
.9389	1	5 0 5	110.25
.9277	2	1 2 20	112.27
.9256	2	3 3 0	112.65

Sodium Acetate Hydrate, $C_2H_3NaO_2 \cdot 3H_2O$

Sample
The sample was reagent material from Allied Chemical and Dye Corp., New York.

Color
Colorless

Optical data
Biaxial (-), N_α = 1.448, N_γ = 1.484, 2V is very large.

Structure
Monoclinic, C2/c (15), Z = 8 [Kálmán, 1965; Mannan and Rahaman, 1972].

Lattice constants of this sample:
a = 12.358(3) Å
b = 10.450(3)
c = 10.414(2)
β = 111.75(2)°

a/b = 1.1826
c/b = 0.9966

Volume
1249.0 Å^3

Density
(calculated) 1.447 g/cm^3

Additional patterns
1. PDF card 24-1043 [Hanawalt et al., 1938]
2. PDF card 28-1030 [Technische Physische Dienst, Delft, Holland, 1976]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Kálmán, A. (1965). Acta Crystallogr. 19, 853.
Mannan, K.M. and Rahaman, Md. O. (1972). Acta Crystallogr. B28, 320.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
7.72	55	1 1 0	11.45
6.94	8	-1 1 1	12.75
5.73	1	2 0 0	15.45
5.41	8	1 1 1	16.37
5.227	20	0 2 0	16.95
4.834	2	0 0 2	18.34
4.653	40	-1 1 2	19.06
3.943	40	-2 2 1	22.53
3.869	5	2 2 0	22.97
3.708	10	1 1 2	23.98
3.593	16	3 1 0	24.76
3.549	20	0 2 2	25.07
3.470	6	-2 2 2	25.65
3.317	13	2 2 1	26.86
3.277	2	-1 1 3	27.19
3.259	5	-1 3 1	27.34
3.166	11	2 0 2	28.16
3.052	10	1 3 1	29.24
3.004	100	-4 0 2	29.72
2.895	5	-1 3 2	30.86
2.869	10	4 0 0	31.15
2.744M	16	0 2 3	32.61
2.744M		1 1 3	32.61
2.708	12	2 2 2	33.05
2.659	30	-3 3 1	33.68
2.610	6	0 4 0	34.33
2.601	6	-2 0 4	34.45
2.554	7	-3 3 2	35.11
2.524	14	0 4 1	35.54
2.498	5	3 1 2	35.92
2.455	20	-1 3 3	36.58
2.420	11	0 0 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 0	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	6	-2 4 3	43.66
2.057+	7	-5 1 4	43.98
2.057+		1 5 0	43.98
2.031	17	0 4 3	44.58
2.001	1	-5 3 1	45.28
1.983	4	4 2 2	45.72
1.932M	8	4 4 0	47.00
1.932M		-5 3 3	47.00
1.915	1	-6 2 2	47.44

d(Å)	I	hkℓ			2θ(°)
1.887	6	-6	2	1	48.18
1.877M	7	-6	0	4	48.47
1.877M		-4	4	3	48.47
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		6	2	0	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 Aluminum Sulfate Hydrate (Soda alum), $NaAl(SO_4)_2 \cdot 12H_2O$

Sample
The sample was prepared by slow evaporation of a 1:1 molar aqueous solution of Na_2SO_4 and $Al_2(SO_4)_3$ at room temperature.

Color
Colorless

Structure
Cubic, Pa3 (205), Z = 4 [Lipson, 1935]. The structure was confirmed by Haussühl [1961].

Lattice constants of this sample:
a = 12.214(1) Å

Volume
1822.0 $Å^3$

Density
(calculated) 1.670 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.6(3)

Additional pattern
1. PDF card 1-397 [Hanawalt et al., 1938]

References
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Haussühl, S. (1961). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 116 371.
Lipson, H. (1935). Proc. Roy. Soc. London, A151, 347.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ			2θ(°)
7.05	7	1	1	1	12.55
6.100	2	2	0	0	14.51
5.457	4	2	1	0	16.23
4.985	4	2	1	1	17.78
4.314	100	2	2	0	20.57
4.066	3	2	2	1	21.84
3.681	4	3	1	1	24.16
3.526	14	2	2	2	25.24
3.387	4	3	0	2	26.29
3.263	6	3	2	1	27.31
3.054	5	4	0	0	29.22
2.962	35	4	1	0	30.15
2.801	1L	3	3	1	31.92
2.733	2	4	2	0	32.74
2.666	2	4	2	1	33.59
2.603	1	3	3	2	34.43
2.493	6	4	2	2	36.00
2.395	6	4	3	1	37.53
2.351	1	5	1	1	38.25
2.268	4	5	0	2	39.71
2.229	2	5	2	1	40.44
2.159	2	4	4	0	41.80
2.127	5	5	2	2	42.47
2.095	2	4	3	3	43.15
2.063	2	5	3	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	3	0	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
1.7264	1	5	4	3	53.00
1.7108	1	7	1	1	53.52
1.6621	1	7	2	1	55.22
1.6322	7	6	4	2	56.32
1.6185	1	7	2	2	56.84
1.5904	1	7	3	1	57.94
1.5641	1	6	5	0	59.01
1.5512	1	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	3	0	65.19
1.4197	1	8	3	1	65.72
1.3655	1	8	4	0	68.68
1.3170	1L	9	2	1	71.59

Sodium Calcium Phosphate, β-$NaCaPO_4$

Sample
The sample was made by heating a 1:2:2 molar mixture of Na_2CO_3, $CaCO_3$ and $(NH_4)_2HPO_4$ to 900 °C, grinding and reheating to 650 °C for 18 hours. This material is also called rhenanite [Ando and Matsuno, 1968].

Color
Colorless

Structure
Orthorhombic, Pnam (62), Z = 4, isostructural with β-K_2SO_4 [Bredig, 1942]. The structure was studied by Bredig [1942].

Lattice constants of this sample:
a = 6.797(1) Å
b = 9.165(2)
c = 5.406(1)

a/b = 0.7416
c/b = 0.5899

Volume
336.8 $Å^3$

Density
(calculated) 3.117 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.1(1)

Additional patterns
1. PDF card 2-904 [Klement and Dihn, 1938].
2. PDF card 3-762 [Bredig, 1942].

Polymorphism
Above about 650° β-$NaCaPO_4$ transforms to an α form. [Bredig, 1942; Ando and Matsuno, 1968].

References
Ando, J. and Matsuno, S. (1968). Bull. Chem. Soc. Jap. 41, 345.
Bredig, M. A. (1942). J. Phys. Chem. 46, 744.
Klement, R. and Dihn, P. (1938). Z. Anorg. Allg. Chem. 240, 40.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.460	7	1 1 0	16.22
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
2.701	55	0 0 2	33.14
2.660	80	0 3 1	33.66
2.437	2	2 2 1	36.86
2.423	5	1 1 2	37.08
2.329	10	0 2 2	38.62
2.272	15	2 3 0	39.63
2.200	35	3 1 0	41.00
2.171	8	1 4 0	41.56
2.115	7	2 0 2	42.72
2.062	7	2 1 2	43.88
2.036	11	3 1 1	44.47
2.031	13	3 2 0	44.58
2.015	30	1 4 1	44.95
1.940	12	1 3 2	46.79
1.921	35	2 2 2	47.28
1.900M	10	3 2 1	47.84
1.900M		2 4 0	47.84
1.8196	3	3 3 0	50.09
1.7695M	6	1 5 0	51.61
1.7695M		0 1 3	51.61
1.7395	11	2 3 2	52.57
1.7058	9	3 1 2	53.69
1.6996	11	4 0 0	53.90
1.6710	2	4 1 0	54.90
1.6290	1	1 2 3	56.44
1.6136	3	2 5 0	57.03
1.5931M	5	4 2 0	57.83
1.5931M		2 0 3	57.83
1.5689	6	2 1 3	58.81
1.5526	12	0 3 3	59.49
1.5443	9	3 4 1	59.84
1.5275M	2	0 6 0	60.57
1.5275M		4 2 1	60.57
1.4853	5	4 3 0	62.48
1.4808	6	1 5 2	62.69
1.4370	6	1 6 1	64.83
1.4319	9	4 3 1	65.09
1.4210	5	4 1 2	65.65
1.3936M	1	2 6 0	67.11
1.3936M		3 1 3	67.11
1.3861	5	1 4 3	67.52
1.3838	5	3 4 2	67.65
1.3517	7	0 0 4	69.48
1.3487	4	2 6 1	69.66
1.3296	4	0 6 2	70.81

Sodium Cobalt Nitrite, $Na_3Co(NO_2)_6$

Sample
The sample was obtained from the City Chemical Corporation, N.Y.

Color
Deep orange yellow

Structure
Hexagonal, $R\bar{3}m$ (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 Å^3

Density
(calculated) 2.559 g/cm^3

Reference intensity
$I/I_{corundum}$ = 0.81(6)

Additional pattern
1. PDF card 12-444 [Shrier, priv. comm.]

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

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.155	85	1 0 1	14.38
5.004	90	0 1 2	17.71
3.904	60	1 1 0	22.76
3.298	8	0 2 1	27.01
3.261	8	1 0 4	27.33
3.078	100	2 0 2	28.99
2.726	4	0 1 5	32.83
2.519	15	2 1 1	35.61
2.504	85	0 2 4	35.84
2.481	11	0 0 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	42.87
2.0536	9	3 0 3	44.06
1.9522	40	2 2 0	46.48
1.9400	7	1 2 5	46.79
1.8618	4	1 3 1	48.88
1.8179M	12	3 1 2	50.14
1.8179M		2 2 3	50.14
1.8005	25	0 2 7	50.66
1.7945	20	0 1 8	50.84
1.6752	18	1 3 4	54.75
1.6688	14	3 0 6	54.98
1.6538	5	0 0 9	55.52
1.6349	4	2 1 7	56.22
1.6304	4	2 0 8	56.39
1.5432	11	3 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	14	4 1 0	62.93
1.4149	4	4 1 3	65.97
1.4068	4	1 3 7	66.40
1.3624	2	0 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
1.3018	12	3 3 0	72.56
1.2864	4	2 1 10	73.57
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		3 3 3	75.40
1.2562	5	2 0 11	75.64
1.2515	3	0 4 8	75.98
1.2404	2	0 0 12	76.78
1.2319	1	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 3 8	80.54
1.1821	3	1 1 12	81.33
1.1549	5	5 1 4	83.67

Sodium Hydrogen Carbonate Hydrate, Trona, $Na_3H(CO_3)_2 \cdot 2H_2O$

Sample
The sample was a natural mineral from Sweetwater County, Wyoming. (U. S. National Museum #117729)

Color
Colorless

Structure
Monoclinic, I2/a (15), Z=4 [Brown et al., 1949]. A partial structure determination was done by Candlin [1956].

Lattice constants of this sample:
a = 20.106(4) Å
b = 3.492(1)
c = 10.333(2)
β = 103.05(2)°

a/b = 5.7577
c/b = 2.9590

Volume
706.7 $Å^3$

Density
(calculated) 2.124 g/cm^3

Reference intensity
$I/I_{corundum}$ = 0.96(2)

Additional pattern
1. PDF card 11-643 [Pabst, 1959].

References

Brown, C.J., Peiser, H. S., and Turner-Jones, A. (1949). Acta Crystallogr. 2, 167.
Candlin, R. (1956). Acta Crystallogr. 9, 545.
Pabst, A. (1959). Amer. Mineral. 44, 274.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ			2θ(°)
9.77	45	2	0	0	9.04
4.892	55	4	0	0	18.12
4.113	2	2	0	2	21.59
3.987	6	-4	0	2	22.28
3.436	2	1	1	0	25.91
3.261	6	6	0	0	27.33
3.196	20	-2	1	1	27.89
3.167	4	4	0	2	28.15
3.071	80	-6	0	2	29.05
2.891	1	-1	1	2	30.91
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
2.510	12	3	1	2	35.74
2.472	6	-5	1	2	36.32
2.444	30	-2	1	3	36.74
2.426	13	-8	0	2	37.02
2.254	30	-6	0	4	39.96
2.185M	2	5	1	2	41.29
2.185M		7	1	0	41.29
2.146	5	-7	1	2	42.08
2.116	2	-6	1	3	42.69
2.057	7	4	0	4	43.99
2.040M	18	4	1	3	44.36
2.040M		-8	1	1	44.36
2.029	30	8	0	2	44.62
1.995	8	-8	0	4	45.42
1.964	9	-5	1	4	46.18
1.959	10	10	0	0	46.31
1.885	7	7	1	2	48.23
1.854M	2	3	1	4	49.11
1.854M		-9	1	2	49.11
1.8480	3	9	1	0	49.27
1.8058	2	6	0	4	50.50
1.7785	10	-2	1	5	51.33
1.7425	16	-10	1	1	52.47
1.7197+	4	-2	0	6	53.22
1.7197+		-1	2	1	53.22
1.6883	2	5	1	4	54.29
1.6806	4	-6	1	5	54.56
1.6618	14	2	1	5	55.23
1.6516	5	-6	0	6	55.60
1.6354	3	9	1	2	56.20
1.6325M	3	12	0	0	56.31
1.6325M		10	1	1	56.31
1.5977	8	-5	2	1	57.65
1.5949M	9	8	1	3	57.76
1.5949M		2	0	6	57.76
1.5846	3	8	0	4	58.17
1.5573M	2	-8	0	6	59.29
1.5573M		-1	2	3	59.29
1.5318M	1	-1	1	6	60.38
1.5318M		1	2	3	60.38
1.5184M	3	-5	1	6	60.97
1.5184M		-6	2	2	60.97
1.4921	2	-7	2	1	62.16
1.4344M	2	0	2	4	64.96
1.4344M		-14	0	2	64.96
1.4214M	1	12	1	1	65.63
1.4214M		8	2	0	65.63
1.3991	9	14	0	0	66.81

Sodium Magnesium Sulfate (Vanthoffite), $Na_6Mg(SO_4)_4$

Sample
The sample was prepared by melting a 3:1 molar mixture of Na_2SO_4 and $MgSO_4$ at about 800 °C. This was followed by heating for 15 hrs. at 450 °C, grinding and reheating again for 15 hrs. at 450 °C. As this phase both melts and dissolves incongruently, it is difficult to prepare pure and several weak peaks of impurities were present. The strongest of these was at 25.05° (2θ) and had an intensity of about 9.

Color
Colorless

Structure
Monoclinic, $P2_1/c(14)$, Z = 2. The structure was determined by Fischer and Hellner [1964].

Lattice constants of this sample:
a = 9.781(2) Å
b = 9.196(2)
c = 8.197(2)
β = 113.61(2)°

a/b = 1.0636
c/b = .8914

Volume
675.5 Å^3

Density
(calculated) 2.687 g/cm^3

Reference intensity
$I/I_{corundum}$ = 0.64(5)

Additional pattern
1. PDF card 21-1138 [Madsen, 1966].

References
Fischer, W., and Hellner, E. (1964). Acta Crystallogr. 17, 1613.
Madsen, B. M. (1966). U. S. Geol. Surv. Prof. Pap. 550B, 125.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
8.94	9	100	9.89
5.81	20	011	15.25
4.595	12	020	19.30
4.478	5	200	19.81
4.241	25	$\bar{2}11$	20.93
4.090	20	$\bar{1}02,120$	21.71
4.032	95	210	22.03
3.917	70	021	22.68
3.754	15	002	23.68
3.477	25	012	25.60
3.431	100	$\bar{2}12$	25.95
3.346	8	$\bar{1}21$	26.62
3.314	3	$\bar{2}21$	26.88
3.114	75	$\bar{2}11$	28.64
3.057	50	$\bar{1}22,102$	29.19
2.995	50	$\bar{3}02$	29.81
2.909	70	022	30.71
2.901	50	130,112	30.80
2.846	60	$\bar{3}12$	31.41
2.832	60	$\bar{1}31$	31.57
2.684	25	$\bar{2}21$	33.36
2.582	40	$\bar{2}13,\bar{2}31$	34.71
2.545	11	$\bar{1}22$	35.23
2.455	25	$\bar{1}32$	36.58
2.377	11	311,032	37.82
2.359	12	$\bar{2}32$	38.12
2.324	12	$\bar{2}23$	38.72
2.315	14	$\bar{4}12$	38.87
2.299	12	040	39.16
2.250	13	231	40.05
2.243	14	400	40.17
2.196	10	$\bar{1}41$	41.07
2.171	18	$\bar{3}23$	41.56
2.149	9	$\bar{4}21$	42.00
2.122	5	$\bar{4}22$	42.58
2.073	6	$\bar{2}41$	43.63
2.048	4	$\bar{2}04$	44.18
2.045	3	$\bar{2}40$	44.25
2.004	8	$\bar{1}04,\bar{1}42$	45.20
2.000	4	$\bar{2}14$	45.31
1.982	4	302	45.73
1.961	12	042,$\bar{1}14$	46.27
1.950	12	$\bar{5}02,\bar{4}23$	46.54
1.945	15	$\bar{3}14$	46.66
1.909	6	232,$\bar{5}12$	47.60
1.886	14	$\bar{5}11,\bar{4}32$	48.21
1.850	12	$\bar{4}04$	49.21
1.837	17	$\bar{1}42$	49.58
1.825	35	$\bar{3}24$	49.93
1.802	5	150	50.61
1.794	6	$\bar{5}22$	50.86
1.777	8	$\bar{5}21$	51.37
1.761	9	$\bar{4}33$	51.89
1.720	11	$\bar{1}51$	53.22
1.7153	10	$\bar{5}23,\bar{4}24$	53.37
1.6789	11	341,$\bar{1}34$	54.62
1.6741	8	$\bar{5}04$	54.79
1.6470	2	$\bar{5}14,\bar{2}52$	55.77

Strontium Vanadium Oxide, $Sr_3(VO_4)_2$

Sample
The sample was prepared by heating a stoichiometric mixture of $Sr(OH)_2$ and V_2O_5 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 $Sr_3(PO_4)_2$ and other similar phosphates, vanadates and arsenates [Durif, 1959]. The structure of $Sr_3(PO_4)_2$ was determined by Zachariasen [1948].

Lattice constants of this sample:
a = 5.6197(2) Å
c = 20.103(2)

c/a = 3.5772

Volume
549.81 Å^3

Density
(calculated) 4.464 g/cm^3

Additional patterns
1. PDF card 19-1289 [Lubin and Rittershaus, Gen. Tel. and Electronics, N. Y. (1966)]
2. Durif [1959]

References
Durif, A. (1959). Acta Crystallogr. 12, 420.
Zachariasen, W. H. (1948). Acta Crystallogr. 1, 263.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
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	1	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
1.2095	6	1·1·15	79.12
1.1892	1	229,318	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	3·0·15	96.39
1.0169	<1	1·3·13	98.49
1.0124	<1	416	99.08

Thallium Lead Sulfate, $Tl_2Pb(SO_4)_2$

Sample
The sample was precipitated by adding an aqueous solution of lead acetate to a concentrated solution of Tl_2SO_4.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Sr_3(PO_4)_2$ and many other double sulfates and chromates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

Lattice constants of this sample:
a = 5.626(1) Å
c = 22.047(3)

c/a = 3.9188

Volume
604.36 $Å^3$

Density
(calculated) 6.661 g/cm^3

Reference intensity
$I/I_{corundum}$ = 9.3(4)

Additional pattern
1. PDF card 20-1262 [Schwarz, 1966]

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
7.34	2	0 0 3	12.05
4.759	20	1 0 1	18.63
4.462	5	0 1 2	19.88
3.676	9	0 0 6	24.19
3.648	19	1 0 4	24.38
3.271	100	0 1 5	27.24
2.812	50	1 1 0	31.80
2.647	3	1 0 7	33.84
2.448	6	0 0 9	36.68
2.401	3	0 1 8	37.43
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	0 0 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

Thallium Strontium Sulfate, $Tl_2Sr(SO_4)_2$

Sample
The sample was precipitated by adding a solution of $Sr(NO_3)_2$ to a concentrated solution of Tl_2SO_4.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Sr_3(PO_4)_2$ and many other double chromates and sulfates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ 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 A^3

Density
(calculated) 5.728 g/cm^3

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.

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

Internal standard W, a = 3.16524 A

d(A)	I	hkℓ	2θ(°)
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	300,1·0·13	57.15
1.5826	3	217	58.25
1.5418	3	1·1·12	59.95
1.5259	1	128	60.64
1.5068	<1	0·1·14	61.49
1.4797	2	0·0·15	62.74
1.4768	2	306	62.88
1.4105	6	2·1·10	66.20
1.3953	3	220,0·2·13	67.02
1.3715	<1	223	68.34
1.3489	1	309	69.65
1.3307	<1	312	70.74
1.3075	5	1·1·15	72.19
1.2834	3	315	73.77
1.2346	<1	137	77.21

Tin Arsenide, $Sn_{3.8}As_3$

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, $R\bar{3}m$ (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) Å
c = 36.079(3)

c/a = 8.822

Volume
522.56 $Å^3$

Density
(calculated) 6.442 g/cm^3

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

References

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

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

d(Å)	I	hkℓ	2θ(°)
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
2.083	25	0 1 14	43.40
2.045	25	1 1 0	44.26
2.005	1L	0 0 18	45.19
1.902	1	1 0 16	47.79
1.821M	1L	1 1 9	50.05
1.821M		0 1 17	50.05
1.7379	1L	0 2 4	52.62
1.7179	5	0 0 21	53.28
1.6912	4	1 1 12	54.19
1.6744M	12	0 2 7	54.78
1.6744M		1 0 19	54.78
1.6084	1L	0 1 20	57.23
1.5037	1L	0 0 24	61.63
1.4599	6	2 0 14	63.69
1.4344	1L	0 1 23	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 19	72.95
1.2924	5	0 1 26	73.17
1.2106M	2	1 1 24	79.03
1.2106M		1 0 28	79.03
1.2026	1	0 0 30	79.66
1.1880	4	1 2 14	80.84
1.1808	2	3 0 0	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	3 0 9	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	1L	1 1 30	95.99
1.0224	1	2 2 0	97.77
1.0182M	1L	1 2 23	98.32
1.0182M		2 0 29	98.32
.9897	1	0 1 35	102.22
.9729	1	3 0 21	104.70
.9678	2	2 2 12	105.48
.9648	2	1 3 7	105.96
.9640	2	1 1 33	106.08

Aluminum Plutonium, Al_3Pu

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 6. The structure was determined by Larson, Cromer and Stambaugh [1957].

Atom positions
12(k) 12 aluminum
6(h) 6 aluminum
4(f) 4 plutonium
2(b) 2 plutonium [ibid.]

Polymorphism
There are altogether 4 polymorphs: α-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 Å
c = 14.411

c/a = 2.3691

(published values: a = 6.083 Å, c = 14.410 [Runnalls, 1965])

Volume
461.8 $Å^3$

Density
(calculated) 6.967 g/cm^3

Thermal parameters
Isotropic: aluminum B = 0.977; plutonium B = 0.366 [Larson et al., 1957].

Scattering factors
Al^0 [International Tables, 1962]
Pu^0 [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, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Larson, A. C., Cromer, D. T. and Stambaugh, C. K. (1957). Acta Crystallogr. 10, 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 (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.946	55	1 0 1	17.92
4.251	100	1 0 2	20.88
3.548	100	1 0 3	25.08
3.042	90	1 1 0	29.34
2.972	50	1 0 4	30.04
2.590	25	2 0 1	34.60
2.528	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 3	38.96
2.126	40	2 0 4	42.48
1.972	10	2 1 1	45.98
1.944	5	2 0 5	46.68
1.919	25	2 1 2+	47.34
1.885	40	1 1 6	48.24
1.839	20	2 1 3	49.52
1.756	15	3 0 0	52.04
1.743	20	2 1 4	52.46
1.704	5	1 0 8	53.74
1.638	1	2 1 5	56.10
1.622	5	2 0 7	56.70
1.550	1	1 1 8	59.60
1.532	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	3 1 1	64.00
1.432	10	3 1 2+	65.10
1.417	15	3 0 6	65.84
1.398	10	3 1 3	66.88
1.390	5	1 0 10	67.30
1.368	10	2 0 9	68.52
1.354	5	3 1 4	69.34
1.336	5	2 1 8	70.44
1.311	1	4 0 1	71.94
1.303	1	3 1 5+	72.50
1.296	5	4 0 2	72.96
1.285	20	2 2 6	73.68
1.270	5	4 0 3	74.68
1.264	5	2 0 10	75.08
1.248	5	2 1 9	76.24
1.237	5	4 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	5	3 2 2+	80.54
1.172	5	3 2 3	82.18
1.167	5	2 1 10	82.58

Aluminum Plutonium, Al_3Pu - (continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.948	50	1	0	1	17.91
4.253	100	1	0	2	20.87
3.550	100	1	0	3	25.07
3.042	95	1	1	0	29.34
2.974	55	1	0	4	30.02
2.591	30	2	0	1	34.59
2.529	5	1	0	5	35.47
2.474	65	2	0	2	36.28
2.402	40	0	0	6	37.41
2.324	1	1	1	4	38.71
2.310	75	2	0	3	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	65.09
1.431	10	2	1	7	65.12
1.418	15	3	0	6	65.83
1.398	10	3	1	3	66.88
1.390	5	1	0	10	67.31
1.368	10	2	0	9	68.52
1.354	10	3	1	4	69.35
1.336	5	2	1	8	70.43
1.312	5	4	0	1	71.93
1.296	5	4	0	2	72.96
1.285	30	2	2	6	73.67
1.270	10	4	0	3	74.67
1.264	10	2	0	10	75.08
1.248	5	2	1	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 Rhenium, AlRe

Structure
Cubic, Pm3m (221), Z = 1, isostructural with CsCl and AlRu [Obrowski, 1960].

Atom positions
1(a) 1 aluminum
1(b) 1 rhenium

Lattice constant
a = 2.88 A [ibid.]

Volume
23.89 $\mathring{A}^3$

Density
(calculated) 14.82 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.0, rhenium B = 0.5

Scattering factors
Al^0 [Cromer and Mann, 1968]
Re^0 [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 2.186 \times 10^{-3}$

References

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.
Obrowski, W. (1960). Naturwissenschaften, 47, 14.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.88	80	1 0 0	31.04
2.04	100	1 1 0	44.46
1.66	20	1 1 1	55.20
1.44	15	2 0 0	64.68
1.29	25	2 1 0	73.46
1.18	25	2 1 1	81.86
1.02	10	2 2 0	98.32
.960	15	2 2 1+	106.72
.911	15	3 1 0	115.52
.868	10	3 1 1	125.02
.831	5	2 2 2	135.80
.799	10	3 2 0	149.32

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.88	75	1 0 0	31.03
2.04	100	1 1 0	44.45
1.66	20	1 1 1	55.20
1.44	15	2 0 0	64.68
1.29	25	2 1 0	73.46
1.18	30	2 1 1	81.86
1.02	10	2 2 0	98.31
.960	5	3 0 0	106.72
.960	15	2 2 1	106.72
.911	20	3 1 0	115.52
.868	15	3 1 1	125.02
.831	10	2 2 2	135.80
.799	25	3 2 0	149.31

Aluminum Rhenium, $Al_{12}Re$

Structure
Cubic, Im3 (204), Z = 2, isostructural with $Al_{12}W$. The structure was determined by Walford [1964].

Atom positions
24(g) 24 aluminum
2(a) 2 rhenium [ibid.]

Lattice constant
a = 7.5275(5) Å
(published value 7.5270(5) Å [ibid.])

Volume
426.53 $Å^3$

Density
(calculated) 3.971 g/cm^3
(measured) 3.90 g/cm^3 [Walford, 1964]

Thermal parameters
Isotropic: aluminum B = 1.0; rhenium B = 0.5

Scattering factors
Al^0, Re^0 [Forsyth and Wells, 1959]

Scale factors (integrated intensities)
$\gamma = 1.375 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 8.28

Additional pattern
1. PDF card 18-55 [d'Alte da Veiga, Cavendish Lab., Cambridge, Eng.]. It gives a space group Im3m which is apparently an error and incompatible with intensities calculated in Im3.

References
Forsyth, J.B. and Wells, M. (1959). Acta Crystallogr. 12, 412.
Walford, L. K. (1964). Acta Crystallogr. 17, 57.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.32	100	1 1 0	16.66
3.764	13	2 0 0	23.62
3.072	44	2 1 1	29.04
2.6605	4	2 2 0	33.66
2.3805	47	3 1 0	37.76
2.1732	21	2 2 2	41.52
2.0120	47	3 2 1+	45.02
1.8821	7	4 0 0	48.32
1.7743	9	4 1 1+	51.46
1.6829	3	4 2 0+	54.48
1.6051	2	3 3 2	57.36
1.5364	8	4 2 2	60.18
1.4764	15	4 3 1+	62.90
1.3743	5	1 2 5+	68.18
1.3307	2	4 4 0	70.74
1.2911	9	0 3 5	73.26
1.2545	5	6 0 0+	75.76
1.2211	13	5 3 2+	78.22
1.1902	1	0 2 6+	80.66
1.1616	3	5 4 1+	83.08
1.1348	1	6 2 2	85.50
1.1099	5	6 3 1+	87.90
1.0646	8	5 4 3+	92.70
1.0440	2	0 4 6+	95.10
1.0244	4	7 2 1+	97.52
1.0058	2	6 4 2+	99.96
.9884	1	0 3 7+	102.40
.9560	3	7 3 2+	107.36
.9265	4	1 4 7+	112.48
.9128	2	6 4 4+	115.10
.8997	5	3 5 6+	117.78
.8871	5	8 2 2+	120.52
.8750	6	1 3 8+	123.36
.8523	3	2 5 7+	129.32
.8313	1	9 1 0+	135.84
.8213	3	2 4 8+	139.40
.8117	5	1 6 7+	143.24
.8024	1	6 6 4	147.46

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
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	3	0	1	3	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	3	3	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	3	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	3	3	73.27
1.2910	11	0	3	5	73.27
1.2546	4	6	0	0	75.76
1.2546	3	4	4	2	75.76
1.2211	14	5	3	2	78.22
1.2211	3	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	3	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	3	3	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
.9560	2	7	3	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	3	117.78
.8997	7	3	5	6	117.78
.8871	3	6	6	0	120.53
.8871	6	8	2	2	120.53
.8751	3	7	5	0	123.35
.8751	5	1	3	8	123.35
.8751	1	8	3	1	123.35
.8751	1	7	4	3	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

Structure
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 $Al_{1.146}Rh_{.854}$ and a lattice constant a = 2.968 [Ferro et al., 1964].

Atom positions
1(a) 1 aluminum
1(b) 1 rhodium

Lattice constant
a = 2.980 Å

Volume
26.46 $Å^3$

Density
(calculated) 8.149 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.0; rhodium B = 0.5

Scattering factors
Al^0 [Cromer and Mann, 1968]
Rh^0 [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 1.344 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Ferro, R., Rambaldi, G., and Capelli, R. (1964). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. 36, 491.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 100.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.98	55	1 0 0	29.96
2.107	100	1 1 0	42.88
1.720	10	1 1 1	53.20
1.490	15	2 0 0	62.26
1.333	15	2 1 0	70.62
1.217	25	2 1 1	78.56
1.054	10	2 2 0	93.96
.993	5	2 2 1+	101.70
.942	10	3 1 0	109.66
.898	5	3 1 1	118.04
.860	5	2 2 2	127.12
.826	5	3 2 0	137.50
.796	20	3 2 1	150.56

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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
1(a) 1 aluminum
1(b) 1 ruthenium

Lattice constant
a = 2.95 Å [ibid.]

Volume
25.67 $Å^3$

Density
(calculated) 8.28 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.0; ruthenium B = 0.5.

Scattering factors
Al^0 [Cromer and Mann, 1968]
Ru^0 [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 (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.95	55	1 0 0	30.28
2.09	100	1 1 0	43.34
1.70	10	1 1 1	53.78
1.48	15	2 0 0	62.96
1.32	10	2 1 0	71.44
1.20	25	2 1 1	79.52
1.04	10	2 2 0	95.22
.983	5	2 2 1+	103.14
.933	10	3 1 0	111.32
.889	5	3 1 1	120.00
.852	5	2 2 2	129.52
.818	5	3 2 0	140.60
.788	25	3 2 1	155.38

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.95	50	1 0 0	30.27
2.09	100	1 1 0	43.34
1.70	10	1 1 1	53.78
1.47	15	2 0 0	62.96
1.32	15	2 1 0	71.45
1.20	30	2 1 1	79.53
1.04	10	2 2 0	95.22
.983	1	3 0 0	103.14
.983	5	2 2 1	103.14
.933	15	3 1 0	111.32
.889	5	3 1 1	120.00
.852	5	2 2 2	129.52
.818	10	3 2 0	140.60
.788	65	3 2 1	155.38

Aluminum Ruthenium, Al_6Ru

Structure
Orthorhombic, Cmcm (63), Z = 4, isostructural with Al_6Mn. The structure was determined by Edshammer [1968].

Atom positions
4(c) 4 ruthenium
8(e) 8 aluminum(1)
8(f) 8 aluminum(2)
8(g) 8 aluminum(3) [ibid.]

Lattice constants
a = 7.4886(4) Å
b = 6.5563(3)
c = 8.9610(5)

(published values: a = 7.4882(4)Å, b = 6.5559(3), c = 8.9605(5) [Edshammar, 1968]).

CD cell: a=7.4886(4)Å, b=8.9610(5), c=6.5563(3), sp. gp. Bmmb(63); a/b = 0.8357; c/b = 0.7316

Volume
439.96 $Å^3$

Density
(calculated) 3.970 g/cm^3

Thermal parameters
Isotropic [Edshammar, 1968]

Scattering factors
Al^0, Ru^0 [Cromer and Mann, 1968]

Scale factors (integrated intensities)
$\gamma = 0.343 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 2.15

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Edshammar, L.-E. (1968). Acta Chem. Scand. 22, 2374.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.9295	100	1 1 0	17.98
4.4803	42	0 0 2	19.80
4.3206	16	1 1 1	20.54
3.7418	26	2 0 0	23.76
3.3166	66	1 1 2	26.86
3.2783	22	0 2 0	27.18
3.0786	8	0 2 1	28.98
2.8734	24	2 0 2	31.10
2.5546	5	1 1 3	35.10
2.4663	12	2 2 0	36.40
2.3329	2	3 1 0	38.56
2.2576	27	3 1 1	39.90
2.2404	22	0 0 4	40.22
2.2078	21	0 2 3	40.84
2.1603	63	2 2 2	41.78
2.0980	30	1 3 0	43.08
2.0688	66	3 1 2	43.72
2.0396	55	1 1 4+	44.38
1.9013	13	2 2 3+	47.80
1.8719	7	4 0 0	48.60
1.8497	9	0 2 4	49.22
1.8385	2	3 1 3	49.54
1.7276	5	4 0 2	52.96
1.7168	4	1 3 3	53.32
1.6582	9	2 2 4	55.36
1.6440	1	3 3 0	55.88
1.6392	2	0 4 0	56.06
1.6259	3	4 2 0	56.56
1.6159	8	3 1 4+	56.94
1.5726	2	0 2 5	58.66
1.5434	5	3 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 3	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

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.2232	9	5 1 4+	78.06
1.2216	6	4 4 1	78.18
1.2167	4	1 3 6	78.56
1.2039	1	4 2 5	79.56
1.2024	1	6 0 2	79.68

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.9329	100	1 1 0	17.97
4.4805	43	0 0 2	19.80
4.3214	16	1 1 1	20.54
3.7443	28	2 0 0	23.74
3.3166	72	1 1 2	26.86
3.2781	21	0 2 0	27.18
3.0786	9	0 2 1	28.98
2.8731	27	2 0 2	31.10
2.5551	6	1 1 3	35.09
2.4664	14	2 2 0	36.40
2.3328	2	3 1 0	38.56
2.2576	32	3 1 1	39.90
2.2402	24	0 0 4	40.22
2.2079	24	0 2 3	40.84
2.1607	76	2 2 2	41.77
2.0979	36	1 3 0	43.08
2.0692	80	3 1 2	43.71
2.0427	23	1 3 1	44.31
2.0398	51	1 1 4	44.38
1.9019	11	2 2 3	47.79
1.9000	7	1 3 2	47.84
1.8721	9	4 0 0	48.59
1.8496	11	0 2 4	49.22
1.8386	2	3 1 3	49.54
1.7274	6	4 0 2	52.97
1.7168	5	1 3 3	53.32
1.6583	11	2 2 4	55.36
1.6443	1	3 3 0	55.87
1.6391	2	0 4 0	56.06
1.6257	3	4 2 0	56.57
1.6173	3	3 3 1	56.89
1.6158	9	3 1 4	56.94
1.6123	1	0 4 1	57.08
1.5725	3	0 2 5	58.66
1.5436	6	3 3 2	59.87
1.5393	1	0 4 2	60.06
1.5313	6	1 3 4	60.40
1.5282	11	4 2 2	60.54
1.4935	4	0 0 6	62.10
1.4809	12	2 4 1	62.69
1.4601	4	5 1 0	63.68
1.4499	1	2 2 5	64.19
1.4366	1	4 0 4	64.85
1.4294	2	1 1 6	65.22
1.4279	5	4 2 3	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 3	70.09
1.3228	7	0 4 4	71.23
1.3158	5	4 2 4	71.67
1.3118	1	5 1 3	71.92
1.2784	2	1 5 1	74.11
1.2775	9	2 2 6	74.16
1.2578	8	3 1 6	75.53
1.2481	5	6 0 0	76.22
1.2473	1	2 4 4	76.28
1.2354	7	5 3 0	77.14
1.2239	4	5 3 1	78.01
1.2232	9	5 1 4	78.06
1.2217	4	4 4 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

Aluminum Samarium, $AlSm_2$

Structure
Orthorhombic, Pnma(62), Z = 4, isostructural with Ni_2Si and $AlHo_2$, from powder data, [Buschow and van der Goot, 1971].

Atom positions
From geometric considerations, the atomic positions used were those for $AlHo_2$. All atoms were located in positions 4(c).

Lattice constants
a = 6.654 Å
b = 5.193
c = 9.632
(published value for c was 9.631 Å [Buschow and van der Goot, 1971])

CD cell: a = 6.654 Å, b = 9.632, c = 5.193, sp. gp. Pnam(62); a/b = 0.6908; c/b = 0.5391

Volume
332.8 $Å^3$

Density
(calculated) 6.540 g/cm^3

Thermal parameters
Isotropic: samarium B = 0.5; aluminum B = 1.0

Scattering factors
Al^0 [International Tables, 1962]
Sm^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.180 \times 10^{-3}$

References

Buschow, K.H.J. and van der Goot, A. S. (1971). J. Less-Common Metals 24, 117.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.474	1	1 0 1	16.18
4.813	1	0 0 2	18.42
4.567	15	0 1 1	19.42
3.901	20	1 0 2	22.78
3.767	45	1 1 1	23.60
3.119	35	1 1 2	28.60
2.892	15	1 0 3	30.90
2.801	30	2 1 0	31.92
2.731	100	0 1 3+	32.76
2.690	75	2 1 1	33.28
2.596	45	0 2 0	34.52
2.527	5	1 1 3	35.50
2.421	1	2 1 2	37.10
2.310	10	2 0 3	38.96
2.264	5	1 0 4	39.78
2.161	15	3 0 1+	41.76
2.075	5	1 1 4	43.58
1.995	1	3 1 1	45.42
1.951	5	2 0 4	46.52
1.932	10	1 2 3	47.00
1.884	20	2 2 2	48.28
1.850	5	1 0 5	49.20
1.825	1	3 0 3	49.94
1.806	1	0 1 5	50.50
1.743	5	1 1 5	52.46
1.726	10	2 2 3	53.02
1.707	5	1 2 4	53.66
1.661	10	3 2 1	55.26
1.651	5	1 3 1	55.64
1.639	5	4 0 1	56.06
1.632	5	3 0 4	56.34
1.605	1	0 0 6	57.36
1.587	5	2 1 5	58.06
1.583	5	1 3 2	58.24
1.573	1	4 0 2	58.66
1.556	20	3 1 4	59.34
1.535	5	2 3 0	60.22
1.524	10	0 3 3	60.74
1.516	10	2 3 1	61.06
1.505	10	4 1 2+	61.58
1.494	10	1 1 6	62.06
1.485	1	1 3 3	62.48
1.477	1	4 0 3	62.86
1.446	1	2 0 6	64.38
1.421	1	4 1 3	65.66
1.400	5	4 2 0+	66.74
1.393	1	2 1 6	67.16
1.386	5	4 2 1	67.52
1.383	5	3 2 4	67.72
1.375	1	1 3 4	68.12
1.366	1	0 2 6	68.68
1.347	1	1 0 7	69.74
1.345	1	4 2 2	69.88

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.475	1	1 0 1	16.18
4.816	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 3	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	10	1 2 2	41.75
2.161	15	3 0 1	41.76
2.111	1	2 1 3	42.81
2.076	5	1 1 4	43.57
1.995	5	3 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
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 3 1	55.64
1.639	5	4 0 1	56.06
1.631	5	3 0 4	56.35
1.605	5	0 0 6	57.35
1.587	5	2 1 5	58.06
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 3 0	60.22
1.524	15	0 3 3	60.74
1.516	15	2 3 1	61.06
1.507	10	1 2 5	61.48
1.505	10	4 1 2	61.58
1.495	10	1 1 6	62.05
1.493	1	3 2 3	62.12
1.485	1	1 3 3	62.48
1.477	1	4 0 3	62.87
1.446	1	2 0 6	64.39
1.421	5	4 1 3	65.67
1.403	1	2 2 5	66.61
1.401	5	4 2 0	66.73
1.401	1	3 1 5	66.74
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, $AlSm_3$

Structure
Cubic, Pm3m(221), Z = 1, isostructural with $AuCu_3$, $AlCe_3$ and $AlLa_3$, from powder data [Iandelli, 1959].

Atom positions
1(a) 1 aluminum
3(c) 3 samarium

Lattice constant
a = 4.901 Å [Iandelli, 1959]

Volume
117.7 $Å^3$

Density
(calculated) 6.743 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.0, samarium B = 0.5

Scattering factors
Al^0 [Cromer and Mann, 1968]
Sm^0 [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 0.737 \times 10^{-3}$

References
Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Iandelli, A. (1959). Physical Chemistry of Metallic Solutions and Intermetallic Compounds, Vol. 1. (HMSO, London), 3F. p. 2.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.), p. 100.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.897	20	1 0 0	18.10
3.464	20	1 1 0	25.70
2.829	100	1 1 1	31.60
2.451	50	2 0 0	36.64
2.191	10	2 1 0	41.16
2.001	5	2 1 1	45.28
1.732	30	2 2 0	52.80
1.634	5	2 2 1+	56.26
1.550	5	3 1 0	59.60
1.478	30	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	77.90
1.189	1	3 2 2+	80.78
1.155	1	4 1 1+	83.64
1.124	10	3 3 1	86.48
1.096	10	4 2 0	89.32
1.069	1	4 2 1	92.16
1.000	10	4 2 2	100.70
.980	1	4 3 0+	103.60
.961	1	4 3 1+	106.54
.943	10	5 1 1+	109.50
.910	1	4 3 2+	115.64
.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 3 1	136.82
.817	10	4 4 2+	141.14
.795	1	5 3 2+	151.34

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.901	20	1	0	0	18.09
3.466	15	1	1	0	25.69
2.830	100	1	1	1	31.59
2.451	50	2	0	0	36.64
2.192	10	2	1	0	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	3	132.83
.828	25	5	3	1	136.82
.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

Structure
Cubic, Fd3m(227), Z = 8, a Laves phase, isostructural with Cu_2Mg [Harris et al., 1965].

Atom positions
8(a) 8 samarium
16(d) 16 aluminum

origin at $\bar{4}3m$ [ibid.]

Lattice constant
a = 7.9423 Å

(published value: 7.9258 kX [ibid.])

Volume
501.00 $Å^3$

Density
(calculated) 5.418 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.0, samarium B = 0.5.

Scattering factors
Al^0 [Cromer and Mann, 1968]
Sm^0 [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(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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 3 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 3 1	70.02
1.2557	10	6 2 0	75.68
1.2113	10	5 3 3	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 3 1+	96.32
.9927	1	8 0 0	101.78
.9703	1	7 3 3	105.10
.9360	10	8 2 2+	110.76
.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 (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.585	60	1 1 1	19.34
2.8080	100	2 2 0	31.84
2.3947	100	3 1 1	37.53
2.2927	5	2 2 2	39.26
1.9856	10	4 0 0	45.65
1.8221	15	3 3 1	50.02
1.6212	35	4 2 2	56.74
1.5285	20	5 1 1	60.52
1.5285	5	3 3 3	60.52
1.4040	20	4 4 0	66.55
1.3425	10	5 3 1	70.03
1.2558	15	6 2 0	75.67
1.2112	10	5 3 3	78.99
1.1973	1	6 2 2	80.08
1.1464	1	4 4 4	84.43
1.1121	5	5 5 1	87.68
1.1121	5	7 1 1	87.68
1.0613	15	6 4 2	93.07
1.0340	10	7 3 1	96.31
1.0340	5	5 5 3	96.31
.9928	5	8 0 0	101.77
.9703	1	7 3 3	105.10
.9360	5	8 2 2	110.76
.9360	5	6 6 0	110.76
.9171	10	7 5 1	114.27
.9171	1	5 5 5	114.27
.8880	5	8 4 0	120.33
.8718	5	9 1 1	124.16
.8718	5	7 5 3	124.16
.8467	10	6 6 4	130.96
.8326	15	9 3 1	135.40
.8106	20	8 4 4	143.71
.7982	5	7 7 1	149.60
.7982	5	9 3 3	149.60
.7982	5	7 5 5	149.60
.7788	25	10 2 0	163.05
.7788	45	8 6 2	163.05

Aluminum Samarium, Al_3Sm

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 2, isostructural with Ni_3Sn and Mg_3Cd [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 = 0.714
These are the positions given by Murray [1956] for Al_3Th; the parameters were modified slightly 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 $Å^3$

Density
(calculated) 4.740 g/cm^3

Thermal parameters
Isotropic: aluminum B = 0.75; samarium B = 1.0

Scattering factors
Al^0 Sm^0 [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 84, 1663.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.521	25	1	0	0	16.04
3.534	100	1	0	1	25.18
3.189	50	1	1	0	27.96
2.763	25	2	0	0	32.38
2.367	90	2	0	1	37.98
2.299	20	0	0	2	39.16
2.122	5	1	0	2	42.56
2.088	10	2	1	0	43.30
1.901	20	2	1	1	47.80
1.865	15	1	1	2	48.80
1.842	5	3	0	0	49.44
1.767	10	2	0	2	51.70
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	60.36
1.476	5	1	0	3	62.90
1.454	15	3	1	1	64.00
1.437	5	3	0	2	64.82
1.381	1	4	0	0	67.78
1.340	10	2	0	3	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	3	77.14
1.222	5	3	2	1	78.16
1.206	5	4	1	0	79.42
1.184	1	4	0	2	81.18
1.149	1	0	0	4	84.18
1.105	1	5	0	0	88.38
1.084	5	3	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	3	0	92.84
1.061	1	2	0	4	93.10
1.044	1	4	2	0	95.08
1.026	5	4	0	3	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	0	101.82
.977	5	3	2	3	104.12
.975	1	3	0	4	104.40
.970	5	5	1	1	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
.911	1	5	1	2	115.44
.908	1	4	3	0	115.98
.907	1	1	0	5	116.28
.891	1	4	3	1	119.64

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.525	25	1 0 0	16.03
3.534	100	1 0 1	25.18
3.190	50	1 1 0	27.95
2.763	25	2 0 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 0	43.29
1.901	25	2 1 1	47.80
1.865	20	1 1 2	48.79
1.842	10	3 0 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 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 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 0 4	84.17
1.105	1	5 0 0	88.39
1.084	5	3 1 3	90.62
1.081	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 0	92.84
1.061	1	2 0 4	93.10
1.044	1	4 2 0	95.07
1.026	5	4 0 3	97.32
1.018	10	4 2 1	98.31
1.007	1	2 1 4	99.82
.996	1	5 0 2	101.33
.992	1	5 1 0	101.83
.977	5	3 2 3	104.12
.975	1	3 0 4	104.38
.970	5	5 1 1	105.14
.965	5	3 3 2	105.91
.951	1	4 2 2	108.24
.932	5	2 2 4	111.41
.921	1	6 0 0	113.54
.919	1	3 1 4	113.82
.911	1	5 1 2	115.45
.908	1	4 3 0	116.00
.907	1	1 0 5	116.28
.896	1	5 0 3	118.50
.891	5	4 3 1	119.63

Aluminum Technetium, Al_6Tc

Structure
Orthorhombic, Ccmm(63), Z = 4, isostructural with Al_6Mn. The structure was determined by Wilkinson [1967].

Atom positions
4(c) 4 technetium
8(e) 8 aluminum (1), y = 0.3257
8(f) 8 aluminum (2), x_2 = .1338, z_2 = .1030
8(g) 8 aluminum (3), x_3 = .2880, y_3 = .3180, z_3 = .25
[Wilkinson, 1978, private communication]

Lattice constants
a = 6.5948(9) Å
b = 7.629(9)
c = 9.0016(11)

(published values: a = 6.5944(9)Å, b = 7.629(9), c = 9.0011(11) [Wilkinson, 1967]).

CD cell: a = 7.629(9); b = 9.0016(11); c = 6.5948(9); a/b = 0.8475; c/b = 0.7326; sp. gp. Bmmb(63).

Volume
452.89 $Å^3$

Density
(calculated) 3.826 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.0, technetium B = 0.5

Scattering factors
Al^0, Tc^0 [Cromer and Mann, 1968]

Scale factors (integrated intensities)
$\gamma = 0.330 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 1.97

References

Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Wilkinson, C. (1967). Acta Crystallogr. 22, 924.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.98	100	1 1 0	17.78
4.50	45	0 0 2	19.72
4.36	21	1 1 1	20.34
3.81	30	0 2 0	23.32
3.341	63	1 1 2	26.66
3.297	21	2 0 0	27.02
3.095	9	2 0 1	28.82
2.910	24	0 2 2	30.70
2.572	5	1 1 3	34.86
2.494	14	2 2 0	35.98
2.372	1	1 3 0	37.90
2.294	35	1 3 1	39.24
2.250	21	0 0 4	40.04
2.219	25	2 0 3	40.62
2.181	62	2 2 2	41.36
2.112	32	3 1 0	42.78
2.099	75	1 3 2	43.06
2.051	66	1 1 4	44.12
1.918	14	2 2 3	47.36
1.913	12	3 1 2	47.48
1.907	11	0 4 0	47.64
1.859	9	2 0 4+	48.96
1.756	6	0 4 2	52.04
1.727	5	3 1 3	52.98
1.671	9	2 2 4	54.90
1.651	3	2 4 0	55.64
1.649	3	4 0 0	55.70
1.633	9	1 3 4+	56.30
1.622	2	4 0 1	56.72
1.580	3	2 0 5	58.36
1.560	5	3 3 2	59.18
1.550	10	2 4 2	59.60
1.540	4	3 1 4	60.02
1.513	1	4 2 0	61.20
1.500	4	0 0 6	61.78
1.493	11	4 2 1	62.14
1.489	7	1 5 0	62.32
1.460	1	2 2 5	63.70
1.446	6	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

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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
1.193	5	5 1 3	80.46
1.186	1	2 6 0	80.98
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

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.99	100	1 1 0	17.76
4.50	45	0 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
2.219	29	2 0 3	40.62
2.182	75	2 2 2	41.35
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	47.35
1.912	5	3 1 2	47.51
1.907	9	0 4 0	47.64
1.861	3	1 3 3	48.90
1.859	9	2 0 4	48.96
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
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
1.437	1	1 1 6	64.84
1.434	4	4 2 2	64.96
1.434	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	3 3 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	3 5 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	78.55
1.208	1	3 5 2	79.28
1.202	2	4 4 2	79.71
1.193	7	5 1 3	80.47
1.186	2	2 6 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	83.95

Aluminum Terbium, Al_2Tb

Structure
Cubic, Fd3m(227), Z = 8, a Laves phase, isostructural with Cu_2Mg [Harris et al., 1965].

Atom positions
8(a) 8 terbium
16(d) 16 aluminum

origin at $\bar{4}3m$ [ibid.]

Lattice constant
a = 7.8658 Å

(published value: 7.8495 kX [ibid.])

Volume
486.66 $Å^3$

Density
(calculated) 5.811 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.0; terbium B = 0.5.

Scattering factors
Al^0 [Cromer and Mann, 1968]
Tb^0 [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 9, 270.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.539	70	1 1 1	19.54
2.7811	100	2 2 0	32.16
2.3708	95	3 1 1	37.92
2.2707	5	2 2 2	39.66
1.9666	10	4 0 0	46.12
1.8045	15	3 3 1	50.54
1.6056	30	4 2 2	57.34
1.5137	25	5 1 1+	61.18
1.3905	15	4 4 0	67.28
1.3294	10	5 3 1	70.82
1.2437	10	6 2 0	76.54
1.1996	10	5 3 3	79.90
1.1858	1	6 2 2	81.02
1.1352	1	4 4 4	85.46
1.1013	5	7 1 1+	88.76
1.0510	15	6 4 2	94.26
1.0241	15	7 3 1+	97.56
.9832	1	8 0 0	103.16
.9610	1	7 3 3	106.56
.9270	10	8 2 2+	112.40
.9082	10	7 5 1+	116.02
.8795	5	8 4 0	122.30
.8634	5	7 5 3+	126.30
.8385	5	6 6 4	133.46
.8246	5	9 3 1	138.20
.8028	10	8 4 4	147.28
.7905	5	7 5 5+	154.02

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.541	65	1 1 1	19.53
2.7810	100	2 2 0	32.16
2.3716	95	3 1 1	37.91
2.2707	5	2 2 2	39.66
1.9665	10	4 0 0	46.12
1.8045	15	3 3 1	50.54
1.6056	35	4 2 2	57.34
1.5138	20	5 1 1	61.18
1.5138	5	3 3 3	61.18
1.3905	20	4 4 0	67.28
1.3296	10	5 3 1	70.81
1.2437	15	6 2 0	76.54
1.1995	10	5 3 3	79.91
1.1858	1	6 2 2	81.02
1.1353	1	4 4 4	85.45
1.1014	5	5 5 1	88.75
1.1014	5	7 1 1	88.75
1.0511	20	6 4 2	94.25
1.0240	10	7 3 1	97.57
1.0240	5	5 5 3	97.57
.9832	5	8 0 0	103.15
.9610	5	7 3 3	106.57
.9270	10	8 2 2	112.40
.9270	5	6 6 0	112.40
.9083	10	7 5 1	116.01
.9083	1	5 5 5	116.01
.8794	5	8 4 0	122.31
.8634	5	7 5 3	126.30
.8634	5	9 1 1	126.30
.8385	10	6 6 4	133.46
.8246	15	9 3 1	138.20
.8028	20	8 4 4	147.28
.7905	5	7 7 1	154.01
.7905	5	9 3 3	154.01
.7905	5	7 5 5	154.01

Aluminum Terbium, Al_2Tb_3

Structure
Tetragonal, $P4_2nm$ (102), Z = 4, isostructural with Al_2Gd_3, from powder data [Buschow, 1965]. Baenziger and Hegenbarth [1964] determined the structure for Al_2Gd_3.

Atom positions
4(c) 4 aluminum(1)
4(c) 4 aluminum(2)
4(c) 4 terbium(1)
4(c) 4 terbium(2)
4(b) 4 terbium(3)

Information on atomic position parameters was not available. From considerations of atomic size, the parameters for Al_2Gd_3 were used instead.

Lattice constants
a = 8.255 Å
c = 7.568 [Buschow, 1965]

c/a = 0.9168

Volume
515.7 g/cm^3

Density
(calculated) 6.836 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.97; terbium(1) B = 1.55; terbium(2) B = 1.65; terbium(3) B = 1.75

Scattering factors
Al^0 [International Tables, 1962]
Tb^0 [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 0.436 \times 10^{-3}$

References

Baenziger, N.C. and Hegenbarth, J. J., Jr. (1964) Acta Crystallogr. 17, 620.
Buschow, K. H. J. (1965). J. Less-Common Metals 8, 209.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.832	10	1 1 0	15.18
5.576	5	1 0 1	15.88
4.619	5	1 1 1	19.20
3.783	5	0 0 2	23.50
3.690	55	2 1 0	24.10
3.175	50	1 1 2	28.08
2.917	40	2 2 0	30.62
2.790	100	2 0 2	32.06
2.723	10	2 2 1	32.86
2.642	75	2 1 2	33.90
2.611	65	3 1 0	34.32
2.468	25	3 1 1	36.38
2.413	5	1 0 3	37.24
2.316	5	1 1 3	38.86
2.311	5	2 2 2	38.94
2.290	1	3 2 0	39.32
2.191	1	3 2 1	41.16
2.148	1	3 1 2	42.02
2.002	15	4 1 0	45.26
1.946	1	3 3 0	46.64
1.936	5	4 1 1	46.90
1.908	1	2 2 3	47.62
1.892	10	0 0 4	48.06
1.860	1	3 0 3	48.94
1.846	5	4 2 0	49.34
1.812	10	4 0 2+	50.32
1.800	1	1 1 4	50.68
1.770	15	4 1 2	51.60
1.731	20	3 3 2	52.86
1.695	1	3 2 3	54.06
1.683	10	2 1 4	54.46
1.659	5	4 2 2	55.34
1.619	5	5 1 0	56.84
1.613	10	4 3 1+	57.04
1.587	10	2 2 4	58.06
1.583	10	5 1 1	58.22
1.568	5	4 1 3	58.84
1.541	1	3 3 3	60.00
1.532	15	3 1 4	60.38
1.513	1	4 3 2	61.20
1.502	5	5 2 1	61.70
1.488	10	5 1 2	62.34
1.465	1	1 1 5	63.44
1.459	5	4 4 0	63.72

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.837	10	1	1	0	15.17
5.578	5	1	0	1	15.87
4.622	5	1	1	1	19.19
3.784	5	0	0	2	23.49
3.692	50	2	1	0	24.09
3.175	45	1	1	2	28.08
2.919	40	2	2	0	30.61
2.789	100	2	0	2	32.06
2.723	10	2	2	1	32.86
2.642	75	2	1	2	33.90
2.610	60	3	1	0	34.32
2.586	1	3	0	1	34.66
2.468	25	3	1	1	36.38
2.413	5	1	0	3	37.24
2.316	5	1	1	3	38.86
2.311	1	2	2	2	38.94
2.290	1	3	2	0	39.32
2.191	1	3	2	1	41.16
2.149	1	3	1	2	42.01
2.002	15	4	1	0	45.26
1.946	1	3	3	0	46.64
1.936	5	4	1	1	46.90
1.909	1	2	2	3	47.61
1.892	15	0	0	4	48.05
1.859	1	3	0	3	48.94
1.846	5	4	2	0	49.33
1.814	5	3	1	3	50.25
1.812	5	4	0	2	50.32
1.800	1	1	1	4	50.68
1.770	15	4	1	2	51.61
1.730	25	3	3	2	52.87
1.720	1	2	0	4	53.21
1.695	1	3	2	3	54.05
1.684	10	2	1	4	54.45
1.659	10	4	2	2	55.33
1.619	5	5	1	0	56.82
1.613	1	5	0	1	57.05
1.613	5	4	3	1	57.05
1.588	10	2	2	4	58.05
1.583	5	5	1	1	58.23
1.568	5	4	1	3	58.84
1.541	1	3	3	3	60.00
1.533	1	5	2	0	60.33
1.532	15	3	1	4	60.37
1.513	1	4	3	2	61.20
1.502	5	5	2	1	61.69
1.488	10	5	1	2	62.33
1.465	1	1	1	5	63.44
1.459	5	4	4	0	63.72

Aluminum Thorium Uranium, Al_6ThU

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 1, isostructural with Al_3Th and Ni_3Sn, from powder data [van Vucht, 1966].

Atom positions
2(c) 1 thorium and 1 uranium
6(h) 6 aluminum, with x = 0.857
From geometric considerations, the atomic positions used were those of Al_3Th, given by Murray [1956], slightly modified.

Lattice constants
a = 6.43 Å
c = 4.61 [van Vucht, 1966]

c/a = 0.7170

Volume
165.1 $Å^3$

Density
(calculated) 6.36 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.0; thorium, uranium B = 0.75

Scattering factors
Al^0, Th^0, U^0 [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 1.843 \times 10^{-3}$

References
International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 212.
Murray, J.R. (1956). J. Inst. Metals 84, 1663.
van Vucht, J. H. N. (1966). J. Less-Common Metals 11, 308).

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.56	35	1 0 0	15.92
3.55	100	1 0 1	25.06
3.21	50	1 1 0	27.74
2.78	20	2 0 0	32.12
2.38	65	2 0 1	37.72
2.30	15	0 0 2	39.06
2.13	5	1 0 2	42.42
2.10	10	2 1 0	42.94
1.91	25	2 1 1	47.46
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	10	2 2 0	57.26
1.55	5	2 1 2	59.42
1.54	1	3 1 0	59.84
1.48	5	1 0 3	62.66
1.46	15	3 1 1	63.48
1.45	5	3 0 2	64.40
1.39	1	4 0 0	67.20
1.35	10	2 0 3	69.86
1.33	5	4 0 1	70.62
1.32	10	2 2 2	71.50
1.28	1	3 1 2	73.80
1.24	5	2 1 3	76.74
1.23	5	3 2 1	77.46
1.22	5	4 1 0	78.68
1.19	1	4 0 2	80.54
1.15	1	0 0 4	83.88
1.11	1	5 0 0	87.52
1.09	5	3 1 3	90.00
1.08	5	1 1 4	90.48
1.08	5	5 0 1	90.74
1.07	5	4 1 2	91.56
1.07	5	3 3 0	91.86
1.06	1	2 0 4	92.66
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	1	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
.924	1	3 1 4	113.02
.918	1	5 1 2	114.18

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.915	1	4 3 0	114.60
.910	1	1 0 5	115.74
.902	1	5 0 3	117.34
.898	1	4 3 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 3	125.04
.861	1	6 0 2	126.94
.851	1	4 3 2	129.74

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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 3	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 3	76.73
1.23	10	3 2 1	77.47
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
1.11	1	5 0 0	87.52
1.09	5	3 1 3	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	3 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	3 3 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	3 1 4	113.01
.917	1	5 1 2	114.19
.915	1	4 3 0	114.58
.910	1	1 0 5	115.74
.902	1	5 0 3	117.34
.898	5	4 3 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

Aluminum Tungsten, Al_5W, δ-phase

Structure
Hexagonal, $P6_3(173)$, Z = 2, probably isostructural with $MoAl_5$; the structure was determined by Adam and Rich [1955]. Previous work [Clark, 1940] had indicated a formula Al_9W_2.

Atom positions
2(b) 2 tungsten
2(b) 2 aluminum(1)
2(a) 2 aluminum(2)
6(c) 6 aluminum(3) [ibid]

Lattice constants
a = 4.9023(3) Å
c = 8.8576(5)

c/a = 1.8068

(published values: a = 4.9020(3) Å, c = 8.8570(5) [Adam and Rich, 1955]).

Volume
184.35 $Å^3$

Density
(calculated) 5.742 g/cm^3
(measured) 5.5 g/cm^3 [Adam and Rich, 1955]

Thermal parameters
Isotropic: aluminum B = 1.0; tungsten B = 0.5

Scattering factors
Al^0, W^0 [International Tables, 1962]

Scale factors (integrated intensities)
γ = 1.129 x 10^{-3}
$I/I_{corundum}$ (calculated) 8.47

References
Adam, J. and Rich, J. B. (1955). Acta Crystallogr. 8, 349.
Clark, W. D. (1940). J. Inst. Metals 66, 271.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 212.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.427	33	0 0 2	20.04
4.243	22	1 0 0	20.92
3.8276	100	1 0 1	23.22
3.0641	18	1 0 2	29.12
2.4507	30	1 1 0	36.64
2.4238	28	1 0 3	37.06
2.3624	7	1 1 1	38.06
2.2140	19	0 0 4	40.72
2.1446	76	1 1 2	42.10
2.1234	5	2 0 0	42.54
2.0643	16	2 0 1	43.82
1.9634	5	1 0 4	46.20
1.9141	4	2 0 2	47.46
1.8857	3	1 1 3	48.22
1.7233	9	2 0 3	53.10
1.6429	15	1 1 4	55.92
1.6349	9	1 0 5	56.22
1.6046	2	2 1 0+	57.38
1.5789	13	1 2 1+	58.40
1.5323	2	2 0 4	60.36
1.5088	4	2 1 2+	61.40
1.4764	1	0 0 6	62.90
1.4356	1	1 1 5	64.90
1.4151	11	3 0 0	65.96
1.4102	10	1 2 3+	66.22
1.3945	1	1 0 6	67.06
1.3600	4	2 0 5	69.00
1.3480	5	3 0 2	69.70
1.2993	2	2 1 4+	72.72
1.2645	10	1 1 6	75.06
1.2256	3	2 2 0	77.88
1.2126	3	1 0 7+	78.88
1.1924	11	3 0 4	80.48
1.1895	10	1 2 5+	80.72
1.1813	8	2 2 2	81.40
1.1671	4	3 1 1+	82.60
1.1380	1	1 3 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+	90.28
1.0723	3	2 2 4	91.84
1.0538	2	4 0 1	93.94
1.0396	1	1 3 4+	95.62
1.0216	2	3 0 6	97.88
1.0090	3	1 1 8	99.54
.9989	1	4 0 3	100.92
.9936	3	1 2 7+	101.66
.9806	3	3 1 5+	103.54
.9681	3	2 3 1+	105.44
.9587	1	1 0 9	106.92

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.429	31	0	0	2	20.03
4.246	21	1	0	0	20.91
3.8285	100	1	0	1	23.21
3.0648	19	1	0	2	29.11
2.4512	33	1	1	0	36.63
2.4240	30	1	0	3	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	3	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	6	75.05
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	1	5	80.74
1.1893	3	1	2	5	80.74
1.1812	11	2	2	2	81.41
1.1672	3	3	1	1	82.59
1.1672	3	1	3	1	82.59
1.1380	1	3	1	2	85.21
1.1380	1	1	3	2	85.21
1.1072	2	0	0	8	88.17
1.0937	2	3	1	3	89.54
1.0937	2	1	3	3	89.54
1.0869	2	2	0	7	90.26
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	3	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	3	5	103.54
.9682	2	3	2	1	105.43
.9682	2	2	3	1	105.43
.9588	2	1	0	9	106.92

Aluminum Vanadium, $Al_{10}V$

Structure
Cubic, Fd3m(227), Z = 16, isostructural with $Mg_3Cr_2Al_{18}$ [Brown, 1957]. The phase exists over a range of composition from $Al_{10}V$ to $Al_{10.25}V$ [Ray and Smith, 1957].

Atom positions
96(g) 96 aluminum
48(f) 48 aluminum
16(d) 16 aluminum
16(c) 16 vanadium [Brown, 1957]

Lattice constant
a = 14.493(4) Å

(published value: 14.492(4) Å [Ray and Smith, 1957])

Volume
3044.2 $Å^3$

Density
(calculated) 2.799 g/cm^3
(measured) 2.79(5) g/cm^3 [Brown, 1957]

Thermal parameters
Isotropic: aluminum B = 1.0; vanadium B = 0.5.

Scattering factors
Al^0, V^0 [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.352 \times 10^{-3}$

References
Brown, P. J. (1957). Acta Crystallogr. 10, 133.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204.
Ray, A. E. and Smith, J. F. (1957). Acta Crystallogr. 10, 604.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.355	100	1 1 1	10.58
5.122	12	2 2 0	17.30
4.367	4	3 1 1	20.32
4.184	9	2 2 2	21.22
3.622	12	4 0 0	24.56
3.324	12	3 3 1	26.80
2.957	9	4 2 2	30.20
2.788	1	5 1 1	32.08
2.562	13	4 4 0	35.00
2.449	31	5 3 1	36.66
2.415	15	4 4 2	37.20
2.292	19	6 2 0	39.28
2.210	62	5 3 3	40.80
2.184	99	6 2 2	41.30
2.092	37	4 4 4	43.22
2.029	55	7 1 1+	44.62
1.936	5	6 4 2	46.88
1.771	2	7 3 3	51.58
1.708	9	8 2 2+	53.62
1.673	3	5 5 5+	54.82
1.663	1	6 6 2	55.20
1.620	7	8 4 0	56.78
1.591	7	7 5 3+	57.92
1.581	2	8 4 2	58.30
1.479	3	8 4 4	62.76
1.456	4	9 3 3+	63.86
1.421	2	10 2 0	65.64
1.3945	19	10 2 2+	67.06
1.3514	2	9 5 3	69.50
1.3457	1	8 6 4	69.84
1.3229	6	10 4 2	71.22
1.2811	26	8 8 0	73.92
1.2662	5	9 5 5+	74.94
1.2616	5	10 4 4	75.26
1.2429	2	8 6 6	76.60
1.2293	11	11 3 3	77.60
1.2077	2	8 8 4+	79.26
1.1954	5	7 7 7+	80.24
1.1755	2	12 2 2+	81.88
1.1459	2	12 4 0	84.48
1.1352	1	9 9 1	85.46
1.1318	1	12 4 2	85.78
1.1182	2	10 8 2	87.08
1.1083	3	11 5 5+	88.06
1.1051	7	10 6 6	88.38
1.0924	7	12 4 4	89.68
1.0833	5	13 3 1+	90.64
1.0378	1	13 5 1+	95.84
1.0249	2	10 8 6+	97.46
1.0173	2	13 5 3+	98.44

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.368	79	1 1 1	10.56
5.124	10	2 2 0	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
3.325	11	3 3 1	26.79
2.958	8	4 2 2	30.19
2.789	1	5 1 1	32.06
2.562	13	4 4 0	34.99
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 3 3	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 3	57.92
1.581	2	8 4 2	58.30
1.479	3	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
1.3946	15	10 2 2	67.06
1.3946	7	6 6 6	67.06
1.3515	2	9 5 3	69.50
1.3456	1	8 6 4	69.84
1.3230	7	10 4 2	71.21
1.2810	31	8 8 0	73.93
1.2663	2	11 3 1	74.94
1.2663	1	9 7 1	74.94
1.2663	3	9 5 5	74.94
1.2615	5	10 4 4	75.27
1.2428	2	8 6 6	76.61
1.2293	13	11 3 3	77.60
1.2249	1	10 6 2	77.93
1.2078	2	8 8 4	79.26
1.1954	1	11 5 1	80.24
1.1954	4	7 7 7	80.24
1.1755	2	12 2 2	81.88
1.1458	3	12 4 0	84.49
1.1352	1	9 9 1	85.46
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 3 1	90.65
1.0833	3	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 3	98.45
1.0172	1	11 9 1	98.45
1.0147	1	10 10 2	98.78

Aluminum Vanadium, $Al_{10.25}V$

Structure
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].

Atom positions
96(g) 96 aluminum
48(f) 48 aluminum
16(d) 16 aluminum
8(b) 4 aluminum
16(c) 16 vanadium

The 8(b) site is 50% occupied [Ray and Smith, 1957].

Lattice constant
a = 14.517 Å

(published value: 14.516 Å [Ray and Smith, 1957])

Volume
3059.4 $Å^3$

Density
(calculated) 2.844 g/cm^3

Thermal parameters
Isotropic: [Ray and Smith, 1957].

Scattering factors
Al^0, V^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.360 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.74

Additional pattern
1. PDF card 7-281 [Carlson, et al., 1955]. It appears to be this phase but is labelled $Al_{11}V$.

References

Brown, P. J. (1957). Acta Crystallogr. 10, 133.
Carlson, O. N. Kenny, D. J. and Wilhelm, H. A. (1955). Trans. Amer. Soc. Metals 47, 520.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204.
Ray, A. E. and Smith, J. F. (1957). Acta Crystallogr. 10, 604.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.371	68	1 1 1	10.56
5.128	4	2 2 0	17.28
4.375	9	3 1 1	20.28
4.188	9	2 2 2	21.20
3.628	6	4 0 0	24.52
3.329	8	3 3 1	26.76
2.963	5	4 2 2	30.14
2.566	16	4 4 0	34.94
2.453	37	5 3 1	36.60
2.419	14	4 4 2	37.14
2.295	24	6 2 0	39.22
2.214	68	5 3 3	40.72
2.188	100	6 2 2	41.22
2.095	34	4 4 4	43.14
2.033	50	7 1 1+	44.54
1.940	3	6 4 2	46.80
1.774	3	7 3 3	51.48
1.760	1	6 4 4	51.90
1.711	11	8 2 2+	53.52
1.676	3	5 5 5	54.72
1.623	6	8 4 0	56.66
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	1	9 3 1	60.82
1.481	3	8 4 4	62.66
1.459	6	9 3 3+	63.74
1.424	3	10 2 0+	65.52
1.397	19	10 2 2+	66.94
1.354	2	9 5 3	69.36
1.348	1	8 6 4	69.70
1.325	6	10 4 2	71.08
1.283	30	8 8 0	73.78
1.268	6	9 5 5+	74.80
1.264	5	10 4 4	75.12
1.245	2	8 6 6	76.46
1.231	14	11 3 3	77.46
1.210	1	8 8 4+	79.10
1.1974	5	7 7 7+	80.08
1.1774	1	12 2 2+	81.72
1.1476	3	12 4 0	84.32
1.1369	1	9 9 1	85.30
1.1337	1	12 4 2	85.60
1.1201	2	10 8 2	86.90
1.1101	5	11 5 5+	87.88
1.1069	8	10 6 6	88.20
1.0943	7	12 4 4	89.48
1.0850	6	13 3 1+	90.46
1.0701	1	12 6 2	92.08
1.0396	1	13 5 1+	95.62

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 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	3 3 1	26.75
2.963	5	4 2 2	30.13
2.566	16	4 4 0	34.93
2.454	36	5 3 1	36.59
2.419	14	4 4 2	37.13
2.295	24	6 2 0	39.22
2.214	68	5 3 3	40.72
2.189	100	6 2 2	41.22
2.095	34	4 4 4	43.14
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 3 3	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	7	8 4 0	56.67
1.593	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	9 3 1	60.82
1.482	4	8 4 4	62.65
1.459	5	9 3 3	63.74
1.459	1	7 5 5	63.74
1.424	3	10 2 0	65.52
1.397	15	10 2 2	66.93
1.397	8	6 6 6	66.93
1.354	2	9 5 3	69.36
1.348	1	8 6 4	69.71
1.325	6	10 4 2	71.08
1.283	36	8 8 0	73.79
1.268	1	9 7 1	74.79
1.268	2	11 3 1	74.79
1.268	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 3 3	77.45
1.227	1	10 6 2	77.78
1.210	1	8 8 4	79.10
1.1973	1	11 5 1	80.08
1.1973	5	7 7 7	80.08
1.1775	1	12 2 2	81.72
1.1477	3	12 4 0	84.32
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 3 1	90.46
1.0851	3	9 7 7	90.46
1.0702	1	12 6 2	92.07
1.0396	1	13 5 1	95.63

Aluminum Vanadium, $Al_{23}V_4$

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 2. The structure was determined by Smith and Ray [1957] and refined by Ray and Smith [1960].

Atom positions
2(a) 2 vanadium(1)
6(h) 6 vanadium(2)
12(k) 12 aluminum(1)
12(k) 12 aluminum(2)
12(k) 12 aluminum(3)
6(h) 6 aluminum(4)
4(f) 4 aluminum(5) [Ray and Smith, 1960].

Lattice constants
*a = 7.6933 Å
*c = 17.041

c/a = 2.2150

*published values: a = 7.6928 Å, c = 17.040 [Ray and Smith, 1960].

Volume
873.48 $Å^3$

Density
(calculated) 3.134 g/cm^3

Thermal parameters
Isotropic: vanadium(1): B = 0.49; vanadium(2): B = 0.57; aluminum(1): B = 1.14; aluminum(2): B = 0.82; aluminum(3): B = 0.87; aluminum(4): B = 0.74; aluminum(5): B = 0.81.

Scattering factors
Al^0, V^0 [International Tables, 1962], corrected for dispersion [Cromer and Liberman, 1970].

Scale factors (integrated intensities)
$\gamma = 0.410 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 2.42

Additional pattern
1. PDF card 7-359 [Carlson et al., 1955]. It is called Al_6V, β-phase, and is the phase described above.

References
Carlson, O. N., Kenny, D.J., and Wilhelm, H. A. (1955). Trans. Amer. Soc. Metals 47, 520.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204.
Ray, A. E. and Smith, J. F. (1960). Acta Crystallogr. 13, 876.
Smith, J. F. and Ray, A. E. (1957). Acta Crystallogr. 10, 169.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.515	33	0 0 2	10.38
6.662	7	1 0 0	13.28
6.197	35	1 0 1	14.28
5.248	23	1 0 2	16.88
4.321	15	1 0 3	20.54
4.259	11	0 0 4	20.84
3.844	1	1 1 0	23.12
3.587	3	1 0 4	24.80
3.504	12	1 1 2	25.40
3.331	4	2 0 0	26.74
3.269	7	2 0 1	27.26
3.034	1	1 0 5	29.42
2.873	1	2 0 3	31.10
2.624	4	2 0 4	34.14
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	6	2 0 5	37.74
2.302	37	2 1 3	39.10
2.286	48	1 0 7	39.38
2.220	19	3 0 0	40.60
2.202	27	3 0 1	40.96
2.167	100	2 1 4	41.64
2.162	95	2 0 6	41.74
2.130	18	0 0 8	42.40
2.068	68	3 0 3	43.74
2.025	33	2 1 5	44.72
1.966	12	2 0 7	46.14
1.923	17	2 2 0	47.22
1.863	2	1 1 8+	48.84
1.837	2	3 1 1	49.58
1.806	1	3 1 2	50.50
1.795	9	2 0 8	50.84
1.757	1	3 1 3	52.00
1.750	2	3 0 6+	52.24
1.704	2	0 0 10	53.74
1.696	1	3 1 4	54.04
1.665	1	4 0 0	55.10
1.651	3	1 0 10	55.62
1.641	3	3 0 7	56.00
1.626	3	2 1 8	56.54
1.598	1	4 0 3	57.62
1.558	3	1 1 10	59.26
1.551	9	4 0 4	59.56
1.549	10	3 1 6	59.64
1.476	4	3 2 3	62.92
1.454	2	4 1 0	63.98
1.450	1	4 1 1	64.18
1.437	1	4 0 6+	64.84
1.433	2	4 1 2	65.02

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.427	4	2 2 8	65.32
1.420	1	0 0 12	65.70
1.408	4	4 1 3	66.32
1.395	2	3 2 5+	67.04
1.352	5	3 0 10	69.46
1.346	2	3 2 6	69.82
1.328	3	5 0 1	70.88
1.319	3	2 1 11	71.44
1.317	3	5 0 2	71.62
1.306	3	2 0 12	72.26
1.297	7	5 0 3	72.86
1.294	22	3 2 7	73.04
1.282	22	3 3 0	73.84
1.271	30	3 0 11+	74.64
1.256	1	4 2 1	75.68

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.520	28	0 0 2	10.37
6.663	6	1 0 0	13.28
6.205	30	1 0 1	14.26
5.249	21	1 0 2	16.88
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 3	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	3 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 0 8	42.40
2.068	74	3 0 3	43.73
2.029	9	1 0 8	44.62
2.025	31	2 1 5	44.71
1.969	2	3 0 4	46.05
1.966	13	2 0 7	46.15
1.923	19	2 2 0	47.22
1.863	2	1 1 8	48.83
1.861	1	3 0 5	48.91
1.837	2	3 1 1	49.58
1.806	1	3 1 2	50.50
1.795	10	2 0 8	50.84
1.757	1	3 1 3	52.00
1.750	2	3 0 6	52.25
1.704	2	0 0 10	53.75
1.695	1	3 1 4	54.05
1.666	1	4 0 0	55.09
1.651	3	1 0 10	55.62
1.641	3	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	3 1 6	59.65
1.476	5	3 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
1.437	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	3 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	3	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	3 2 7	73.03
1.282	27	3 3 0	73.85
1.272	14	5 0 4	74.56
1.271	31	3 0 11	74.64
1.268	1	3 3 2	74.82

Aluminum Vanadium, $Al_{45}V_7$, α'-phase

Structure
Monoclinic, C2/m (12), Z = 2. The structure was determined by Brown [1959].

Atom positions
2(a) 2 vanadium(0)
2(d) 2 aluminum(0)
4(i) 4 vanadium(1)
4(i) 4 each of aluminum(3), (4), (5) (6), (7), (8), (9), and (10)
8(j) 8 each of aluminum(11), (12), (13) (14), (15), (16), and (17) [ibid]

Lattice constants
a = 25.605(14) Å
b = 7.6218(18)
c = 11.082(12)
β = 128.92(3)°

(published values: a=25.604(14)Å, b=7.6213(18), c=11.081(12), β=128° 55(2)' [Brown, 1959]).

CD cell: a = 20.540(14)Å, b = 7.6218(18), c = 11.082(12), β = 104.10(3)°, sp. gp. I2/m; a/b = 2.6949, c/b = 1.4540.

Volume
1682.6 $Å^3$

Density
(calculated) 3.100 g/cm^3
(measured) 3.10(3) g/cm^3 [Brown, 1959]

Thermal parameters
Isotropic: aluminum B = 1.0; vanadium B = 0.5

Scattering factors
Al^0, V^0 [Cromer and Mann, 1968]

Scale factors (integrated intensities)
$\gamma = 0.0786 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 0.45

References
Brown, P. J. (1959). Acta Crystallogr. 12, 995.
Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
10.59	33	-2 0 1	8.34
9.95	8	2 0 0	8.88
8.61	2	0 0 1	10.26
7.11	2	1 1 0	12.44
6.38	19	-4 0 1	13.86
6.21	70	-1 1 1	14.24
5.37	1	-2 0 2	16.50
5.30	2	-4 0 2	16.72
5.12	15	2 0 1	17.32
4.968	8	1 1 1	17.84
4.480	1	-3 1 2	19.80
4.308	11	0 0 2	20.60
4.188	23	-6 0 2+	21.20
4.118	2	-1 1 2	21.56
4.074	2	-6 0 1	21.80
3.684	4	-4 0 3	24.14
3.645	1	3 1 1	24.40
3.584	4	-2 2 1	24.82
3.559	2	2 2 0	25.00
3.531	3	5 1 0	25.20
3.469	2	4 0 1	25.66
3.383	3	-2 0 3	26.32
3.368	4	1 1 2	26.44
3.307	5	6 0 0+	26.94
3.274	2	-4 2 1	27.22
3.241	1	-3 1 3	27.50
3.108	3	-2 2 2+	28.70
3.040	5	-7 1 3	29.36
2.932	1	-8 0 1	30.46
2.901	2	-1 1 3	30.80
2.873	1	0 0 3	31.10
2.820	3	-6 2 2	31.70
2.771	3	5 1 1	32.28
2.695	11	3 1 2	33.22
2.650	5	-8 0 4+	33.80
2.627	8	-9 1 3	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 3 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

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.281	10	-10	0	1	39.48
2.254	15	-1	3	2	39.96
2.244	40	-5	3	2	40.16
2.226	54	-11	1	3	40.50
2.207	61	7	1	1+	40.86
2.196	51	-4	2	4+	41.06
2.175	37	-8	2	4	41.48
2.167	52	3	3	1	41.64
2.155	29	0	0	4	41.88
2.142	22	5	3	0	42.16
2.120	18	-10	0	5	42.62
2.099	40	-12	0	4+	43.06
2.092	58	-10	2	2	43.20
2.085	92	8	2	0+	43.36
2.072	100	-3	3	3+	43.64
2.070	98	-5	1	5	43.70
2.037	12	-12	0	2+	44.44
2.025	23	2	2	3+	44.72
2.004	3	4	0	3	45.22
1.992	2	10	0	0	45.50
1.945	1	1	1	4	46.66
1.932	2	5	3	1	47.00
1.906	9	0	4	0	47.68
1.895	7	7	3	0	47.96
1.876	2	0	2	4+	48.48
1.861	3	-12	0	1+	48.90
1.853	3	-10	2	5	49.14
1.834	3	-10	0	6+	49.66
1.824	2	9	1	1	49.96
1.814	1	-13	1	5	50.26
1.806	3	-9	3	1+	50.50
1.802	3	-14	0	3	50.60
1.796	3	-12	2	2+	50.80
1.792	3	-6	0	6+	50.92
1.780	1	4	4	0	51.28
1.773	1	-14	0	5+	51.50
1.766	1	10	2	0	51.72
1.758	1	-11	1	6	51.98
1.743	3	-12	2	5	52.46
1.725	1	0	0	5+	53.06
1.708	2	-14	0	2	53.62
1.703	2	5	3	2	53.78
1.683	2	2	2	4+	54.46
1.670	2	-7	3	5+	54.94

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
10.60	44	-2	0	1	8.33
9.96	10	2	0	0	8.87
8.62	2	0	0	1	10.25
7.12	2	1	1	0	12.42
6.39	23	-4	0	1	13.85
6.22	97	-1	1	1	14.23
5.37	1	-2	0	2	16.48
5.30	3	-4	0	2	16.71
5.12	21	2	0	1	17.31
5.01	5	3	1	0	17.70
4.980	1	4	0	0	17.80
4.969	8	1	1	1	17.84
4.481	2	-3	1	2	19.80
4.311	16	0	0	2	20.59
4.198	21	-6	0	2	21.15
4.185	18	-5	1	1	21.21
4.120	2	-1	1	2	21.55
4.073	2	-6	0	1	21.80
3.686	6	-4	0	3	24.12
3.644	2	3	1	1	24.40
3.586	6	-2	2	1	24.81
3.559	1	2	2	0	25.00
3.531	3	5	1	0	25.20
3.470	3	4	0	1	25.65
3.385	4	-2	0	3	26.30
3.368	4	1	1	2	26.44
3.320	5	6	0	0	26.83
3.305	5	-5	1	3	26.96
3.295	1	-7	1	2	27.04
3.273	2	-4	2	1	27.23
3.242	1	-3	1	3	27.49
3.117	2	-7	1	1	28.62
3.109	4	-2	2	2	28.69
3.057	2	2	2	1	29.19
3.041	7	-7	1	3	29.35
3.027	3	4	2	0	29.49
2.934	1	-8	0	1	30.45
2.901	4	-1	1	3	30.80
2.874	1	0	0	3	31.09
2.822	5	-6	2	2	31.68
2.783	3	-6	2	1	32.14
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	12	-9	1	3	34.10
2.591	5	-6	2	3	34.59
2.589	4	-5	1	4	34.61
2.566	6	4	2	1	34.94
2.531	3	-2	2	3	35.44

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.520	2	1	3	0	35.59
2.504	15	-10	0	2	35.83
2.503	6	6	2	0	35.84
2.490	10	8	0	0	36.04
2.484	1	2	2	2	36.12
2.479	1	1	1	3	36.21
2.472	31	-1	3	1	36.31
2.449	11	-2	0	4	36.67
2.448	8	-8	2	2	36.68
2.445	1	-3	1	4	36.73
2.432	1	-3	3	1	36.94
2.403	7	-9	1	4	37.40
2.393	15	-10	0	4	37.55
2.390	24	2	0	3	37.60
2.386	1	-8	2	3	37.67
2.373	2	3	3	0	37.89
2.369	18	1	3	1	37.95
2.325	2	-8	2	1	38.70
2.309	12	-3	3	2	38.97
2.295	22	0	2	3	39.23
2.281	13	-10	0	1	39.48
2.266	4	-5	3	1	39.75
2.255	16	-1	3	2	39.94
2.244	56	-5	3	2	40.15
2.240	8	-6	2	4	40.22
2.226	86	-11	1	3	40.49
2.209	29	-8	0	5	40.82
2.207	68	7	1	1	40.86
2.205	1	-1	1	4	40.90
2.197	10	5	1	2	41.05
2.196	52	-4	2	4	41.07
2.195	7	-6	0	5	41.09
2.176	50	-8	2	4	41.47
2.167	70	3	3	1	41.65
2.156	32	0	0	4	41.88
2.154	1	-11	1	4	41.90
2.147	4	6	2	1	42.05
2.142	27	5	3	0	42.15
2.126	1	9	1	0	42.49
2.120	25	-10	0	5	42.61
2.104	13	1	3	2	42.95
2.100	1	3	1	3	43.04
2.099	40	-12	0	4	43.06
2.093	54	-10	2	2	43.20
2.089	3	-5	3	3	43.29
2.086	51	-7	3	2	43.34
2.085	70	8	2	0	43.37
2.084	13	-4	0	5	43.39
2.075	44	6	0	2	43.59
2.072	100	-3	3	3	43.64

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.071	2	8	0	1	43.68
2.069	66	-5	1	5	43.72
2.060	6	-2	2	4	43.92
2.039	7	-7	3	1	44.40
2.037	9	-12	0	2	44.45
2.027	9	-10	2	4	44.68
2.025	30	2	2	3	44.72
2.017	5	-7	3	3	44.91
2.003	3	4	0	3	45.23
1.992	2	10	0	0	45.50
1.945	1	1	1	4	46.65
1.932	4	5	3	1	47.00
1.913	3	-2	0	5	47.49
1.911	1	-8	2	5	47.54
1.906	2	3	3	2	47.68
1.905	13	0	4	0	47.69
1.895	9	7	3	0	47.96
1.877	1	2	0	4	48.46
1.876	2	0	2	4	48.48
1.862	2	-12	0	1	48.88
1.861	2	-7	3	4	48.91
1.853	4	-10	2	5	49.14
1.839	2	-12	2	4	49.54
1.835	1	7	1	2	49.63
1.834	3	-10	0	6	49.67
1.827	1	-14	0	4	49.86
1.824	1	9	1	1	49.96
1.814	2	-13	1	5	50.25
1.806	3	-9	3	1	50.50
1.803	2	-14	0	3	50.59
1.796	2	-12	2	2	50.79
1.796	1	-2	4	2	50.80
1.793	1	5	1	3	50.88
1.791	1	-6	0	6	50.94
1.780	1	4	4	0	51.30
1.773	1	-14	0	5	51.50
1.765	1	10	2	0	51.74
1.758	2	-11	1	6	51.97
1.743	5	-12	2	5	52.45
1.743	1	0	4	2	52.46
1.735	1	8	0	2	52.71
1.724	2	0	0	5	53.06
1.708	3	-14	0	2	53.62
1.703	1	5	3	2	53.79
1.684	2	2	2	4	54.45
1.684	1	-11	3	2	54.45
1.683	1	-11	3	4	54.49
1.674	1	-13	1	6	54.78
1.673	1	-12	2	1	54.84
1.670	1	4	4	1	54.93

Aluminum Ytterbium, Al_2Yb

Structure
Cubic, Fd3m(227), Z = 8, isostructural with Cu_2Mg [Havinga et al., 1973].

Atom positions
16(d) 16 aluminum
8(a) 8 ytterbium

Lattice constants
a = 7.875 Å [ibid.]

Volume
488.4 $Å^3$

Density
(calculated) 6.175 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.0; ytterbium B = 0.5

Scattering factors
Al^0 [Cromer and Mann, 1968]
Yb^0 [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 1.770 \times 10^{-3}$

References

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.

Havinga, E. E., Buschow, K.H.J. and van Daal, H. J. (1973). Solid State Commun. 13, 621.

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

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.544	75	1 1 1	19.52
2.784	100	2 2 0	32.12
2.374	90	3 1 1	37.86
2.273	5	2 2 2	39.62
1.969	10	4 0 0	46.06
1.806	15	3 3 1	50.48
1.608	35	4 2 2	57.26
1.515	25	5 1 1+	61.10
1.392	15	4 4 0	67.20
1.331	10	5 3 1	70.72
1.245	10	6 2 0	76.44
1.201	10	5 3 3	79.80
1.187	1	6 2 2	80.90
1.137	1	4 4 4	85.32
1.103	5	7 1 1+	88.62
1.052	15	6 4 2	94.10
1.025	15	7 3 1+	97.42
.984	1	8 0 0	102.98
.962	1	7 3 3	106.38
.928	10	8 2 2+	112.20
.909	10	7 5 1+	115.80
.880	5	8 4 0	122.06
.864	5	7 5 3+	126.04
.839	5	6 6 4	133.16
.826	5	9 3 1	137.84
.804	5	8 4 4	146.82
.791	5	7 5 5+	153.44

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.547	65	1 1 1	19.51
2.784	100	2 2 0	32.12
2.374	95	3 1 1	37.86
2.273	5	2 2 2	39.61
1.969	10	4 0 0	46.07
1.807	20	3 3 1	50.47
1.607	35	4 2 2	57.27
1.516	20	5 1 1	61.10
1.516	5	3 3 3	61.10
1.392	20	4 4 0	67.19
1.331	10	5 3 1	70.72
1.245	15	6 2 0	76.43
1.201	10	5 3 3	79.80
1.187	1	6 2 2	80.91
1.137	1	4 4 4	85.33
1.103	5	5 5 1	88.62
1.103	5	7 1 1	88.62
1.052	20	6 4 2	94.11
1.025	10	7 3 1	97.41
1.025	5	5 5 3	97.41
.984	5	8 0 0	102.98
.962	5	7 3 3	106.39
.928	10	8 2 2	112.20
.928	5	6 6 0	112.20
.909	10	7 5 1	115.80
.909	1	5 5 5	115.80
.880	5	8 4 0	122.06
.864	5	7 5 3	126.03
.864	5	9 1 1	126.03
.839	10	6 6 4	133.15
.826	15	9 3 1	137.85
.804	20	8 4 4	146.83
.791	5	9 3 3	153.44
.791	5	7 7 1	153.44
.791	5	7 5 5	153.44

Aluminum Yttrium, Al_3Y

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 2, isostructural with Ni_3Sn. The structure refinement was based on two-dimensional data [Bailey, 1967].

Atom positions
2(c) 2 yttrium
6(h) 6 aluminum, x = 0.8534

These are a transformation of positions from those given by Bailey [1967], to show more clearly the relation to the isostructural compounds.

Polymorphism
This form occurs in small quantities in the residues of preparations of the high temperature rhombohedral polymorph [ibid.]. A third form with cubic cell a = 4.323 was found by Dagerhamn [1967].

Lattice constants
a = 6.276(2) Å
c = 4.582(1) [ibid.]

c/a = 0.7301

Volume
156.3 $Å^3$

Density
(calculated) 3.609 g/cm^3

Thermal parameters
Isotropic: aluminum B = 1.38; yttrium B = 0.16 [ibid.]

Scattering factors
Al^0, Y^0 [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.986 \times 10^{-3}$

References

Bailey, D. M. (1967). Acta Crystallogr. 23, 729.
Dagerhamn, T. (1967). Ark. Kemi 27, 363.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 211.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.434	10	1 0 0	16.30
3.501	65	1 0 1	25.42
3.138	30	1 1 0	28.42
2.717	25	2 0 0	32.94
2.338	100	2 0 1	38.48
2.291	25	0 0 2	39.30
2.111	1	1 0 2	42.80
2.055	10	2 1 0	44.04
1.875	10	2 1 1	48.52
1.850	10	1 1 2	49.20
1.812	5	3 0 0	50.32
1.752	10	2 0 2	52.18
1.685	1	3 0 1	54.42
1.569	15	2 2 0	58.80
1.530	5	2 1 2	60.48
1.507	1	3 1 0	61.46
1.470	5	1 0 3	63.18
1.432	10	3 1 1	65.08
1.421	5	3 0 2	65.64
1.359	1	4 0 0	69.06
1.331	10	2 0 3	70.70
1.303	10	4 0 1	72.50
1.294	15	2 2 2	73.04
1.259	1	3 1 2	75.42
1.226	5	2 1 3	77.88
1.203	5	3 2 1	79.62
1.186	5	4 1 0	81.00
1.169	1	4 0 2	82.46
1.145	1	0 0 4	84.52
1.0871	1	5 0 0	90.24
1.0761	1	1 1 4	91.42
1.0730	5	3 1 3	91.76
1.0555	1	2 0 4	93.74
1.0533	5	4 1 2	94.00
1.0460	1	3 3 0	94.86
1.0271	1	4 2 0	97.18
1.0151	5	4 0 3	98.72
1.0023	5	4 2 1	100.44
.9999	5	2 1 4	100.78
.9821	1	5 0 2	103.32
.9762	1	5 1 0	104.20
.9682	1	3 0 4	105.42
.9659	5	3 2 3	105.78
.9548	5	5 1 1	107.56
.9515	5	3 3 2	108.10
.9373	1	4 2 2	110.54
.9251	5	2 2 4	112.74
.9059	1	6 0 0	116.50
.9036	1	1 0 5	116.96

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
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	0	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	3	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	3	1	0	61.46
1.470	5	1	0	3	63.19
1.432	10	3	1	1	65.09
1.421	5	3	0	2	65.65
1.359	1	4	0	0	69.07
1.331	15	2	0	3	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	3	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
1.0870	1	5	0	0	90.25
1.0760	1	1	1	4	91.43
1.0729	5	3	1	3	91.77
1.0556	1	2	0	4	93.73
1.0533	5	4	1	2	94.00
1.0460	1	3	3	0	94.86
1.0272	1	4	2	0	97.17
1.0152	5	4	0	3	98.71
1.0023	10	4	2	1	100.45
1.0005	1	2	1	4	100.70
.9821	1	5	0	2	103.32
.9762	1	5	1	0	104.20
.9682	1	3	0	4	105.42
.9659	5	3	2	3	105.78
.9548	5	5	1	1	107.57
.9515	5	3	3	2	108.10
.9373	1	4	2	2	110.54
.9252	5	2	2	4	112.73
.9121	1	3	1	4	115.25
.9059	1	6	0	0	116.50
.9036	1	1	0	5	116.96

Amobarbital, form I, $C_{11}H_{18}N_2O_3$

Synonyms
5-Ethyl-5-isoamylbarbituric acid
Amytal

Structure
Monoclinic, C2/c (15), Z = 8. The structure was determined by Craven and Vizzini [1969].

Atom positions
Seven hydrogen positions were not located in the structure determination. All other atoms were in general positions 8(f). The data for H(112) apparently had errors and was omitted from the powder data calculations here.

Polymorphism
A polymorph called form II is also monoclinic with similar cell volume and space group $P2_1/c$ (14). The two forms crystallize simultaneously from the same aqueous ethanol solution by slow evaporation at room temperature [Craven and Vizzini, 1969].

Lattice constants
a = 21.481(10) Å
b = 11.591(6)
c = 10.371(6)
β = 97.07(3)°

a/b = 1.8532
c/b = 0.8947

(published values: a = 21.480(10)Å, b = 11.590(6), c = 10.370(6), β = 97° 4(2)' [Craven and Vizzini, 1969]).

Volume
2562.6 $Å^3$

Density
(calculated) 1.173 g/cm^3
(measured) 1.167 (7) g/cm^3[Craven and Vizzini, 1969]

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

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 2.742 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 1.08

Additional patterns
1. Williams [1959]

PDF card 27-1596 is labelled form I but is either form II or a mixture of the two forms.

References

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.
Williams, P. P. (1959). Anal. Chem. 31, 140.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
10.64	34	2 0 0	8.30
10.18	100	1 1 0	8.68
7.46	32	-1 1 1	11.86
7.03	79	1 1 1	12.58
6.05	6	3 1 0	14.62
5.79	2	0 2 0	15.28
5.47	22	-3 1 1	16.18
5.32	16	4 0 0	16.64
5.15	6	0 0 2	17.22
5.09	4	2 2 0	17.40
4.996	2	3 1 1	17.74
4.870	21	-2 0 2	18.20
4.672	12	-2 2 1	18.98
4.458	10	2 2 1	19.90
4.423	10	2 0 2	20.06
4.141	1	-3 1 2	21.44
4.001	7	5 1 0	22.20
3.802	35	1 3 0	23.38
3.733	10	3 1 2+	23.82
3.590	5	5 1 1	24.78
3.542	4	6 0 0+	25.12
3.517	4	2 2 2	25.30
3.394	1	3 3 0	26.24
3.351	4	-5 1 2	26.58
3.264	1	-4 2 2	27.30
3.193	6	1 1 3	27.92
3.108	3	-6 0 2	28.70
3.026	2	1 3 2	29.50
2.992	4	-6 2 1+	29.84
2.951	5	0 2 3	30.26
2.925	2	-7 1 1+	30.54
2.897	7	0 4 0	30.84
2.819	1	6 2 1+	31.72
2.796	6	2 4 0	31.98
2.769	2	2 2 3+	32.30
2.698	5	-7 1 2	33.18
2.676	3	2 4 1	33.46
2.595	3	-5 3 2	34.54
2.573	5	0 0 4	34.84
2.546	1	4 4 0	35.22
2.529	1	-1 1 4	35.46
2.494	2	-8 0 2+	35.98
2.474	1	4 2 3	36.28
2.468	1	5 1 3	36.38
2.438	1	-4 0 4+	36.84
2.418	1	-8 2 1+	37.16
2.399	1	-6 2 3	37.46
2.379	1	-7 1 3	37.78
2.336	1	-4 4 2	38.50
2.282	1	7 3 1+	39.46

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.253	1	-7 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 0	44.44
2.015	1	-3 1 5	44.96
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
1.890	1	10 0 2+	48.10
1.881	1	8 2 3	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

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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
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
5.05	1	0 2 1	17.55
4.997	1	3 1 1	17.74
4.875	23	-2 0 2	18.18
4.706	1	-1 1 2	18.84
4.674	13	-2 2 1	18.97
4.488	1	1 1 2	19.77
4.461	10	2 2 1	19.89
4.426	10	2 0 2	20.05
4.142	1	-3 1 2	21.43
4.001	8	5 1 0	22.20
3.884	1	-5 1 1	22.88
3.802	41	1 3 0	23.38
3.734	7	3 1 2	23.81
3.731	4	-2 2 2	23.83
3.592	5	5 1 1	24.77
3.553	2	6 0 0	25.04
3.541	2	1 3 1	25.13
3.517	5	2 2 2	25.30
3.493	1	4 0 2	25.48
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	7	1 1 3	27.90
3.169	1	3 3 1	28.14
3.108	3	-6 0 2	28.70
3.090	1	-1 3 2	28.87
3.026	2	1 3 2	29.49
2.992	4	-6 2 1	29.84
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	0 4 0	30.83
2.827	1	6 2 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
2.771	1	2 2 3	32.28
2.769	1	6 0 2	32.31
2.701	1	5 3 1	33.14
2.699	6	-7 1 2	33.17
2.677	3	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
2.573	6	0 0 4	34.84
2.546	1	4 4 0	35.23
2.530	1	-1 1 4	35.45
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	-3 3 3	36.08
2.474	1	4 2 3	36.29
2.467	1	5 1 3	36.38
2.418	1	-8 2 1	37.16
2.399	1	-6 2 3	37.46
2.379	1	-7 1 3	37.78
2.337	1	-4 4 2	38.49
2.288	1	-5 1 4	39.35
2.282	1	7 3 1	39.46
2.255	1	-1 5 1	39.94
2.254	1	-7 3 2	39.97
2.246	1	6 4 0	40.12
2.243	2	1 5 1	40.18

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

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.218	1	-6	0	4	40.65
2.214	1	0	4	3	40.73
2.207	1	9	1	1	40.85
2.204	1	3	5	0	40.92
2.172	1	-3	5	1	41.54
2.159	1	6	4	1	41.80
2.153	1	-1	3	4	41.93
2.119	1	-6	4	2	42.62
2.093	1	7	3	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	3	5	2	45.34
1.995	1	1	1	5	45.43
1.972	1	6	0	4	45.99
1.951	1	-9	3	2	46.52
1.949	1	-2	2	5	46.57
1.932	1	0	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	3	48.34
1.837	1	-9	1	4	49.58
1.823	1	9	1	3	49.99

Amobarbital, form II, $C_{11}H_{18}N_2O_3$

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) Å
b = 22.602(10)
c = 11.680(6)
β = 109.1(3)°

(published values: a = 10.281(6)Å, b = 22.601(10), c = 11.679(6), β = 109° 6(2)' [Craven and Vizzini, 1969])

CD cell: a = 11.680(6)Å, b = 22.602(10), c = 10.282(6), β = 109.1(3)°; sp. gp. $P2_1/a$; a/b = 0.5167; c/b = 0.4549.

Volume
2564.9 $Å^3$

Density
(calculated) 1.172 g/cm^3
(measured) 1.185(7) g/cm^3 [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^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 2.847 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 1.12

Additional patterns
1. PDF card 23-1682 [Eli Lilly and Co., Indianapolis, Ind.]
2. 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.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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 3 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 3	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 3 3+	27.82
3.166	3	2 0 2	28.16
3.097	13	0 7 1	28.80
3.050	9	2 2 2	29.26
3.026	6	-3 3 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	0 7 2+	32.10
2.759	1	0 0 4	32.42
2.730	2	1 4 3	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 3	35.22
2.510	1	2 7 1	35.74
2.448	1	0 9 1+	36.68
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

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.981	2	-4 1 5+	45.76
1.883	1	0 12 0+	48.30
1.774	1	3 3 4	51.46

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
11.30	100	0 2 0	7.82
9.92	53	0 1 1	8.91
8.93	12	1 1 0	9.90
7.37	1	1 2 0	12.00
6.98	60	-1 2 1	12.67
6.22	1	0 3 1	14.22
5.95	16	1 3 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
4.979	3	-2 1 1	17.80
4.959	5	0 2 2	17.87
4.858	24	2 0 0	18.25
4.766	10	-1 4 1	18.60
4.525	6	-1 3 2	19.60
4.463	2	2 2 0	19.88
4.452	1	0 3 2	19.93
4.437	11	-2 0 2	20.00
4.354	1	-2 1 2	20.38
4.217	3	1 4 1	21.05
4.183	13	0 5 1	21.22
4.130	2	-2 2 2	21.50
3.767	25	0 6 0	23.60
3.684	3	2 4 0	24.14
3.676	5	-1 2 3	24.19
3.631	5	0 1 3	24.49
3.565	1	0 6 1	24.96
3.501	2	-2 1 3	25.42
3.490	5	-2 4 2	25.50
3.270	6	-3 1 2	27.25
3.207	1	-2 3 3	27.80
3.168	3	2 0 2	28.14
3.099	14	0 7 1	28.79
3.092	2	1 5 2	28.85
3.064	3	1 7 0	29.12
3.051	9	2 2 2	29.25
3.026	6	-3 3 2	29.49
3.007	1	1 2 3	29.69
2.992	2	2 5 1	29.84
2.929	2	-3 4 1	30.49
2.921	1	2 3 2	30.59
2.872	2	-2 6 2	31.12
2.825	6	0 8 0	31.64
2.787	1	0 7 2	32.09
2.759	1	0 0 4	32.42
2.731	2	1 4 3	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 3	35.29
2.510	1	2 7 1	35.74
2.425	1	2 6 2	37.05
2.341	1	3 3 2	38.42
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 3 6	49.79
1.775	1	3 3 4	51.45

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

Synonyms
(+)-Methylphenethylamine sulfate
d-Benzedrine sulfate
Dexedrine sulfate
d-1-Phenyl-2-aminopropane sulfate

Structure
Monoclinic, $P2_1$ (4), Z = 4. The structure was determined by Bergin and Carlström [1971].

Atom positions
25 atoms in general positions 2(a). The hydrogen atom positions were not determined [ibid.].

Lattice constants
a = 10.509(2) Å
b = 6.350(1)
c = 31.338(5)
β = 94.99(6)°

(published values: a=10.508(2) Å, b=6.350(1), c=31.336(5), β=94.99(6)° [Bergin and Carlström, 1971]).

CD cell: a=31.338(5) Å, b=10.509(2), c=10.509(2), β=94.99(6)°; sp. gp. $P2_1$; a/b=4.9351; c/b=1.6550.

Volume
2083.3 $Å^3$

Density
(calculated) 1.175 g/cm^3
(measured) 1.172(2) g/cm^3 [Bergin and Carlström, 1971]

Thermal parameters
Isotropic B_i, estimated from β_{11}, β_{22}, β_{33} for each atom.

Scattering factors
C^0, N^0, O^0, S^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.318 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 1.16

Additional pattern
1. Folen [1975]

References

Bergin, R. and Carlström, D. (1971). Acta Crystallogr. B27, 2146.
Folen, V. A. (1975). J. Forens. Sci. 20, 348.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
15.60	100	0 0 2	5.66
7.80	9	0 0 4	11.34
6.215	3	0 1 1	14.24
5.878	7	0 1 2	15.06
5.420	18	0 1 3+	16.34
5.298	4	1 1 1	16.72
5.199	26	-1 1 2+	17.04
5.093	33	-2 0 2+	17.40
5.058	31	1 1 2	17.52
4.908	14	-1 1 3+	18.06
4.844	7	-2 0 3+	18.30
4.726	18	1 1 3	18.76
4.535	8	-2 0 4+	19.56
4.449	4	0 1 5	19.94
4.363	46	1 1 4	20.34
4.191	23	-2 0 5	21.18
4.037	7	2 1 0+	22.00
4.008	5	1 1 5	22.16
3.973	4	2 1 1+	22.36
3.897	2	0 0 8	22.80
3.844	16	-1 1 6+	23.12
3.675	3	1 1 6	24.20
3.548	6	-2 0 7	25.08
3.498	2	3 0 0+	25.44
3.435	1	3 0 1	25.92
3.371	3	1 1 7	26.42
3.293	1	-3 0 4+	27.06
3.257	1	2 0 7+	27.36
3.239	2	-1 1 8	27.52
3.173	3	0 2 0	28.10
3.110	10	0 2 2	28.68
3.064	5	-3 1 1	29.12
3.019	6	3 1 1+	29.56
2.996	6	-3 1 3	29.80
2.940	7	0 2 4	30.38
2.875	4	3 1 3	31.08
2.833	1	-3 1 5+	31.56
2.759	1	-1 1 10+	32.42
2.714	2	2 2 0+	32.98
2.695	1	-2 2 2+	33.22
2.656	2	-2 2 3+	33.72
2.618	1	-3 1 7+	34.22
2.589	2	4 0 1+	34.62
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 0 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

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.0519	1	1 3 2	44.10
2.0137	1	-1 3 4+	44.98
2.0078	1	-2 2 11+	45.12
1.9886	1	-4 2 4+	45.58
1.9157	1	1 3 6+	47.42
1.8850	1	4 2 5+	48.24

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
15.61	100	0 0 2	5.66
7.80	9	0 0 4	11.33
7.72	1	-1 0 3	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 3	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	7	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
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	0 0 10	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	3 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 10	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 11	36.34
2.4526	1	-2 2 6	36.61
2.3060	1	1 1 12	39.03
2.2585	2	-2 0 13	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 3 4	44.98
1.8849	1	4 2 5	48.24

Structure
Hexagonal, $P6_3/mmc(194)$, isostructural with NiAs, from powder data [Fürst and Halla, 1938].

Atom positions
2(c) 2 antimony
2(a) 2 cobalt

Lattice constants
a = 3.880 Å
c = 5.185 [Rosenqvist, 1953]

c/a = 1.3363

Volume
67.6 $Å^3$

Density
(calculated) 8.876 g/cm^3

Thermal parameters
Isotropic: cobalt B = 1.0; antimony B = 0.75

Scattering factors
Co^0, Sb^0 [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. Abt. B40, 285.
Rosenqvist, T. (1953). Acta Met. 1, 761.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.819	100	1 0 1	31.72
2.592	5	0 0 2	34.58
2.053	50	1 0 2	44.08
1.940	45	1 1 0	46.80
1.598	15	2 0 1	57.62
1.553	5	1 1 2	59.46
1.537	10	1 0 3	60.16
1.410	10	2 0 2	66.24
1.296	5	0 0 4	72.92
1.234	10	2 1 1	77.28
1.205	5	2 0 3	79.50
1.141	10	2 1 2	84.96
1.120	5	3 0 0	86.90
1.078	10	1 1 4	91.24
1.028	1	3 0 2	97.04
1.023	5	2 1 3	97.64
.991	1	1 0 5	102.04
.970	5	2 2 0	105.14
.917	5	3 1 1	114.24
.909	1	2 2 2	115.96
.882	1	2 0 5	121.60
.877	5	3 1 2	122.88
.848	5	3 0 4	130.70
.837	1	1 0 6	133.96
.829	1	4 0 1	136.54
.820	5	3 1 3	139.78
.803	5	2 1 5	147.06
.799	1	4 0 2	149.12
.789	1	1 1 6	154.74

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.820	100	1 0 1	31.71
2.593	5	0 0 2	34.57
2.053	50	1 0 2	44.08
1.940	50	1 1 0	46.79
1.598	15	2 0 1	57.63
1.553	5	1 1 2	59.46
1.537	15	1 0 3	60.16
1.410	15	2 0 2	66.23
1.296	5	0 0 4	72.92
1.234	10	2 1 1	77.28
1.205	5	2 0 3	79.50
1.141	10	2 1 2	84.97
1.120	5	3 0 0	86.90
1.078	10	1 1 4	91.24
1.028	1	3 0 2	97.04
1.023	5	2 1 3	97.64
.991	5	1 0 5	102.04
.970	5	2 2 0	105.14
.917	5	3 1 1	114.24
.908	1	2 2 2	115.97
.882	5	2 0 5	121.60
.877	5	3 1 2	122.88
.848	10	3 0 4	130.71
.837	5	1 0 6	133.96
.829	5	4 0 1	136.54
.820	10	3 1 3	139.79
.803	10	2 1 5	147.06
.799	5	4 0 2	149.12
.789	5	1 1 6	154.75

Antimony Cobalt, $CoSb_2$

Structure
Monoclinic, $P2_1/c$ (14), Z = 4, isostructural with $CoAs_2$ and FeAsS. The structure was determined by Zhdanov and Kuz'min [1962], and confirmed by Kjekshus [1971]. Previously, the structure was assumed to be orthorhombic.

Atom positions
All atoms were in general positions.

Lattice constants
a = 6.5081(3)Å
b = 6.3883(4)
c = 6.5434(3)
β = 117.660(4)°

CD cell: a = 6.5434(3), b = 6.3883(4), c = 6.5081(3), β = 117.660(4)°; Sp.Gp. $P2_1/a$(14); a/b = 1.0243, c/b = 1.0188

(Published values: a = 6.5077(3), b = 6.3879(4), c = 6.5430(3), β = 117.660(4) [Kjekshus, 1971].)

Volume
240.96 Å^3

Density
(calculated) 8.337 g/cm^3
(measured) 8.30 [Kjekshus, 1971]

Thermal parameters
Isotropic: overall B = 0.16

Scattering factors
Co^0, Sb^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.329 \times 10^{-3}$

Additional pattern
1. PDF card 4-0890 [Fürst and Halla, 1938].

References

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Fürst, U. and Halla, F. (1938). Z. Phys. Chem. Abt. B, 40, 285.
Kjekshus, A. (1971). Acta Chem. Scand. 25, 411.
Zhdanov, G. S. and Kuz'min, R. N. (1961). Sov. Phys. Crystallogr. 6, 704.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.764	1	1 0 0	15.36
4.203	1	-1 1 1	21.12
2.986	20	1 1 1	29.90
2.897	25	0 0 2	30.84
2.882	30	2 0 0	31.00
2.773	100	-1 2 1	32.26
2.638	55	0 1 2	33.96
2.627	65	2 1 0	34.10
2.557	20	-2 1 2	35.06
2.210	5	1 0 2	40.80
2.146	1	0 2 2	42.08
2.140	5	2 2 0	42.20
2.102	10	-2 2 2	43.00
2.089	1	1 1 2	43.28
2.045	25	-1 1 3	44.26
2.033	25	-3 1 1	44.52
2.016	5	-2 1 3	44.92
1.989	10	-1 3 1	45.56
1.849	1	0 1 3	49.24
1.801	35	1 3 1	50.64
1.787	25	-3 1 3+	51.06
1.782	20	-3 2 1	51.22
1.716	5	0 3 2	53.36
1.713	10	2 3 0	53.46
1.689	15	2 0 2	54.28
1.653	1	0 2 3	55.56
1.634	5	-2 0 4	56.24
1.626	5	-4 0 2	56.56
1.608	5	-3 2 3	57.24
1.5969	5	0 4 0	57.68
1.5834	5	-2 1 4	58.22
1.5755	5	-4 1 2	58.54
1.5355	1	-1 4 1+	60.22
1.5318	1	2 3 1	60.38
1.5159	5	-1 3 3	61.08
1.5115	5	-3 3 1+	61.28
1.4548	1	-2 2 4	63.94
1.4488	5	-4 2 2+	64.24
1.4443	10	1 2 3	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	3 0 2	70.16
1.3194	1	0 2 4	71.44
1.3137	1	4 2 0	71.80
1.2889	1	1 3 3	73.40
1.2859	5	3 3 1	73.60
1.2791	1	-2 1 5+	74.06

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.764	1	1 0 0	15.36
4.204	1	-1 1 1	21.12
2.986	20	1 1 1	29.90
2.910	1	-1 1 2	30.70
2.898	20	0 0 2	30.83
2.882	25	2 0 0	31.00
2.792	15	-2 0 2	32.03
2.773	100	-1 2 1	32.26
2.639	50	0 1 2	33.94
2.627	50	2 1 0	34.10
2.558	20	-2 1 2	35.05
2.210	5	1 0 2	40.80
2.146	1	0 2 2	42.07
2.140	1	2 2 0	42.20
2.102	10	-2 2 2	42.99
2.088	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 3 1	45.55
1.849	1	0 1 3	49.24
1.801	40	1 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 3 2	53.35
1.713	5	2 3 0	53.46
1.693	1	-2 3 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 3	57.24
1.5971	5	0 4 0	57.67
1.5833	5	-2 1 4	58.22
1.5757	5	-4 1 2	58.53
1.5355	1	-1 4 1	60.22
1.5316	1	2 3 1	60.39
1.5159	5	-1 3 3	61.08
1.5114	5	-3 3 1	61.28
1.5106	1	-3 1 4	61.32
1.4549	1	-2 2 4	63.94
1.4490	1	-4 2 2	64.23
1.4489	1	0 0 4	64.23
1.4442	10	1 2 3	64.47
1.4411	1	4 0 0	64.62
1.4404	10	3 2 1	64.66
1.4130	1	0 1 4	66.07
1.4058	5	4 1 0	66.45
1.4014	5	-3 3 3	66.69
1.3959	1	-4 0 4	66.99
1.3863	10	-2 4 2	67.51
1.3637	5	-4 1 4	68.78
1.3403	1	3 0 2	70.16
1.3195	1	0 2 4	71.43
1.3136	1	4 2 0	71.81
1.2889	1	1 3 3	73.40
1.2861	5	3 3 1	73.59

Structure
Cubic, $F\bar{4}3m$ (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 $Å^3$

Density
(calculated) 7.454 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Sb^0, Ti^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.660 \times 10^{-3}$

References
Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Webster, P. J. and Ziebeck, K. R. A. (1973). J. Phys. Chem. Solids 34, 1647.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.396	55	1 1 1	26.22
2.942	35	2 0 0	30.36
2.081	100	2 2 0	43.46
1.774	20	3 1 1	51.48
1.698	5	2 2 2	53.94
1.471	15	4 0 0	63.16
1.350	5	3 3 1	69.60
1.316	5	4 2 0	71.68
1.201	20	4 2 2	79.78
1.1324	5	5 1 1+	85.72
1.0401	5	4 4 0	95.56
.9946	5	5 3 1	101.52
.9806	5	4 4 2+	103.54
.9304	10	6 2 0	111.78
.8973	1	5 3 3	118.28
.8871	1	6 2 2	120.54
.8493	5	4 4 4	130.18
.8239	5	7 1 1+	138.42
.8160	1	6 4 0	141.48
.7863	15	6 4 2	156.86

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.397	50	1 1 1	26.21
2.942	30	2 0 0	30.36
2.080	100	2 2 0	43.47
1.774	20	3 1 1	51.47
1.699	5	2 2 2	53.94
1.471	15	4 0 0	63.16
1.350	5	3 3 1	69.59
1.316	10	4 2 0	71.67
1.201	25	4 2 2	79.78
1.1324	5	5 1 1	85.73
1.1324	1	3 3 3	85.73
1.0402	5	4 4 0	95.56
.9946	5	5 3 1	101.52
.9807	5	4 4 2	103.53
.9807	1	6 0 0	103.53
.9303	10	6 2 0	111.78
.8973	1	5 3 3	118.29
.8870	5	6 2 2	120.54
.8493	5	4 4 4	130.19
.8239	5	5 5 1	138.43
.8239	5	7 1 1	138.43
.8160	5	6 4 0	141.48
.7863	50	6 4 2	156.86

Structure
Cubic, $F\bar{4}3m(216)$, Z = 4, isostructural with AgAsMg, from powder data [Kripyakevich and Markiv, 1963].

Atom positions
4(d) 4 antimony
4(a) 4 cobalt
4(c) 4 vanadium

Lattice constant
a = 5.796 Å [ibid.]

Volume
194.71 $Å^3$

Density
(calculated) 7.902 g/cm^3

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.
Terada, M., Endo, K., Fujita, Y., and Kimura, R. (1972). J. Phys. Soc. Jap. 32, 91.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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	5	2 2 2	54.82
1.449	10	4 0 0	64.22
1.330	5	3 3 1	70.80
1.296	5	4 2 0	72.94
1.183	20	4 2 2	81.24
1.115	5	5 1 1+	87.36
1.025	5	4 4 0	97.50
.980	5	5 3 1	103.68
.966	5	4 4 2+	105.76
.916	10	6 2 0	114.40
.884	1	5 3 3	121.26
.874	1	6 2 2	123.66
.837	5	4 4 4	134.08
.812	5	7 1 1+	143.28
.804	1	6 4 0	146.82

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.346	45	1 1 1	26.62
2.898	30	2 0 0	30.83
2.049	100	2 2 0	44.16
1.748	20	3 1 1	52.31
1.673	5	2 2 2	54.82
1.449	15	4 0 0	64.23
1.330	5	3 3 1	70.80
1.296	10	4 2 0	72.93
1.183	25	4 2 2	81.25
1.115	5	5 1 1	87.35
1.115	1	3 3 3	87.35
1.025	5	4 4 0	97.49
.980	5	5 3 1	103.67
.966	5	4 4 2	105.77
.966	1	6 0 0	105.77
.916	10	6 2 0	114.40
.884	1	5 3 3	121.27
.874	5	6 2 2	123.66
.837	5	4 4 4	134.08
.812	5	5 5 1	143.28
.812	5	7 1 1	143.28
.804	5	6 4 0	146.82

Barbital, form I, $C_8H_{12}N_2O_3$

Synonyms
5,5-Diethylbarbituric acid, form I
Diemal
Veronal
Diethylmalonylurea

Structure
Hexagonal, $R\bar{3}$ (148), Z = 18. The structure was determined by Craven, Vizzini, and Rodrigues [1969].

Atom positions
All atoms are in general positions 18(f).

Polymorphism
Six forms of barbital have been reported though forms V and VI have not been isolated as single crystals. Form I described here is the most stable. Crystals of forms I, II, and IV were obtained from the same ethanol solution by slow evaporation at room temperature [ibid.].

Lattice constants
a = 26.923(6) Å
c = 6.828(9)

c/a = 0.2536

(published values: a = 26.921(6)Å, c = 6.828(9) [Craven et al., 1969]).

Volume
4286.2 $Å^3$

Density
(calculated) 1.284 g/cm^3
(measured) 1.287(7) g/cm^3 [Craven et al., 1969]

Thermal parameters
Isotropic B_i, estimated from β_{11}, β_{22}, β_{33} for each atom.

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 2.484 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 1.02

Additional patterns
1. PDF card 5-129 [Huang, T.-Y., 1951]
2. Williams [1959]. The pattern appears to represent a mixture of forms I and II.

References

Craven, B.M., Vizzini, E.A., and Rodrigues, M.M. [1969]. Acta Crystallogr. B25, 1978.
Huang, T.-Y. (1951). Acta Pharm. Int. 2, 95.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Williams, P. P. (1959). Anal. Chem. 31, 140.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
13.46	14	1 1 0	6.56
7.77	100	3 0 0	11.38
6.72	7	2 2 0	13.16
6.54	8	1 0 1	13.52
5.89	5	0 2 1	15.04
5.39	70	1 2 -1+	16.42
5.09	65	1 4 0	17.42
4.69	25	3 1 -1+	18.90
4.48	9	3 3 0	19.78
4.21	8	3 2 1+	21.10
3.88	6	6 0 0	22.88
3.85	7	0 5 1	23.08
3.73	7	2 5 0	23.82
3.70	5	4 2 -1+	24.02
3.57	8	5 1 1+	24.94
3.36	14	4 4 0	26.48
3.34	12	3 4 -1+	26.66
3.28	2	2 0 2	27.20
3.18	8	1 2 2	28.02
3.15	9	6 1 -1+	28.28
3.09	23	1 7 0+	28.90
3.02	10	1 3 -2+	29.58
2.994	5	5 3 -1+	29.82
2.938	4	0 4 2+	30.40
2.877	3	2 3 2	31.06
2.754	4	5 0 2	32.48
2.735	2	4 5 -1+	32.72
2.645	4	1 5 2	33.86
2.629	11	7 2 -1	34.08
2.590	4	9 0 0	34.60
2.543	8	2 8 0	35.26
2.490	2	4 6 1	36.04
2.418	1	4 7 0	37.16
2.301	5	1 9 1+	39.12
2.276	2	0 0 3	39.56
2.244	4	1 1 3+	40.16
2.213	3	1 10 0+	40.74
2.178	1	9 2 1+	41.42
2.155	2	2 2 3+	41.88
2.079	2	7 3 -2+	43.50
2.024	1	0 11 1	44.74
2.002	1	10 2 -1+	45.26
1.943	2	2 5 -3+	46.72
1.939	2	9 4 -1+	46.82
1.923	1	2 11 0+	47.22
1.867	1	10 4 0+	48.74
1.851	1	8 4 -2	49.18
1.846	1	8 6 -1	49.34
1.739	1	9 4 2+	52.58
1.735	2	8 7 1	52.72

d(Å)	I	hkℓ	2θ(°) λ = 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	2θ(°) λ = 1.540598Å
13.46	14	1 1 0	6.56
7.77	100	3 0 0	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	3 3 0	19.77
4.21	5	3 2 1	21.08
4.21	4	2 3 -1	21.08
3.89	7	6 0 0	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	3	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	3	1 6 1	28.28
3.15	6	6 1 -1	28.28
3.09	8	7 1 0	28.89
3.09	19	1 7 0	28.89
3.02	4	3 1 2	29.56
3.02	7	1 3 -2	29.56
2.994	2	7 0 1	29.82
2.994	2	5 3 -1	29.82
2.946	2	0 4 2	30.32
2.938	2	6 3 0	30.40
2.938	2	3 6 0	30.40
2.922	2	6 2 1	30.57
2.878	3	2 3 2	31.05
2.755	4	5 0 2	32.48
2.735	2	4 5 -1	32.71
2.646	3	1 5 2	33.85
2.629	13	7 2 -1	34.08
2.591	5	9 0 0	34.60
2.544	9	2 8 0	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	4 7 0	37.16
2.301	2	1 9 1	39.11
2.301	2	6 5 1	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	9 2 1	41.44
2.156	1	2 2 3	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 11 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	3 10 2	53.50
1.658	1	5 9 2	55.35
1.634	1	1 12 -2	56.26
1.618	1	0 14 1	56.86

Barbital, form II, $C_8H_{12}N_2O_3$

Synonyms
5,5-Diethyl barbituric acid
Diemal
Veronal
Diethylmalonylurea

Structure
Monoclinic, C2/c (15), Z = 4. The structure was determined by Craven, Vizzini, and Rodrigues [1969].

Atom positions
4(e) 4 C(2)
4(e) 4 C(5)
4(e) 4 O(2)
All other atoms in general positions 8(f) [ibid.]

Polymorphism
Six forms of barbital have been reported though forms V and VI have not been isolated as single crystals. The hexagonal form I is the most stable. Form II described here is the 2nd most stable. Crystals of forms I, II, and IV were obtained from the same ethanol solution by slow evaporation at room temperature [ibid.].

Lattice constants
a = 7.120(5) Å
b = 14.163(10)
c = 9.810(7)
β = 89.23(3)°
(published values: a = 7.120(5)Å, b = 14.162(10), c = 9.810(7), β = 89° 14(2)' [Craven et al., 1969]).

CD cell: a = 9.810(7)Å, b = 14.163(10), c = 7.120(5), β = 90.77(3)°, sp. gp. A2/a; a/b = 0.6926; c/b = 0.5027

Volume
989.2 $Å^3$

Density
(calculated) 1.237 g/cm^3
(measured) 1.238(7) g/cm^3 [Craven et al., 1969]

Thermal parameters
Isotropic B_i estimated from β_{11}, β_{22}, β_{33} for each atom.

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 5.144 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 2.12

Additional patterns
1. PDF card 14-953 [Huang, 1951]
2. Williams [1959]. The pattern appears to represent a mixture of forms I and II

References

Craven, B. M., Vizzini, E. A., and Rodrigues, M.M. (1969). Acta.Crystallogr. B25, 1978.
Huang, T.-Y. (1951). Acta Pharm. Int. 2, 95.
International Tables of X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Williams, P. P. (1959). Anal. Chem. 31, 140.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
7.08	4	0 2 0	12.50
6.36	4	1 1 0	13.92
5.73	20	0 2 1	15.44
5.36	36	1 1 1	16.54
5.30	100	-1 1 1	16.70
4.90	5	0 0 2	18.08
3.90	1	1 1 2	22.76
3.86	2	-1 1 2	23.02
3.66	5	1 3 1	24.30
3.54	5	0 4 0	25.14
3.33	1	0 4 1	26.76
3.08	4	1 3 2	28.98
3.04	9	2 2 1	29.40
2.968	9	0 2 3	30.08
2.893	2	-1 1 3	30.88
2.863	14	-2 0 2	31.22
2.682	3	2 2 2	33.38
2.653	5	-2 2 2	33.76
2.543	2	1 5 1	35.26
2.524	6	1 3 3	35.54
2.340	1	3 1 0	38.44
2.294	1	2 2 3+	39.24
2.278	1	-1 1 4	39.52
2.243	1	2 4 2	40.18
2.226	3	-2 4 2	40.50
1.953	1	2 2 4	46.46
1.947	1	1 7 0	46.62
1.931	1	2 6 1+	47.02
1.891	2	-3 1 3	48.08
1.762	1	2 4 4+	51.84

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
7.08	4	0 2 0	12.49
6.36	4	1 1 0	13.91
5.74	20	0 2 1	15.42
5.37	26	1 1 1	16.51
5.31	100	-1 1 1	16.69
4.90	5	0 0 2	18.07
3.91	1	1 1 2	22.74
3.86	2	-1 1 2	23.01
3.66	6	1 3 1	24.29
3.54	6	0 4 0	25.13
3.33	1	0 4 1	26.75
3.08	4	1 3 2	28.96
3.04	10	2 2 1	29.39
2.969	10	0 2 3	30.08
2.894	1	-1 1 3	30.87

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

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
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	33.74
2.545	2	1	5	1	35.23
2.524	6	1	3	3	35.54
2.340	1	3	1	0	38.43
2.294	1	2	2	3	39.25
2.279	1	-1	1	4	39.51
2.243	1	2	4	2	40.17
2.226	3	-2	4	2	40.49
1.953	1	2	2	4	46.45
1.946	1	1	7	0	46.63
1.891	3	-3	1	3	48.07
1.763	1	2	4	4	51.83

Barbital, form IV, $C_8H_{12}N_2O_3$

Synonyms
5,5-Diethylbarbituric acid
Diemal
Veronal
Diethylmalonylurea

Structure
Monoclinic, $P2_1$ (4), Z = 8. The structure was determined by Craven and Vizzini [1971].

Atom positions
All atoms were in general positions 2(a). Positions for hydrogen(72)(molecule 3) appeared to be in error and were omitted from these calculations.

Polymorphism
Six forms of barbital have been reported though forms V and VI have not been isolated as single crystals. The phase described as form III may not exist [Craven and Vizzini, 1971]. Crystals described here were hand-picked from the mixture of forms I, II, and IV, obtained from the same ethanol solution by slow evaporation at room temperature.

Lattice constants
a = 12.586(8) Å
b = 22.084(10)
c = 6.788(9)
β = 90.92(3)°

a/b = 0.5699
c/b = 0.3074

(published values: a = 12.585(8)Å; b = 22.083(10), c = 6.788(9), β = 90°55(2)' [Craven and Vizzini, 1971]).

Volume
1886.5 $Å^3$

Density
(calculated) 1.297 g/cm^3
(measured) 1.296(7) g/cm^3 [Craven and Vizzini, 1971]

Thermal parameters
Isotropic for hydrogens; anisotropic for all others [Craven and Vizzini, 1971]

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.804 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 0.743

Additional pattern
1. PDF card 5-0083 [Huang, 1951]

References
Craven, B. M. and Vizzini, E. A. (1971). Acta Crystallogr. B27, 1917.
Huang, T.-Y. (1951). Acta Pharm. Int. 2, 95.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598A
11.04	77	0 2 0	8.00
6.49	100	0 1 1	13.64
5.93	9	1 0 1	14.94
5.78	58	0 2 1	15.32
5.47	69	2 2 0	16.20
5.28	3	-1 2 1	16.78
5.22	5	1 2 1	16.96
4.98	42	0 3 1	17.78
4.78	13	2 3 0	18.54
4.65	10	-2 0 1+	19.06
4.55	14	-2 1 1	19.50
4.48	15	2 1 1	19.80
4.28	2	0 4 1+	20.72
4.23	1	2 2 1	21.00
4.15	10	2 4 0	21.40
4.04	5	1 4 1	21.98
3.678	5	0 6 0	24.18
3.613	21	2 5 0	24.62
3.548	13	-3 1 1+	25.08
3.498	2	3 1 1	25.44
3.373	9	3 2 1	26.40
3.257	4	1 0 2	27.36
3.245	4	0 2 2	27.46
3.175	5	2 6 0	28.08
3.144	13	4 0 0	28.36
3.116	6	4 1 0	28.62
3.081	10	0 3 2	28.96
3.004	17	-1 3 2+	29.72
2.982	11	1 3 2+	29.94
2.968	10	2 0 2	30.08
2.940	4	2 1 2	30.38
2.901	10	-2 2 2	30.80
2.864	10	2 2 2	31.20
2.824	11	-1 4 2	31.66
2.820	11	2 7 0+	31.70
2.812	9	1 4 2	31.80
2.793	8	-1 7 1	32.02
2.784	9	-2 3 2+	32.12
2.753	6	2 3 2+	32.50
2.735	2	4 4 0	32.72
2.659	4	-3 0 2	33.68
2.639	6	-3 1 2+	33.94
2.624	6	1 5 2	34.14
2.599	5	3 1 2	34.48
2.572	1	-3 6 1	34.86
2.548	3	3 2 2	35.20
2.528	4	2 8 0	35.48
2.502	4	1 8 1+	35.86
2.466	2	3 3 2	36.40
2.453	1	-1 6 2	36.60

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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	0 7 2+	38.96
2.275	2	-4 2 2+	39.58
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	0 8 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
2.017	1	6 3 0+	44.90
2.003	2	-5 2 2	45.24
1.998	3	5 1 2+	45.36
1.979	2	5 6 1+	45.82
1.973	2	-3 2 3+	45.96
1.962	2	6 4 0+	46.24
1.926	2	0 6 3+	47.14
1.910	2	3 3 3+	47.56
1.901	2	-2 9 2+	47.80
1.891	1	2 9 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	-3 9 2+	50.58
1.798	1	-6 0 2+	50.72
1.772	1	2 10 2+	51.54
1.750	1	6 2 2+	52.24
1.746	1	-6 3 2+	52.36
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 (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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	10	2 4 0	21.39
4.04	5	1 4 1	21.97
3.681	5	0 6 0	24.16
3.615	23	2 5 0	24.61
3.560	1	-1 5 1	24.99
3.557	1	-2 4 1	25.01
3.548	12	-3 1 1	25.08
3.524	1	2 4 1	25.25
3.498	1	3 1 1	25.44
3.374	10	3 2 1	26.40
3.354	4	0 1 2	26.55
3.263	3	1 0 2	27.31
3.254	1	-1 1 2	27.39
3.244	2	0 2 2	27.47
3.177	5	2 6 0	28.06
3.153	2	-1 2 2	28.28
3.146	11	4 0 0	28.35
3.130	4	1 2 2	28.50
3.128	1	1 6 1	28.51
3.115	4	4 1 0	28.64
3.082	10	0 3 2	28.95
3.026	3	4 2 0	29.50
3.007	8	-2 0 2	29.68
3.004	11	-1 3 2	29.72
2.983	6	1 3 2	29.93
2.982	2	3 4 1	29.94
2.980	2	-2 1 2	29.97
2.967	8	2 0 2	30.10
2.941	3	2 1 2	30.37
2.901	10	-2 2 2	30.79
2.893	2	4 3 0	30.88

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.865	10	2 2 2	31.19
2.861	1	0 7 1	31.24
2.848	1	-4 1 1	31.38
2.826	10	-1 4 2	31.63
2.820	3	2 7 0	31.70
2.814	1	4 1 1	31.77
2.809	5	1 4 2	31.83
2.794	5	-1 7 1	32.01
2.784	5	-2 3 2	32.13
2.780	1	-4 2 1	32.18
2.761	2	0 8 0	32.41
2.752	5	2 3 2	32.51
2.733	1	4 4 0	32.74
2.659	4	-3 0 2	33.68
2.641	1	-2 4 2	33.92
2.640	4	-3 1 2	33.93
2.638	1	-1 5 2	33.95
2.625	5	1 5 2	34.13
2.614	1	2 4 2	34.28
2.600	5	3 1 2	34.47
2.572	1	-3 6 1	34.86
2.547	3	3 2 2	35.20
2.528	4	2 8 0	35.48
2.503	4	1 8 1	35.85
2.467	2	3 3 2	36.40
2.453	1	-1 6 2	36.61
2.371	1	-3 7 1	37.92
2.359	1	-5 1 1	38.12
2.356	1	3 7 1	38.17
2.348	2	5 0 1	38.31
2.311	4	0 7 2	38.95
2.276	1	-4 2 2	39.57
2.258	1	-5 3 1	39.89
2.241	1	4 2 2	40.20
2.218	1	-4 3 2	40.65
2.186	1	4 3 2	41.27
2.141	1	0 8 2	42.16
2.115	1	-1 8 2	42.72
2.088	1	6 1 0	43.30
2.017	1	6 3 0	44.90
2.003	1	-5 2 2	45.22
1.998	2	5 1 2	45.35
1.979	1	5 6 1	45.81
1.972	1	-3 2 3	45.97
1.961	1	6 4 0	46.27
1.927	1	0 6 3	47.11
1.910	1	3 3 3	47.56
1.891	1	2 9 2	48.08
1.866	1	-4 9 1	48.77
1.856	1	4 9 1	49.05
1.803	1	-3 9 2	50.57
1.746	1	-6 3 2	52.36
1.722	1	6 3 2	53.13
1.693	1	5 7 2	54.13
1.589	1	4 12 0	58.01

Bufotenine, $C_{12}H_{16}N_2O$

Synonyms
5-Hydroxy-N,N-dimethyltryptamine
3-(2-Dimethylaminoethyl)-indol-5-ol
Mappine

Structure
Monoclinic, $P2_1/a$ (14), Z = 8. The structure was determined by Falkenburg [1972].

Atom positions
All atoms were in general positions 4(e) [ibid.].

Lattice constants
a = 17.95(1) Å
b = 11.52(1)
c = 14.24(2)
β = 131.29(3)°

CD cell: a=14.24(2)Å, b=11.52(1), c=13.70(1), β = 100.07(2)°; sp. gp. $P2_1/n$; a/b = 1.2361; c/b = 1.1891

Volume
2212.5 $Å^3$

Density
(calculated) 1.226 g/cm^3
(measured) 1.205 g/cm^3 [Falkenburg, 1972]

Thermal parameters
For hydrogens: overall B = 5.0; for other atoms, isotropic B_i estimated from β_{11}, β_{22}, β_{33} for each atom.

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.845 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 0.602

Additional pattern
1. PDF card 26-1586 [Physical Data of Indole and Dihydroindole Alkaloids, Eli Lilly Co., edited by N. Neuss]

References

Falkenburg, G. (1972). Acta Crystallogr. B28, 3219.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
10.70	1	0 0 1	8.26
8.89	11	-1 1 1	9.94
7.84	1	0 1 1	11.28
7.08	26	-2 1 1	12.50
6.74	12	2 0 0	13.12
5.98	40	-2 1 2	14.80
5.81	16	2 1 0	15.24
5.76	11	0 2 0	15.36
5.32	51	-1 2 1	16.64
5.19	18	-3 1 2	17.08
5.07	21	0 2 1	17.48
4.85	67	0 1 2	18.28
4.48	5	-4 0 2	19.80
4.37	18	-1 2 2+	20.30
4.32	19	-3 1 3+	20.52
4.19	46	-4 0 3+	21.18
4.08	100	-4 0 1	21.78
3.94	53	-4 1 3	22.54
3.89	5	1 1 2	22.86
3.69	3	1 3 0+	24.08
3.63	3	-2 2 3	24.52
3.54	27	3 2 0	25.12
3.50	15	-4 0 4	25.40
3.36	7	-2 0 4+	26.50
3.33	3	-4 2 1	26.76
3.27	17	3 1 1	27.22
3.24	19	4 1 0	27.54
3.02	2	-3 2 4	29.56
2.994	2	-4 2 4	29.82
2.967	1	-3 3 3+	30.10
2.903	12	-6 0 4+	30.78
2.843	6	2 2 2+	31.44
2.820	9	-6 1 4+	31.70
2.766	4	-6 1 2+	32.34
2.741	3	-2 4 1	32.64
2.725	5	-5 1 5	32.84
2.688	2	-3 1 5+	33.30
2.656	2	-2 4 2+	33.72
2.609	2	3 1 2+	34.34
2.587	2	-4 3 4+	34.64
2.552	3	-4 2 5+	35.14
2.528	3	-2 3 4+	35.48
2.489	2	2 3 2	36.06
2.485	2	-5 3 4	36.12
2.474	2	-7 1 3	36.28
2.443	4	5 2 0	36.76
2.425	2	0 2 4+	37.04
2.388	1	-7 1 5	37.64
2.374	3	-1 3 4+	37.86
2.361	2	-2 2 5+	38.08

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.345	3	-6	2	1	38.36
2.252	1	0	5	1	40.00
2.239	2	-5	4	3+	40.24
2.212	2	-8	0	5+	40.76
2.186	2	-2	4	4+	41.26
2.097	2	-8	0	6+	43.10
2.063	2	-8	1	6	43.84
2.040	1	-8	0	2	44.38
2.023	2	-7	2	1+	44.76
2.019	3	-1	3	5+	44.86
2.001	1	1	3	4	45.28
1.997	2	-6	3	6+	45.38
1.969	1	5	4	0+	46.06
1.933	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	3	7+	52.32
1.722	1	7	3	0+	53.16
1.702	1	-10	1	7+	53.82
1.665	1	-5	2	8+	55.12
1.628	1	-10	0	8+	56.46
1.577	1	-9	2	1+	58.46

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
10.70	1	0	0	1	8.26
8.97	1	-2	0	1	9.85
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	3	-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	3	2	1	1	21.11
4.19	32	-4	0	3	21.16
4.19	13	3	1	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	3	-2	2	3	24.50
3.54	25	3	2	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	3	-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	3	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	3	-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
2.473	1	-7	1	3	36.29

Bufotenine, $C_{12}H_{16}N_2O$ - (continued)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
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	3	37.86
2.345	2	-6	2	1	38.36
2.252	1	0	5	1	40.00
2.212	2	-8	0	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	3	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	8	56.47
1.577	1	-9	2	1	58.46

Calcium Borate, CaB_2O_4

Structure
Orthorhombic, Pnca(60), Z = 4. The structure was determined by Marezio et al. [1963].

Atom positions
4(c) 4 calcium
8(d) 8 boron
8(d) 8 oxygen(1)
8(d) 8 oxygen(2) [ibid.]

Lattice constants
a = 6.214(3) Å
b = 11.605(4)
c = 4.285(1) [ibid.]

a/b = 0.5355
c/b = 0.3692

Volume
309.0 $Å^3$

Density
(calculated) 2.702 g/cm^3

Thermal parameters
Anisotropic [Marezio et al., 1963]

Scattering factors
Ca^0, B^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.289 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.05
(hkℓ = 210 as scale reflection)

Additional patterns
1. PDF card 18-281 [Stojanovic, Inst. for Refractories, Kraljevo, Yugoslavia]
2. PDF card 23-407 [Fletcher et al., 1974]

References

Fletcher, B. L., Stevenson, J.R. and Whitaker, A. (1974). J. Am. Ceram. Soc. 53, 95.

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204.

Marezio, M., Plettinger, H. A., and Zachariasen, W. H. (1963). Acta Crystallogr. 16, 390.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.80	13	0 2 0	15.26
4.019	1	0 1 1	22.10
3.373	50	1 1 1	26.40
3.106	19	2 0 0	28.72
3.002	100	2 1 0	29.74
2.901	20	0 4 0	30.80
2.872	16	0 3 1	31.12
2.738	13	2 2 0	32.68
2.606	39	1 3 1	34.38
2.458	1	2 1 1	36.52
2.308	2	2 2 1	39.00
2.240	12	1 4 1	40.22
2.143	28	0 0 2	42.14
2.121	22	2 4 0	42.60
2.040	3	0 5 1	44.36
2.025	1	1 0 2	44.72
2.010	9	0 2 2	45.08
1.995	2	1 1 2	45.42
1.939	46	1 5 1	46.82
1.912	6	1 2 2	47.52
1.901	7	2 4 1	47.82
1.859	2	2 5 0	48.96
1.841	37	3 1 1	49.46
1.763	3	2 0 2	51.80
1.743	5	2 1 2	52.44
1.723	3	0 4 2	53.10
1.696	1	1 6 1	54.04
1.687	6	2 2 2	54.32
1.680	9	3 3 1	54.58
1.661	1	1 4 2	55.26
1.642	8	2 6 0	55.96
1.605	1	2 3 2	57.36
1.569	1	3 4 1	58.82
1.553	1	4 0 0	59.46
1.546	1	0 7 1	59.76
1.533	2	2 6 1	60.32
1.507	8	2 4 2	61.48
1.500	13	4 2 0+	61.78
1.489	1	3 0 2	62.30
1.477	1	3 1 2	62.86
1.454	1	3 5 1	64.00
1.450	1	4 1 1	64.18
1.442	2	4 3 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 3 2	67.32
1.382	1	1 1 3	67.74
1.369	2	4 4 0	68.46

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.353	1	1 2 3	69.38
1.340	2	0 3 3	70.18
1.325	1	3 4 2	71.10
1.314	2	2 8 0	71.76
1.310	4	1 3 3	72.04
1.303	5	2 6 2	72.46
1.290	1	2 1 3	73.34
1.283	1	1 7 2	73.80
1.267	1	2 2 3	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
1.211	6	1 9 1+	79.00
1.201	1	0 8 2	79.78
1.196	1	4 3 2	80.20
1.194	2	1 5 3	80.38
1.191	3	2 9 0	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	3	0 10 0	83.18
1.154	2	4 4 2	83.76
1.145	1	3 8 1	84.56
1.141	2	5 3 1	84.96
1.133	1	2 5 3+	85.68
1.125	1	3 3 3	86.42
1.120	2	2 8 2	86.88
1.102	1	1 10 1	88.66
1.0871	1	2 10 0	90.24
1.0820	1	0 7 3	90.78
1.0776	1	2 6 3	91.26
1.0712	1	0 0 4	91.96
1.0660	2	1 7 3	92.54
1.0604	4	4 8 0+	93.18
1.0543	3	4 6 2	93.88
1.0536	2	0 2 4	93.96
1.0490	1	3 5 3	94.50
1.0471	1	4 1 3	94.72
1.0410	1	2 9 2	95.46
1.0385	1	1 2 4+	95.76
1.0357	1	6 0 0	96.10
1.0317	1	6 1 0	96.60
1.0217	1	2 7 3	97.86
1.0203	2	0 10 2	98.04
1.0196	2	6 2 0	98.14

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.0127	1	2 0 4	99.04
1.0108	1	1 11 1	99.30
1.0082	1	5 4 2	99.64
1.0045	1	1 8 3+	100.14
1.0020	1	4 7 2+	100.48
.9990	1	2 11 0	100.90
.9977	1	2 2 4	101.08
.9920	1	1 4 4+	101.88
.9854	1	3 10 1	102.84
.9797	1	2 3 4	103.68
.9754	1	6 4 0+	104.32
.9687	2	5 7 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	4 8 2	108.32
.9459	1	1 9 3	109.04
.9390	1	3 2 4	110.24
.9346	1	5 1 3	111.02
.9325	1	6 0 2	111.40
.9266	1	1 6 4	112.46
.9257	1	5 2 3	112.64
.9234	1	2 12 0+	113.06
.9207	2	6 2 2	113.58
.9183	4	3 11 1	114.04
.9130	1	6 6 0+	115.06
.9112	1	5 3 3	115.42
.9041	1	3 4 4	116.86
.9020	1	5 7 2+	117.30
.9004	1	4 9 2	117.64
.8972	1	2 6 4	118.32
.8929	1	6 6 1	119.24
.8922	1	5 4 3	119.40
.8905	1	1 7 4	119.76

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.80	13	0 2 0	15.26
4.020	1	0 1 1	22.10
3.375	53	1 1 1	26.39
3.107	20	2 0 0	28.71
3.014	29	1 2 1	29.61
3.001	100	2 1 0	29.74
2.901	21	0 4 0	30.79
2.871	16	0 3 1	31.12
2.739	15	2 2 0	32.67
2.607	44	1 3 1	34.38
2.458	1	2 1 1	36.52
2.308	2	2 2 1	39.00
2.241	14	1 4 1	40.21
2.143	33	0 0 2	42.14
2.121	25	2 4 0	42.60
2.109	2	2 3 1	42.85
2.041	4	0 5 1	44.35
2.025	1	1 0 2	44.70
2.010	11	0 2 2	45.07
1.995	2	1 1 2	45.42
1.939	56	1 5 1	46.82
1.934	1	0 6 0	46.94
1.912	6	1 2 2	47.51
1.901	7	2 4 1	47.82
1.859	1	2 5 0	48.95
1.841	46	3 1 1	49.46
1.764	4	2 0 2	51.79
1.744	6	2 1 2	52.43
1.723	4	0 4 2	53.10
1.696	1	1 6 1	54.03
1.688	7	2 2 2	54.32
1.680	10	3 3 1	54.59
1.661	1	1 4 2	55.27
1.642	9	2 6 0	55.95
1.605	1	2 3 2	57.37
1.569	1	3 4 1	58.82
1.553	1	4 0 0	59.45
1.546	1	0 7 1	59.76
1.533	2	2 6 1	60.32
1.526	1	1 5 2	60.63
1.507	10	2 4 2	61.47
1.501	8	4 2 0	61.77
1.500	8	1 7 1	61.78
1.489	1	3 0 2	62.30
1.477	1	3 1 2	62.87
1.454	1	3 5 1	63.99
1.449	1	4 1 1	64.23
1.442	1	3 2 2	64.56
1.442	2	4 3 0	64.60
1.436	1	0 6 2	64.90
1.418	1	0 1 3	65.83
1.416	1	4 2 1	65.90
1.404	1	2 5 2	66.53
1.399	1	1 6 2	66.83
1.390	1	3 3 2	67.32
1.384	1	2 7 1	67.63
1.382	2	1 1 3	67.74
1.370	3	4 4 0	68.45
1.366	1	4 3 1	68.63
1.354	1	1 2 3	69.37
1.342	1	3 6 1	70.03
1.342	1	1 8 1	70.08
1.340	3	0 3 3	70.18
1.325	1	3 4 2	71.10
1.314	2	2 8 0	71.75
1.310	4	1 3 3	72.04
1.303	6	2 6 2	72.46
1.290	1	2 1 3	73.35
1.283	1	1 7 2	73.80
1.266	1	2 2 3	74.92
1.257	1	2 8 1	75.61
1.255	1	1 4 3	75.72
1.253	1	3 5 2	75.84
1.239	1	3 7 1	76.88
1.236	1	4 5 1	77.09
1.230	1	2 3 3	77.52
1.229	3	4 2 2	77.61
1.216	1	0 5 3	78.58
1.211	2	4 6 0	78.99
1.211	5	1 9 1	79.00
1.201	1	0 8 2	79.77
1.196	1	4 3 2	80.19
1.194	3	1 5 3	80.37
1.191	3	2 9 0	80.60
1.187	2	5 1 1	80.90
1.185	3	2 4 3	81.12
1.179	1	1 8 2	81.56
1.170	5	3 1 3	82.36
1.169	1	5 2 1	82.43
1.161	4	0 10 0	83.18
1.154	3	4 4 2	83.76
1.145	1	3 8 1	84.56
1.141	3	5 3 1	84.97
1.134	1	4 7 0	85.61
1.133	1	2 5 3	85.69
1.125	2	3 3 3	86.42
1.120	3	2 8 2	86.87
1.104	1	5 4 1	88.51
1.102	1	1 10 1	88.66
1.0871	1	2 10 0	90.23

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.0821	1	0 7 3	90.77
1.0777	1	2 6 3	91.25
1.0750	1	5 0 2	91.54
1.0713	1	0 0 4	91.95
1.0661	3	1 7 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	2 9 2	95.46
1.0391	1	3 8 2	95.69
1.0386	1	1 2 4	95.74
1.0358	1	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	2 7 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 11 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	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	3	5 7 1	105.35
.9672	1	2 8 3	105.58
.9671	1	0 12 0	105.60
.9666	1	4 9 1	105.67
.9591	1	3 7 3	106.86
.9578	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 3	109.04

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.9390	1	3 2 4	110.24
.9345	1	5 1 3	111.03
.9327	1	1 12 1	111.36
.9324	1	6 0 2	111.40
.9294	1	6 1 2	111.95
.9266	1	1 6 4	112.46
.9256	1	5 2 3	112.66
.9234	1	2 12 0	113.07
.9217	1	5 8 1	113.38
.9206	3	6 2 2	113.59
.9182	5	3 11 1	114.04
.9154	1	3 10 2	114.60
.9147	1	2 9 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	5 7 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
Hexagonal, $P6_3/mmc(194)$, Z = 4, a ternary Laves phase, isostructural with $MgZn_2$, from powder data [Ganglberger et al., 1965].

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 $Å^3$

Density
(calculated) 8.409 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Cr^0, Nb^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.320 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Faller, J. G. and Skolnick, L. P. (1963). Trans. AIME 227, 687.
Friauf, J. B. (1927). Phys. Rev. 29, 34.
Ganglberger, E., Nowotny, H., and Benesovsky, F. (1965). Monatsh. Chem. 96, 1658.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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 0 0	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 3	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	3 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	3 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	3 0 8	145.12
.800	5	5 0 3	148.56
.794	1	4 2 0	152.16
.792	5	3 3 2	153.24

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
3.709	1	1	0	1	23.97
2.879	5	1	0	2	31.04
2.424	50	1	1	0	37.05
2.232	85	1	0	3	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	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	3	0	2	71.43
1.318	5	0	0	6	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	6	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	96.39
1.014	1	2	1	6	98.88
1.003	1	3	1	4	100.28
.962	5	1	0	8	106.39
.938	5	3	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	3	116.71
.893	10	4	1	2	119.28
.892	5	2	2	6	119.40
.875	10	4	0	5	123.45
.873	1	3	1	6	123.93
.866	1	3	2	4	125.61
.860	1	1	0	9	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	8	145.13
.800	5	5	0	3	148.56
.794	5	4	2	0	152.16
.792	10	3	3	2	153.24

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 4, a ternary Laves phase, isostructural with $MgZn_2$, 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 Å
c = 7.952 [Kuo (1953), table II]

c/a = 1.6376

Volume
162.4 $Å^3$

Density
(calculated) 11.94 g/cm^3

Thermal parameters
Isotropic: tantalum B = 0.75; chromium B = 1.0; cobalt B = 1.0

Scattering factors
Co^0, Cr^0, Ta^0 [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. 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 (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.203	20	1 0 0	21.12
3.973	15	0 0 2	22.36
3.717	20	1 0 1	23.92
2.888	20	1 0 2	30.94
2.428	75	1 1 0	37.00
2.243	100	1 0 3	40.18
2.103	15	2 0 0	42.98
2.072	90	1 1 2	43.64
2.033	45	2 0 1	44.54
1.988	5	0 0 4	45.60
1.797	5	1 0 4	50.76
1.647	5	2 0 3	55.76
1.589	5	2 1 0	57.98
1.559	5	2 1 1	59.24
1.487	10	1 0 5	62.38
1.476	5	2 1 2	62.92
1.402	10	3 0 0	66.66
1.363	30	2 1 3	68.82
1.325	5	0 0 6	71.08
1.322	20	3 0 2	71.28
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	3 1 0	82.66
1.163	5	1 1 6	82.92
1.161	5	2 2 2	83.14
1.154	1	3 1 1	83.74
1.124	10	2 1 5	86.50
1.121	10	2 0 6	86.78
1.119	5	3 1 2	87.04
1.097	1	1 0 7	89.24
1.068	15	3 1 3	92.36
1.051	1	4 0 0	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 3	104.04
.967	5	1 0 8	105.56
.965	1	3 2 0	105.94
.963	1	3 0 6	106.24
.941	5	3 1 5	109.96
.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	3 2 3	116.34
.899	1	2 0 8	118.00
.895	5	2 2 6	118.74
.894	10	4 1 2	118.96
.877	5	4 0 5	122.88
.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
.814	1	3 1 7	142.36
.811	5	3 0 8	143.62
.809	5	3 3 0	144.28
.802	5	5 0 3	147.82
.795	1	4 2 0+	151.50
.793	5	3 3 2	152.48
.791	5	4 2 1	153.82

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.205	20	1 0 0	21.11
3.976	10	0 0 2	22.34
3.718	15	1 0 1	23.92
2.889	15	1 0 2	30.93
2.428	70	1 1 0	36.99
2.242	100	1 0 3	40.18
2.103	15	2 0 0	42.98
2.072	90	1 1 2	43.65
2.033	45	2 0 1	44.53
1.988	5	0 0 4	45.59
1.797	5	1 0 4	50.76
1.647	10	2 0 3	55.76
1.589	5	2 1 0	57.97
1.559	5	2 1 1	59.23
1.488	15	1 0 5	62.37
1.476	5	2 1 2	62.92
1.402	10	3 0 0	66.67
1.363	35	2 1 3	68.81
1.325	5	0 0 6	71.07
1.322	20	3 0 2	71.28
1.268	20	2 0 5	74.79
1.264	5	1 0 6	75.09
1.241	1	2 1 4	76.70
1.214	15	2 2 0	78.77
1.166	1	3 1 0	82.66
1.163	1	1 1 6	82.93
1.161	1	2 2 2	83.12
1.154	1	3 1 1	83.75
1.124	10	2 1 5	86.50
1.121	5	2 0 6	86.79
1.119	1	3 1 2	86.98
1.097	1	1 0 7	89.24
1.068	15	3 1 3	92.36
1.051	1	4 0 0	94.22
1.042	5	4 0 1	95.30
1.036	1	2 2 4	96.06
1.018	5	2 1 6	98.36
.977	1	4 0 3	104.04
.967	5	1 0 8	105.56
.965	1	3 2 0	105.96
.963	1	3 0 6	106.23
.958	1	3 2 1	107.08
.941	10	3 1 5	109.97
.938	1	3 2 2	110.49
.924	5	2 1 7	112.91
.920	10	1 1 8	113.73
.918	10	4 1 0	114.15
.907	15	3 2 3	116.35
.899	1	2 0 8	118.00
.895	5	2 2 6	118.74
.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	3 2 5	138.08
.824	5	4 0 6	138.52
.823	1	5 0 2	138.82
.814	5	3 1 7	142.36
.811	10	3 0 8	143.61
.809	5	3 3 0	144.27
.802	10	5 0 3	147.83
.795	1	0 0 10	151.25
.795	5	4 2 0	151.50
.793	10	3 3 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 $MgZn_2$, from powder data [Teslyuk et al., 1964].

Atom positions
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 for $Ge_{0.5}Ni_{1.5}Ta$ [ibid.]

Lattice constants
a = 4.870 Å
c = 7.893 [ibid., table II]

c/a = 1.6207

Volume
162.1 $Å^3$

Density
(calculated) 8.857 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ga^0, Nb^0 [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. A24, 321.
Teslyuk, M. Yu., Markiv, V. Ya., and Gladyshevs'kii, E. I. (1964). J. Struct. Chem. USSR 5, 364.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.881	5	1 0 2	31.02
2.435	45	1 1 0	36.88
2.232	80	1 0 3	40.38
2.108	15	2 0 0	42.86
2.072	100	1 1 2	43.64
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 1 4	76.80
1.217	15	2 2 0	78.50
1.122	5	2 1 5	86.74
1.116	5	2 0 6	87.28
1.089	1	1 0 7	90.00
1.069	10	3 1 3	92.22
1.054	1	4 0 0	93.86
1.045	5	4 0 1	94.96
1.036	5	2 2 4	96.04
1.015	1	2 1 6	98.78
1.006	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 3	116.04
.896	10	4 1 2	118.50
.894	5	2 2 6	119.08
.877	5	4 0 5	122.94
.875	5	3 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	1	3 2 5	138.06
.823	5	4 0 6	138.86
.812	5	3 1 7+	143.22
.808	1	3 0 8	145.04
.803	5	5 0 3	147.08

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

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

Cobalt Gallium Tantalum, $Co_{1.5}Ga_{0.5}Ta$

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 4, a ternary Laves phase, isostructural with $MgZn_2$, from powder data [Teslyuk et al., 1964].

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 $Ge_{0.5}Ni_{1.5}Ta$ [ibid.]

Lattice constants
a = 4.860 Å
c = 7.861 [ibid., table II]

c/a = 1.6175

Volume
160.8 $Å^3$

Density
(calculated) 12.57 g/cm^3

Thermal parameters
Isotropic: cobalt B = 1.0; gallium B = 1.0; tantalum B = 0.75

Scattering factors
Co^0, Ga^0 [Cromer and Mann, 1968]
Ta^0 [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 0.632 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
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 (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.207	15	1 0 0	21.10
3.928	10	0 0 2	22.62
3.708	15	1 0 1	23.98
2.872	15	1 0 2	31.12
2.430	70	1 1 0	36.96
2.224	100	1 0 3	40.52
2.105	15	2 0 0	42.94
2.067	95	1 1 2	43.76
2.033	50	2 0 1	44.54
1.965	5	0 0 4	46.16
1.781	5	1 0 4	51.26
1.641	5	2 0 3	56.00
1.591	1	2 1 0	57.92
1.559	1	2 1 1	59.22
1.473	15	1 0 5+	63.06
1.403	10	3 0 0	66.60
1.360	30	2 1 3	69.00
1.321	15	3 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	3 1 3	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 3	104.16
.957	5	1 0 8+	107.22
.937	5	3 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	3 2 3	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	3 1 6	124.20
.855	1	1 0 9	128.50
.836	5	2 1 8	134.26
.823	5	3 2 5	138.84
.821	5	4 0 6	139.64
.810	5	3 3 0	143.98
.809	1	3 1 7	144.28
.805	5	3 0 8	146.30
.801	5	5 0 3	147.96
.795	1	4 2 0	151.14
.793	5	3 3 2	152.32
.791	5	4 2 1	153.50
.786	1	0 0 10	156.98

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.209	15	1 0 0	21.09
3.931	10	0 0 2	22.60
3.711	15	1 0 1	23.96
2.873	15	1 0 2	31.11
2.430	70	1 1 0	36.96
2.224	100	1 0 3	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 3	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 3	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	3 1 0	82.58
1.161	1	2 2 2	83.15
1.155	1	3 1 1	83.69
1.153	1	1 1 6	83.82
1.119	1	3 1 2	87.00
1.118	10	2 1 5	87.08
1.112	5	2 0 6	87.67
1.085	1	1 0 7	90.46
1.066	15	3 1 3	92.51
1.052	1	4 0 0	94.12
1.043	5	4 0 1	95.22
1.033	5	2 2 4	96.38
1.011	5	2 1 6	99.22
1.004	1	3 1 4	100.26
.976	1	4 0 3	104.16
.958	1	3 0 6	107.11
.957	5	1 0 8	107.22
.938	1	3 2 2	110.47
.937	5	3 1 5	110.55
.918	10	4 1 0	114.00
.917	5	2 1 7	114.20
.911	10	1 1 8	115.47
.906	15	3 2 3	116.47
.894	15	4 1 2	118.92
.891	5	2 2 6	119.69
.890	1	2 0 8	119.80

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.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	3 2 5	138.84
.820	5	4 0 6	139.75
.810	5	3 3 0	143.97
.809	5	3 1 7	144.28
.805	10	3 0 8	146.30
.801	10	5 0 3	147.95
.795	5	4 2 0	151.13
.793	15	3 3 2	152.32
.791	15	4 2 1	153.50
.786	5	0 0 10	156.99

Cobalt Germanium, Co_5Ge_7

Structure
Tetragonal, I4mm (107), Z = 2, from powder data [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.]

Lattice constants
a = 7.641 Å
c = 5.814 [ibid.]

c/a = 0.7609

Volume
339.45 $Å^3$

Density
(calculated) 7.854 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ge^0 [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. A24, 321.
Stolz, E. and Schubert, K. (1962). Chem. Erde 22, 709.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.624	35	1 0 1	19.18
3.818	1	2 0 0	23.28
2.946	35	2 1 1	30.32
2.906	10	0 0 2	30.74
2.701	10	2 2 0	33.14
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	25	3 2 1	45.52
1.979	100	2 2 2	45.82
1.910	40	4 0 0	47.56
1.878	10	1 0 3	48.42
1.765	5	4 1 1	51.74
1.708	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	3 0 3	59.92
1.478	5	4 3 1+	62.82
1.474	5	4 2 2	63.02
1.454	5	0 0 4	64.00
1.379	5	5 2 1	67.94
1.359	1	2 0 4	69.08
1.351	10	4 4 0	69.54
1.339	5	4 1 3	70.22
1.280	1	2 2 4	74.00
1.228	1	6 1 1	77.72
1.200	5	5 0 3+	79.88
1.195	1	5 3 2	80.30
1.169	1	5 4 1	82.44
1.166	1	6 0 2	82.66
1.157	10	4 0 4	83.50
1.145	1	5 2 3	84.58
1.116	15	6 2 2	87.34
1.107	1	4 2 4	88.18
1.101	1	2 1 5	88.82
1.073	1	7 0 1	91.78
1.033	5	7 2 1	96.46
1.019	5	3 2 5	98.16
1.016	5	5 4 3	98.58
.996	1	6 4 2	101.38
.990	5	4 4 4	102.24
.955	1	8 0 0	107.50
.939	1	2 0 6	110.20
.935	1	7 4 1+	110.88
.927	1	8 2 0	112.46
.912	5	2 2 6	115.24

Cobalt Germanium, Co_5Ge_7 - (continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
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	45.52
1.979	100	2	2	2	45.82
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	3	0	3	59.93
1.478	1	5	0	1	62.82
1.478	5	4	3	1	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	0	3	79.87
1.200	1	4	3	3	79.87
1.195	1	5	3	2	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	3	1	87.12
1.116	15	6	2	2	87.33
1.107	1	4	2	4	88.18
1.101	1	2	1	5	88.81
1.073	1	7	0	1	91.78
1.060	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	6	4	2	101.38
.989	5	4	4	4	102.25
.955	1	8	0	0	107.51
.939	1	2	0	6	110.19
.935	1	7	4	1	110.87
.927	1	8	2	0	112.47
.912	5	2	2	6	115.24

Cobalt Germanium Niobium, $Co_{1.5}Ge_{0.5}Nb$

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 4, a ternary Laves phase, isostructural with $MgZn_2$, 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(f) 4 niobium
The positions assigned were those given for $Ge_{0.5}Ni_{1.5}Ta$ [ibid.]

Lattice constants
a = 4.860 Å
c = 7.832 [ibid.]

c/a = 1.6115

Volume
160.2 $Å^3$

Density
(calculated) 9.022 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ge^0, Nb^0 [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. A24, 321.
Teslyuk, M. Yu., Markiv, V. Ya., and Gladyshevs'kii, E. I. (1964). J. Struct. Chem. USSR 5, 364.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.866	5	1 0 2	31.18
2.430	45	1 1 0	36.96
2.218	80	1 0 3	40.64
2.105	15	2 0 0	42.94
2.064	100	1 1 2	43.82
2.033	75	2 0 1	44.54
1.958	15	0 0 4	46.34
1.854	10	2 0 2	49.10
1.775	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	0 0 6	72.34
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	15	2 2 0	78.70
1.116	5	2 1 5	87.28
1.109	5	2 0 6	87.96
1.081	1	1 0 7	90.86
1.066	10	3 1 3	92.58
1.052	1	4 0 0	94.12
1.043	5	4 0 1	95.24
1.032	5	2 2 4	96.52
1.009	1	2 1 6	99.52
1.003	1	3 1 4	100.40
.988	1	2 0 7	102.48
.954	5	1 0 8	107.76
.936	1	3 1 5	110.76
.918	5	4 1 0	114.00
.915	1	2 1 7	114.64
.908	5	1 1 8	116.06
.906	5	3 2 3	116.54
.894	10	4 1 2	118.96
.889	5	2 2 6	120.02
.873	5	4 0 5	123.74
.870	1	3 1 6	124.56
.866	1	3 2 4	125.62
.852	1	1 0 9	129.36
.834	5	2 1 8	135.00
.822	1	3 2 5	139.16
.819	5	4 0 6	140.20
.810	1	3 3 0	143.98
.808	1	3 1 7	144.96
.803	1	3 0 8	147.26
.801	5	5 0 3	148.10

Cobalt Germanium Niobium, $Co_{1.5}Ge_{0.5}Nb$ - (continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.867	5	1	0	2	31.17
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
1.775	10	1	0	4	51.43
1.474	1	2	1	2	63.02
1.468	5	1	0	5	63.30
1.403	5	3	0	0	66.60
1.358	25	2	1	3	69.09
1.321	20	3	0	2	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
1.109	5	2	0	6	87.96
1.081	1	1	0	7	90.86
1.066	10	3	1	3	92.58
1.052	1	4	0	0	94.12
1.043	5	4	0	1	95.23
1.032	5	2	2	4	96.51
1.016	1	4	0	2	98.58
1.009	1	2	1	6	99.52
1.003	1	3	1	4	100.39
.988	1	2	0	7	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	1	1	8	116.05
.906	10	3	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
.870	1	3	1	6	124.57
.866	1	3	2	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
.808	5	3	1	7	144.97
.804	1	2	0	9	146.62
.803	5	3	0	8	147.26
.801	5	5	0	3	148.09

Cobalt Germanium Tantalum, $Co_{1.5}Ge_{0.5}Ta$

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 4, a ternary Laves phase, isostructural with $MgZn_2$, 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(f) 4 tantalum
The positions assigned were those given for $Ge_{0.5}Ni_{1.5}Ta$ [ibid.]

Lattice constants
a = 4.875 Å
c = 7.817 [ibid., table II]

c/a = 1.6035

Volume
160.9 $Å^3$

Density
(calculated) 12.62 g/cm^3

Thermal parameters
Isotropic: cobalt B = 1.0; germanium B = 1.0; tantalum B = 0.75

Scattering factors
Co^0, Ge^0 [Cromer and Mann, 1968]
Ta^0 [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 (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.219	15	1 0 0	21.04
3.907	10	0 0 2	22.74
3.714	15	1 0 1	23.94
2.868	15	1 0 2	31.16
2.438	75	1 1 0	36.84
2.217	100	1 0 3	40.66
2.111	15	2 0 0	42.80
2.068	100	1 1 2	43.74
2.038	50	2 0 1	44.42
1.954	5	0 0 4	46.44
1.774	5	1 0 4	51.48
1.640	5	2 0 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 0	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	2 0 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	2 2 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 6	88.02
1.080	1	1 0 7	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	2 2 4	96.30
1.009	1	2 1 6	99.50
1.004	1	3 1 4	100.16
.978	1	4 0 3	103.90
.956	1	3 0 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 0	113.46
.915	1	2 1 7	114.68
.908	10	3 2 3	116.10
.907	5	1 1 8	116.26
.897	10	4 1 2	118.42
.890	5	2 2 6	119.88
.887	1	2 0 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	3 3 0	142.90
.808	1	3 1 7	144.80
.803	5	5 0 3	147.08
.803	5	3 0 8	147.36
.798	1	4 2 0	149.80
.795	5	3 3 2	151.08
.794	5	4 2 1	152.10

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.222	15	1	0	0	21.03
3.908	10	0	0	2	22.73
3.715	15	1	0	1	23.94
2.868	15	1	0	2	31.16
2.438	75	1	1	0	36.84
2.217	100	1	0	3	40.66
2.111	15	2	0	0	42.80
2.068	100	1	1	2	43.73
2.038	50	2	0	1	44.42
1.954	5	0	0	4	46.43
1.773	5	1	0	4	51.49
1.640	5	2	0	3	56.02
1.596	1	2	1	0	57.73
1.563	1	2	1	1	59.03
1.477	5	2	1	2	62.85
1.466	10	1	0	5	63.39
1.407	10	3	0	0	66.37
1.361	35	2	1	3	68.95
1.324	20	3	0	2	71.15
1.303	5	0	0	6	72.49
1.256	25	2	0	5	75.63
1.245	5	1	0	6	76.45
1.236	1	2	1	4	77.10
1.219	20	2	2	0	78.40
1.171	1	3	1	0	82.27
1.163	1	2	2	2	82.91
1.158	1	3	1	1	83.39
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	6	88.02
1.080	1	1	0	7	91.04
1.068	15	3	1	3	92.31
1.055	1	4	0	0	93.74
1.046	5	4	0	1	94.86
1.034	5	2	2	4	96.30
1.009	5	2	1	6	99.51
1.004	1	3	1	4	100.15
.978	1	4	0	3	103.89
.956	1	3	0	6	107.36
.952	5	1	0	8	108.03
.940	1	3	2	2	110.04
.937	5	3	1	5	110.55
.921	10	4	1	0	113.46
.915	5	2	1	7	114.69
.908	15	3	2	3	116.09
.907	10	1	1	8	116.27
.897	15	4	1	2	118.41
.890	10	2	2	6	119.87
.887	1	2	0	8	120.61
.875	10	4	0	5	123.42
.871	5	3	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	3	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	3	0	8	147.37
.798	5	4	2	0	149.79
.795	15	3	3	2	151.08
.794	15	4	2	1	152.08

Cobalt Holmium, $Co_{9.2}Ho_{12}$

Structure
Hexagonal, $P6_3/m$ (176), Z = 1. The structure was determined by Lemaire et al. [1969]. One of the 3 cobalt sites is only partially filled at random.

Atom positions

6(h)	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 constants
a = 11.411 Å
c = 3.984
(published values: a = 11.410 Å, c = 3.984 [ibid., table 4])

c/a = 0.3491

Volume
449.3 $Å^3$

Density
(calculated) 9.319 g/cm^3

Thermal parameters
Isotropic [Lemaire et al., 1969]

Scattering factors
Co^0, Ho^0 [Cromer and Mann, 1968]

Scale factors (integrated intensities)
$\gamma = 0.948 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 9.96

References
Cromer, D. T. and Mann, J. B. (1969). Acta Crystallogr. A24, 321.
Lemaire, P. R., Schweizer, J., and Yakinthos, J. (1969). Acta Crystallogr. B25, 710.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.940	1	2 0 0	17.94
3.733	7	2 1 0	23.82
3.693	6	1 0 1	24.08
3.293	1	3 0 0	27.06
3.266	2	1 1 1	27.28
2.852	6	2 2 0	31.34
2.740	42	3 1 0	32.66
2.725	100	2 1 1+	32.84
2.538	23	3 0 1	35.34
2.470	5	4 0 0	36.34
2.319	9	2 2 1	38.80
2.266	3	2 3 0+	39.74
2.258	5	1 3 1+	39.90
2.156	19	1 4 0+	41.86
2.100	4	4 0 1	43.04
1.992	13	0 0 2	45.50
1.971	5	2 3 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 3 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	3 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 3 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	3	2 4 2	68.86
1.331	1	5 3 1+	70.74
1.325	3	1 5 2	71.08
1.296	2	6 2 1+	72.94
1.265	3	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	3 0 3	77.40
1.204	1	2 2 3	79.58
1.202	2	1 6 2+	79.72
1.188	2	3 6 1	80.82
1.157	1	8 1 0+	83.52
1.152	1	5 3 2+	83.94
1.111	3	1 8 1+	87.82
1.090	2	4 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 3	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

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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
3.266	3	1 1 1	27.28
2.853	8	2 2 0	31.33
2.741	42	3 1 0	32.65
2.725	100	2 1 1	32.84
2.725	23	1 2 1	32.84
2.539	31	3 0 1	35.33
2.471	6	4 0 0	36.33
2.319	12	2 2 1	38.79
2.267	2	2 3 0	39.73
2.258	1	3 1 1	39.89
2.258	5	1 3 1	39.89
2.156	5	4 1 0	41.86
2.156	21	1 4 0	41.86
2.100	5	4 0 1	43.05
1.992	18	0 0 2	45.50
1.976	1	5 0 0	45.88
1.970	6	2 3 1	46.02
1.896	1	1 4 1	47.93
1.868	6	2 4 0	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 3 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
1.621	7	1 5 1	56.73
1.611	12	3 1 2	57.11
1.582	3	5 2 0	58.26
1.582	3	2 5 0	58.26
1.551	1	4 0 2	59.57
1.522	1	6 0 1	60.81
1.507	1	6 1 0	61.48
1.507	2	1 6 0	61.48
1.496	1	3 2 2	61.96
1.496	2	2 3 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	71.08

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.296	2	6 2 1	72.94
1.296	1	2 6 1	72.94
1.265	4	4 5 0	75.00
1.251	7	2 1 3	75.99
1.251	1	1 2 3	75.99
1.244	3	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 3	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 3 3	84.48
1.112	1	7 3 0	87.71
1.111	4	1 8 1	87.81
1.090	1	6 4 1	89.90
1.090	3	4 6 1	89.90
1.082	2	2 4 3	90.75
1.078	1	8 2 0	91.19
1.071	2	7 3 1	91.99
1.071	1	3 7 1	91.99
1.068	4	4 5 2	92.31
1.063	2	1 5 3	92.84
1.059	1	9 0 1	93.39
1.050	3	8 0 2	94.40
1.0172	6	5 2 3	98.44

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 4, a Laves phase, isostructural with $MgZn_2$, 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 C14 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 $Å^3$

Density
(calculated) 5.811 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Mg^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.187 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Friauf, J. B. (1927). Phys. Rev. 29, 34.
Smith, J. F. and Smith, M. J. (1964). ASM (Amer. Soc. Metals) Trans. Quart. 57, 337.
Stadelmaier, H. H. and Yun, T. S. (1961). Z. Metallk. 52, 477.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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	15	1 0 4	50.88
1.647	20	2 0 3	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 3	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	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	1	3 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 3	92.22
1.044	5	4 0 1	95.06
1.037	10	2 2 4	95.98
1.018	5	4 0 2	98.32
1.017	1	2 1 6	98.50
1.007	5	3 1 4	99.84
.9974	5	2 0 7	101.12
.9908	1	0 0 8	102.06
.9786	1	4 0 3	103.84
.9668	1	3 2 0	105.64
.9644	1	1 0 8	106.02
.9622	1	3 0 6	106.36
.9229	1	2 1 7	113.16
.9079	1	3 2 3	116.08
.8958	5	4 1 2	118.62
.8949	5	2 2 6	118.80
.8774	5	4 0 5	122.78
.8689	1	3 2 4	124.88

Cobalt Magnesium, Co_2Mg - (continued)

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

Cobalt Molybdenum, Co_2Mo_3

Structure
Tetragonal, $P4_2/mnm$ (136), Z = 6, σ-phase, isostructural with σ-CrFe. The structure was determined by Forsyth and d'Alte da Veiga [1963].

Atom positions
2(a) 2 cobalt(1)
8(i) 8 cobalt(2)
8(i) 1 cobalt(3) and 7 molybdenum(2)
8(i) 1 cobalt(4) and 7 molybdenum(4)
4(g) 4 molybdenum(1)

Lattice constants
a = 9.2292(4)Å
c = 4.8271(6)
(published values: a = 9.2287(4), c = 4.8269(6) [ibid.])

c/a = 0.5230

Volume
411.16 $Å^3$

Density
(calculated) 9.831 g/cm^3

Thermal parameters
Isotropic: overall B = 2.0

Scattering factors
Co^{2+}, Mo^{+} [Forsyth and Wells, 1959], corrected for the real part of the anomalous dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.231 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 2.97

References
Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
Forsyth, J. B. and d'Alte da Veiga, L. M. (1962). Acta Crystallogr. 15, 543.
Forsyth, J. B. and Wells, M. (1959). Acta Crystallogr. 12, 412.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.275	5	1 0 1	20.76
4.126	3	2 1 0	21.52
3.880	2	1 1 1	22.90
3.262	2	2 2 0	27.32
3.136	1	2 1 1	28.44
2.917	6	3 1 0	30.62
2.593	5	3 0 1	34.56
2.559	4	3 2 0	35.04
2.497	18	3 1 1	35.94
2.414	18	0 0 2	37.22
2.306	3	4 0 0	39.02
2.262	9	1 1 2+	39.82
2.238	95	4 1 0	40.26
2.175	46	3 3 0	41.48
2.139	47	2 0 2	42.22
2.083	81	2 1 2	43.40
2.031	100	4 1 1	44.58
1.983	44	3 3 1	45.72
1.940	9	2 2 2	46.78
1.860	9	3 1 2	48.94
1.724	1	4 3 1	53.08
1.569	1	4 2 2	58.82
1.466	4	4 3 2	63.38
1.459	1	6 2 0	63.72
1.448	3	5 1 2+	64.28
1.442	2	5 4 0	64.60
1.409	2	3 1 3	66.28
1.3971	9	5 2 2+	66.92
1.3811	2	5 4 1	67.80
1.3236	16	5 3 2	71.18
1.3064	16	4 1 3+	72.26
1.2971	8	6 0 2	72.86
1.2938	10	3 3 3	73.08
1.2844	5	6 1 2	73.70
1.2677	12	7 2 0	74.84
1.2599	4	5 5 1	75.38
1.2487	2	6 2 2	76.18
1.2374	2	5 4 2+	77.00
1.2261	3	7 2 1	77.84
1.2067	6	0 0 4	79.34
1.1224	1	7 2 2	86.68
1.1193	5	8 2 0	86.98
1.0903	3	8 2 1	89.90
1.0877	3	6 6 0	90.18
1.0809	1	6 2 3	90.90
1.0623	7	4 1 4	92.96
1.0553	4	3 3 4	93.76
1.0408	4	8 0 2	95.48
1.0343	7	7 4 2	96.28
1.0136	1	5 5 3	98.92
.9959	1	7 2 3	101.34
.9247	3	7 6 2+	112.82
.9188	2	8 2 3+	113.94
.9065	1	8 6 1+	116.36
.9023	3	9 3 2+	117.24
.9011	2	6 6 3	117.48
.8964	1	9 5 0	118.48
.8864	4	4 1 5+	120.68
.8824	1	3 3 5	121.60
.8740	6	7 2 4+	123.60
.8620	1	8 6 2+	126.66
.8583	1	10 1 2	127.66
.8532	2	9 6 0	129.06
.8402	1	9 6 1	132.92
.8356	2	11 1 0	134.40
.8255	1	10 5 0	137.86
.8233	1	11 1 1	138.64
.8206	3	8 2 4	139.66
.8137	1	10 5 1	142.42
.8079	1	6 6 4	144.90

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.277	4	1 0 1	20.75
4.127	3	2 1 0	21.51
3.881	2	1 1 1	22.90
3.263	2	2 2 0	27.31
3.137	1	2 1 1	28.43
2.919	6	3 1 0	30.61
2.594	5	3 0 1	34.55
2.560	4	3 2 0	35.03
2.498	18	3 1 1	35.93
2.414	18	0 0 2	37.22
2.307	2	4 0 0	39.01
2.264	5	1 1 2	39.79
2.261	2	3 2 1	39.83
2.238	92	4 1 0	40.26
2.175	44	3 3 0	41.48
2.139	45	2 0 2	42.22
2.083	79	2 1 2	43.40
2.031	100	4 1 1	44.58
1.983	44	3 3 1	45.71
1.940	9	2 2 2	46.78
1.860	9	3 1 2	48.93
1.724	1	4 3 1	53.08
1.569	1	4 2 2	58.83
1.466	4	4 3 2	63.39
1.459	1	6 2 0	63.72
1.448	3	5 1 2	64.28
1.441	1	5 4 0	64.61
1.409	2	3 1 3	66.28
1.3974	8	5 2 2	66.91
1.3968	3	6 2 1	66.93
1.3811	2	5 4 1	67.80
1.3236	17	5 3 2	71.18
1.3065	15	4 1 3	72.26
1.3052	5	5 5 0	72.34
1.2972	7	6 0 2	72.86
1.2936	7	3 3 3	73.09
1.2845	5	6 1 2	73.69
1.2677	14	7 2 0	74.84
1.2600	4	5 5 1	75.38
1.2488	3	6 2 2	76.17
1.2375	2	5 4 2	76.99
1.2261	4	7 2 1	77.84
1.2068	7	0 0 4	79.33
1.1223	1	7 2 2	86.68
1.1192	5	8 2 0	86.98
1.0903	4	8 2 1	89.90
1.0877	2	6 6 0	90.18
1.0809	1	6 2 3	90.90
1.0622	8	4 1 4	92.97
1.0611	2	6 6 1	93.10
1.0553	4	3 3 4	93.77
1.0409	4	8 0 2	95.47
1.0343	8	7 4 2	96.28
1.0136	2	5 5 3	98.92
.9958	2	7 2 3	101.35
.9389	1	9 1 2	110.25
.9247	2	9 2 2	112.83
.9247	2	7 6 2	112.83
.9188	2	8 2 3	113.94
.9065	1	8 6 1	116.37
.9023	3	9 3 2	117.23
.9022	1	10 1 1	117.26
.9011	2	6 6 3	117.48
.8964	1	9 5 0	118.48
.8865	4	4 1 5	120.67
.8861	3	5 5 4	120.76
.8824	2	3 3 5	121.60
.8741	9	7 2 4	123.59
.8736	3	9 4 2	123.72
.8620	2	8 6 2	126.65
.8583	1	10 1 2	127.65
.8532	3	9 6 0	129.06
.8402	1	9 6 1	132.92
.8356	3	11 1 0	134.41
.8255	3	10 5 0	137.86
.8233	2	11 1 1	138.65
.8206	6	8 2 4	139.67
.8137	3	10 5 1	142.42
.8095	1	11 3 0	144.21
.8079	3	6 6 4	144.89
.8052	1	6 2 5	146.15
.8045	1	9 6 2	146.49
.8006	1	8 6 3	148.39
.7983	1	11 3 1	149.56
.7976	1	10 1 3	149.94
.7926	2	2 0 6	152.78
.7897	5	2 1 6	154.58
.7896	2	11 1 2	154.62
.7888	1	10 2 3	155.14

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, μ-phase, isostructural with Fe_7W_6. The structure was determined by Forsyth and d'Alte da Veiga [1962].

Atom positions
3(a) 3 cobalt(1)
18(h) 18 cobalt(2)
6(c) 6 molybdenum(1)
6(c) 6 molybdenum(2)
6(c) 6 molybdenum(3)

Lattice constants
a = 4.762(1) Å
c = 25.617(5)
(published values: a = 4.762(1)Å, c = 25.615(5) [ibid.])

c/a = 5.3795

Volume
503.1 $Å^3$

Density
(calculated) 9.785 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^{2+}, Mo^{+} [Forsyth and Wells, 1959], corrected for the real part of the dispersion effects [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.223 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 3.15

References
Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
Forsyth, J. B. and d'Alte da Veiga, L. M. (1962). Acta Crystallogr. 15, 543.
Forsyth, J. B. and Wells, M. (1959). Acta Crystallogr. 12, 412.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.532	4	0 0 3	10.36
4.267	1	0 0 6	20.80
4.070	4	1 0 1	21.82
3.466	4	1 0 4	25.68
2.529	5	0 1 8	35.46
2.381	98	1 1 0	37.76
2.293	5	1 1 3	39.26
2.176	72	1 0 10	41.46
2.135	18	0 0 12	42.30
2.080	100	1 1 6	43.48
2.055	42	0 2 1	44.02
2.027	60	0 1 11	44.66
1.9626	21	0 2 4	46.22
1.9126	32	2 0 5	47.50
1.8261	12	1 1 9	49.90
1.7965	13	0 2 7	50.78
1.7782	4	1 0 13	51.34
1.7336	5	2 0 8	52.76
1.6061	3	0 2 10	57.32
1.5439	1	2 0 11	59.86
1.4926	1	1 0 16	62.14
1.4015	1	1 2 8	66.68
1.3876	2	1 1 15	67.44
1.3747	12	3 0 0	68.16
1.3317	20	2 1 10	70.68
1.3086	15	0 3 6+	72.12
1.2953	18	1 2 11	72.98
1.2814	1	1 0 19	73.90
1.2645	7	0 2 16	75.06
1.2379	2	3 0 9+	76.96
1.2216	12	1 1 18+	78.18
1.2198	9	0 0 21	78.32
1.2167	10	2 0 17	78.56
1.1905	20	2 2 0	80.64
1.1168	1	2 1 16	87.22
1.0880	3	2 0 20	90.14
1.0856	6	1 1 21	90.40
1.0752	1	0 1 23	91.52
1.0708	1	3 0 15+	92.00
1.0674	1	0 0 24	92.38
1.0445	9	1 3 10	95.04
1.0398	5	2 2 12	95.60
1.0301	2	4 0 1	96.80
1.0266	8	3 1 11	97.24
1.0197	1	2 1 19	98.12
1.0179	2	4 0 4	98.36
1.0139	1	0 2 22	98.88
1.0108	2	0 4 5	99.30
.9923	1	4 0 7	101.84
.9895	5	1 2 20	102.24
.9888	6	0 3 18+	102.34
.9739	1	1 1 24	104.54
.9564	1	4 0 10	107.30
.9124	3	0 3 21+	115.18
.9063	1	1 2 23	116.42
.8999	7	4 1 0	117.74
.8875	6	3 2 10	120.44
.8806	9	4 1 6+	122.04
.8765	6	2 3 11	123.00
.8723	1	1 3 19	124.04
.8669	2	4 0 16	125.40
.8638	1	0 1 29	126.20
.8581	1	1 4 9+	127.72
.8531	3	3 1 20	129.10
.8520	8	2 2 21	129.40
.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

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.8031	2	0 4 20	147.12
.8012	1	2 3 17	148.08
.7980	1	3 1 23	149.74
.7961	1	1 4 15+	150.76
.7947	3	2 2 24	151.52
.7937	3	3 3 0	152.12
.7851	3	0 5 10	157.70

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.539	3	0 0 3	10.35
4.270	1	0 0 6	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 1 6	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 1 9	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 2 8	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 0 6	72.13
1.3085	8	0 3 6	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 3 9	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
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
1.0397	6	2 2 12	95.61
1.0302	3	4 0 1	96.79
1.0267	9	3 1 11	97.23
1.0197	1	2 1 19	98.12
1.0179	2	4 0 4	98.36
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 20	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	115.18
.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 21	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
.8031	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	157.71

Cobalt Molybdenum Silicide, Co_3Mo_2Si

Structure
Hexagonal, $P6_3/mmc(194)$, Z = 2, a ternary Laves phase, isostructural with $MgZn_2$, 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_3Nb_2Si [Kuz'ma et al., 1964]

Lattice constants
a = 4.70 Å
c = 7.67 [Bardos et al., (1961), table III]

c/a = 1.6319

Volume
146.7 $Å^3$

Density
(calculated) 8.98 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Mo^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 (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.07	10	1 0 0	21.82
3.83	1	0 0 2	23.18
3.59	1	1 0 1	24.76
2.79	25	1 0 2	32.04
2.35	40	1 1 0	38.28
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	80	2 0 1	46.12
1.92	10	0 0 4	47.38
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 3	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	3 1 3	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	1	2 1 6	103.16
.933	1	1 0 8	111.26
.909	5	3 1 5	115.82
.907	1	3 2 2	116.24
.892	1	2 1 7	119.34
.888	5	1 1 8+	120.38
.877	10	3 2 3	122.86
.865	15	4 1 2+	125.82
.848	10	4 0 5	130.58
.834	1	1 0 9	134.88
.814	5	2 1 8	142.42
.798	1	3 2 5	149.92

Cobalt Molybdenum Silicide, Co_3Mo_2Si - (continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.07	10	1	0	0	21.82
3.84	1	0	0	2	23.17
3.60	1	1	0	1	24.74
2.79	25	1	0	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	1	4	0	0	98.40
1.01	5	4	0	1	99.57
1.00	5	2	2	4	100.50
.983	1	2	1	6	103.16
.973	1	3	1	4	104.71
.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	0	120.28
.888	5	1	1	8	120.39
.877	10	3	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
.814	10	2	1	8	142.41
.798	5	3	2	5	149.91

Cobalt Niobium Silicide, $Co_3Nb_4Si_7$

Structure
Tetragonal, I4/mmm (139), Z = 4, isostructural with $NiTiSi_2$. The structure was determined by Yarmolyuk and Kripyakevich [1969].

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 $Å^3$

Density
(calculated) 6.294 g/cm^3

Thermal parameters
Isotropic: overall B = 3.4

Scattering factors
Co^0, Nb^0, Si^0 [Cromer and Mann, 1968]

Scale factors (integrated intensities)
$\gamma = 0.191 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.99

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Yarmolyuk, Ya. P. and Kripyakevich, P.I. (1969). Sov. Phys. Crystallogr. 13, 862.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.874	45	1 1 0	9.96
6.276	10	2 0 0	14.10
4.440	10	2 2 0	19.98
3.969	5	3 1 0	22.38
3.204	5	3 0 1	27.82
3.140	10	4 0 0	28.40
2.959	15	3 3 0	30.18
2.855	30	3 2 1	31.30
2.808	5	4 2 0	31.84
2.599	35	4 1 1	34.48
2.491	10	0 0 2	36.02
2.464	1	5 1 0	36.44
2.399	15	1 1 2	37.46
2.243	100	4 3 1+	40.18
2.220	40	4 4 0	40.60
2.173	10	2 2 2	41.52
2.111	65	3 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	5	3 3 2+	47.66
1.864	5	4 2 2	48.82
1.776	5	5 5 0	51.40
1.688	5	7 0 1	54.30
1.658	1	4 4 2	55.38
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 3 3+	67.54
1.375	15	7 3 2	68.12
1.324	5	9 3 0	71.16
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 3 1+	82.40
1.166	5	10 4 0	82.68
1.155	1	6 5 3	83.62
1.150	5	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

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
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	0	22.37
3.206	10	3	0	1	27.81
3.140	15	4	0	0	28.40
2.960	20	3	3	0	30.16
2.855	45	3	2	1	31.30
2.809	5	4	2	0	31.84
2.599	45	4	1	1	34.48
2.492	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	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	10	4	0	2	46.49
1.908	5	6	1	1	47.63
1.906	10	3	3	2	47.66
1.864	5	4	2	2	48.82
1.825	1	5	4	1	49.92
1.776	5	5	5	0	51.40
1.742	1	6	4	0	52.50
1.688	10	7	0	1	54.29
1.658	1	4	4	2	55.38
1.630	1	7	2	1	56.39
1.603	1	6	0	2	57.45
1.570	5	8	0	0	58.76
1.530	10	6	5	1	60.44
1.523	1	8	2	0	60.76
1.500	5	3	2	3	61.82
1.487	5	8	1	1	62.40
1.487	1	7	4	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
1.446	1	5	5	2	64.36
1.428	5	6	4	2	65.31
1.404	5	8	4	0	66.53
1.386	10	4	3	3	67.54
1.386	5	5	0	3	67.54
1.375	25	7	3	2	68.12
1.324	5	9	3	0	71.16
1.314	1	7	6	1	71.77
1.300	1	8	2	2	72.70
1.260	1	7	5	2	75.39
1.246	5	0	0	4	76.37
1.223	5	8	4	2	78.05
1.219	1	7	0	3	78.38
1.212	5	10	1	1	78.90
1.212	1	9	1	2	78.93
1.169	1	10	3	1	82.40
1.166	5	10	4	0	82.68
1.155	5	6	5	3	83.62
1.150	5	8	7	1	84.14
1.136	1	8	1	3	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_2NbSn

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy, isostructural with $AlCu_2Mn$, 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 $Å^3$

Density
(calculated) 9.394 g/cm^3
(measured) 9.80 [Ziebeck and Webster, 1974]

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Nb^0, 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. A24, 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 (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.551	1	1 1 1	25.06
3.077	15	2 0 0	29.00
2.175	100	2 2 0	41.48
1.855	1	3 1 1	49.06
1.776	5	2 2 2	51.40
1.538	15	4 0 0	60.10
1.3757	5	4 2 0	68.10
1.2559	20	4 2 2	75.66
1.0877	5	4 4 0	90.18
1.0255	1	4 4 2+	97.38
.9729	10	6 2 0	104.70
.9276	1	6 2 2	112.28
.8881	1	4 4 4	120.30
.8533	1	6 4 0	129.04
.8222	10	6 4 2	139.06

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.552	1	1 1 1	25.05
3.076	15	2 0 0	29.00
2.175	100	2 2 0	41.48
1.855	1	3 1 1	49.07
1.776	5	2 2 2	51.40
1.538	15	4 0 0	60.10
1.3759	5	4 2 0	68.09
1.2560	25	4 2 2	75.66
1.0877	5	4 4 0	90.18
1.0255	1	4 4 2	97.38
.9729	10	6 2 0	104.70
.9276	1	6 2 2	112.28
.8881	5	4 4 4	120.30
.8533	1	6 4 0	129.05
.8222	25	6 4 2	139.06

Cobalt Platinum, CoPt (disordered)

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 = 1.3765

Volume
26.41 $Å^3$

Density
(calculated) 15.97 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Pt^0 [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.
Newman, R. W. and Hren, J. J. (1967). Surface Sci. 8, 373.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.684	25	0 0 1	24.14
2.676	20	1 0 0	33.46
2.165	100	1 0 1	41.68
1.893	30	1 1 0	48.02
1.843	15	0 0 2	49.42
1.683	10	1 1 1	54.46
1.518	5	1 0 2	61.00
1.3386	10	2 0 0	70.26
1.3204	15	1 1 2	71.38
1.2579	5	2 0 1	75.52
1.1971	1	2 1 0	80.10
1.1387	15	2 1 1	85.14
1.1164	10	1 0 3	87.26
1.0830	5	2 0 2	90.68
1.0304	1	1 1 3	96.76
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 3	116.68
.8711	1	1 0 4	124.32
.8672	5	3 0 1	125.30
.8573	10	2 1 3	127.92
.8465	5	3 1 0	131.00
.8419	5	2 2 2	132.40
.8284	5	1 1 4	136.84
.8250	1	3 1 1	138.02
.8031	1	3 0 2	147.14

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.685	20	0 0 1	24.13
2.677	20	1 0 0	33.45
2.166	100	1 0 1	41.67
1.893	30	1 1 0	48.03
1.843	15	0 0 2	49.43
1.684	10	1 1 1	54.45
1.518	5	1 0 2	61.00
1.3385	10	2 0 0	70.27
1.3203	15	1 1 2	71.38
1.2581	5	2 0 1	75.51
1.2283	1	0 0 3	77.67
1.1972	5	2 1 0	80.09
1.1386	20	2 1 1	85.15
1.1164	10	1 0 3	87.26
1.0829	10	2 0 2	90.69
1.0304	1	1 1 3	96.76
1.0039	5	2 1 2	100.23
.9465	5	2 2 0	108.95
.9213	1	0 0 4	113.47
.9167	1	2 2 1	114.34
.9050	1	2 0 3	116.67
.8923	1	3 0 0	119.37
.8711	1	1 0 4	124.32
.8673	5	3 0 1	125.29
.8573	15	2 1 3	127.92
.8465	5	3 1 0	130.99
.8419	5	2 2 2	132.40
.8284	5	1 1 4	136.84
.8251	5	3 1 1	138.02
.8031	1	3 0 2	147.13

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
1(a) 1 cobalt
1(d) 1 platinum

Lattice constants
a = 2.682 Å
c = 3.675
[Newman and Hren, 1967]

c/a = 1.3702

Volume
26.44 $Å^3$

Density
(calculated) 15.96 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Pt^0 [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	2θ(°) λ = 1.540598Å
3.675	30	0 0 1	24.20
2.682	25	1 0 0	33.38
2.166	100	1 0 1	41.66
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 3	77.92
1.1994	5	2 1 0	79.92
1.1402	15	2 1 1	85.00
1.1143	10	1 0 3	87.46
1.0831	5	2 0 2	90.66
1.0290	1	1 1 3	96.94
1.0044	5	2 1 2	100.16
.9482	1	2 2 0	108.66
.9182	1	2 2 1+	114.06
.9044	1	2 0 3	116.80
.8940	1	3 0 0	119.00
.8687	5	3 0 1+	124.94
.8570	10	2 1 3	128.00
.8481	5	3 1 0	130.52
.8427	5	2 2 2	132.16
.8268	5	1 1 4+	137.40
.8039	1	3 0 2	146.76

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.675	30	0 0 1	24.20
2.682	25	1 0 0	33.38
2.166	100	1 0 1	41.66
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
1.3410	10	2 0 0	70.12
1.3197	15	1 1 2	71.42
1.2598	5	2 0 1	75.39
1.2250	1	0 0 3	77.93
1.1994	5	2 1 0	79.92
1.1402	20	2 1 1	85.00
1.1143	10	1 0 3	87.47
1.0832	10	2 0 2	90.65
1.0290	1	1 1 3	96.94
1.0044	5	2 1 2	100.16
.9482	5	2 2 0	108.65
.9188	1	0 0 4	113.95
.9182	1	2 2 1	114.06
.9044	1	2 0 3	116.79
.8940	1	3 0 0	119.00
.8692	1	1 0 4	124.81
.8687	5	3 0 1	124.94
.8570	15	2 1 3	128.00
.8481	5	3 1 0	130.53
.8426	5	2 2 2	132.17
.8268	10	1 1 4	137.38
.8264	5	3 1 1	137.53
.8039	5	3 0 2	146.75

Cobalt Platinum, $CoPt_3$ (disordered)

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) 1 cobalt
4(a) 3 platinum

Lattice constant
a = 3.8532(3) Å
(published value, 3.8530(3) [Berg and Cohen, 1972]).

Volume
57.209 $Å^3$

Density
(calculated) 18.694 g/cm^3

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

Scattering factors
Co^0, Pt^0 [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. 3, 1797.
Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Geisler, A. H. and Martin, D. L. (1952). J. Appl. Phys. 23, 375.

Calculated Pattern (Peak heights)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
2.224	100	1	1	1	40.52
1.926	45	2	0	0	47.14
1.3624	25	2	2	0	68.86
1.1618	30	3	1	1	83.06
1.1123	10	2	2	2	87.66
.9633	5	4	0	0	106.20
.8840	15	3	3	1	121.24
.8616	15	4	2	0	126.76
.7865	20	4	2	2	156.68

Calculated Pattern (Integrated)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
2.225	100	1	1	1	40.52
1.927	50	2	0	0	47.13
1.3623	30	2	2	0	68.87
1.1618	35	3	1	1	83.06
1.1123	10	2	2	2	87.66
.9633	5	4	0	0	106.19
.8840	25	3	3	1	121.24
.8616	25	4	2	0	126.77
.7865	55	4	2	2	156.68

Cobalt Platinum, $CoPt_3$ (ordered)

Structure
Cubic, Pm3m (221), Z = 1, isostructural with $AuCu_3$, from powder data. There is also a disordered phase with very similar size and structure, found when the sample is heated to 800 °C, then quenched [Geisler and Martin, 1952].

Atom positions
1(a) 1 cobalt
3(c) 3 platinum

Lattice constant
a = 3.8541(4) Å
(published value, a = 3.8539(4) [Berg and Cohen, 1972]).

Volume
57.249 $Å^3$

Density
(calculated) 18.686 g/cm^3

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

Scattering factors
Co^0, Pt^0 [Cromer and Mann, 1968], corrected for dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)
$\gamma = 1.633 \times 10^{-3}$

References

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

Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.

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

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
3.854	15	1	0	0	23.06
2.725	10	1	1	0	32.84
2.224	100	1	1	1	40.52
1.927	45	2	0	0	47.12
1.723	5	2	1	0	53.10
1.574	5	2	1	1	58.62
1.3627	25	2	2	0	68.84
1.2847	1	2	2	1+	73.68
1.2188	1	3	1	0	78.40
1.1620	30	3	1	1	83.04
1.1125	10	2	2	2	87.64
1.0689	1	3	2	0	92.22
1.0301	1	3	2	1	96.80
.9635	5	4	0	0	106.16
.9348	1	3	2	2+	110.98
.9084	1	4	1	1+	115.98
.8842	15	3	3	1	121.20
.8618	15	4	2	0	126.72
.8411	1	4	2	1	132.66
.8217	1	3	3	2	139.26
.7867	20	4	2	2	156.54

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
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	30	2	2	0	68.85
1.2847	1	2	2	1	73.68
1.2188	1	3	1	0	78.40
1.1621	35	3	1	1	83.04
1.1126	10	2	2	2	87.63
1.0689	1	3	2	0	92.21
1.0301	5	3	2	1	96.80
.9635	5	4	0	0	106.16
.9348	1	4	1	0	110.99
.9348	1	3	2	2	110.99
.9084	1	4	1	1	115.98
.8842	25	3	3	1	121.19
.8618	25	4	2	0	126.72
.8410	5	4	2	1	132.67
.8217	1	3	3	2	139.26
.7867	55	4	2	2	156.55

Cobalt Plutonium, $CoPu_3$

Structure
Orthorhombic, Cmcm (63), Z = 4, isostructural with BRe_3 and Al_2CuMg. The structure was refined by Larson, Cromer, and Roof [1963].

Atom positions
4(c) 4 cobalt
4(c) 4 plutonium(1)
8(f) 8 plutonium(2) [ibid.]

Lattice constants
a = 3.475(4) Å
b = 10.977(10)
c = 9.221(8)

(published values: a = 3.475(4)Å, b = 10.976(10), c = 9.220(8) [Larson et al., 1963]).

CD cell: a=9.221(8)Å, b=10.977(10), c=3.475(4); sp. gp. Amam; a/b = 0.8400; c/b = 0.3166

Volume
351.7 $Å^3$

Density
(calculated) 14.823 g/cm^3
(measured) 14.82 g/cm^3 [Larson et al., 1963]

Thermal parameters
Isotropic [Larson et al., 1963]

Scattering factors
Co^0 [Forsyth and Wells, 1959], corrected for dispersion by $\Delta f' = -2.2$
Pu^0 [Larson et al., 1963], modified for use with Cu λ.

Scale factors (integrated intensities)
$\gamma = 0.413 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 8.07

References
Forsyth, J.B. and Wells, M. (1959). Acta Crystallogr. 12, 412.
Larson, A. C., Cromer, D. T., and Roof, R. B., Jr. (1963). Acta Crystallogr. 16, 835.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.61	2	0 0 2	19.24
3.53	5	0 2 2	25.22
3.312	3	1 1 0	26.90
3.116	16	1 1 1	28.62
2.745	24	0 4 0	32.60
2.688	88	1 1 2	33.30
2.682	100	0 2 3	33.38
2.630	14	0 4 1	34.06
2.520	19	1 3 0	35.60
2.430	35	1 3 1	36.96
2.358	11	0 4 2	38.14
2.305	7	0 0 4	39.04
2.253	11	1 1 3	39.98
2.211	15	1 3 2	40.78
2.047	2	0 4 3	44.22
1.892	2	1 1 4	48.04
1.795	1	0 6 1	50.84
1.765	1	0 4 4	51.76
1.748	3	0 2 5	52.30
1.737	10	2 0 0	52.64
1.722	7	1 5 2	53.16
1.700	4	0 6 2	53.88
1.611	8	1 1 5	57.12
1.589	10	1 5 3	58.00
1.572	3	0 6 3	58.68
1.559	1	2 2 2	59.22
1.537	3	0 0 6	60.16
1.531	3	0 4 5	60.42
1.488	10	1 3 5	62.34
1.468	4	2 4 0	63.30
1.458	11	2 2 3	63.78
1.450	3	2 4 1	64.18
1.429	7	1 7 0	65.22
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 3	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

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.61	2	0 0 2	19.24
3.53	6	0 2 2	25.21
3.313	4	1 1 0	26.89
3.118	21	1 1 1	28.61
2.744	32	0 4 0	32.60
2.690	100	1 1 2	33.27
2.682	78	0 2 3	33.39
2.630	18	0 4 1	34.06
2.520	26	1 3 0	35.60
2.431	49	1 3 1	36.95
2.358	15	0 4 2	38.13
2.305	10	0 0 4	39.04
2.253	15	1 1 3	39.98
2.211	21	1 3 2	40.78
2.047	3	0 4 3	44.21
1.892	4	1 1 4	48.04
1.856	1	1 5 0	49.04
1.795	1	0 6 1	50.84
1.765	1	0 4 4	51.75
1.748	4	0 2 5	52.29
1.737	14	2 0 0	52.63
1.722	11	1 5 2	53.15
1.701	6	0 6 2	53.87
1.611	12	1 1 5	57.12
1.589	15	1 5 3	58.00
1.572	5	0 6 3	58.68
1.559	1	2 2 2	59.22
1.537	4	0 0 6	60.16
1.531	3	0 4 5	60.43
1.488	16	1 3 5	62.34
1.468	7	2 4 0	63.30
1.458	16	2 2 3	63.78
1.450	4	2 4 1	64.19
1.433	1	0 6 4	65.03
1.429	10	1 7 0	65.22
1.399	4	2 4 2	66.83
1.388	3	2 0 4	67.44
1.341	1	0 4 6	70.13
1.325	1	2 4 3	71.11
1.315	4	0 8 2	71.71
1.312	1	1 3 6	71.90
1.308	2	1 5 5	72.15
1.299	3	0 6 5	72.75
1.281	3	0 2 7	73.94
1.232	2	2 2 5	77.37
1.215	3	2 6 2	78.67
1.215	2	1 7 4	78.71
1.166	2	2 6 3	82.72
1.151	2	2 0 6	84.00
1.149	2	2 4 5	84.24
1.130	1	1 7 5	85.97
1.118	3	3 1 2	87.14
1.106	1	2 6 4	88.34
1.104	1	3 3 0	88.46
1.096	2	3 3 1	89.26
1.090	1	0 10 1	89.93
1.089	3	1 1 8	90.08

Cobalt Samarium, Co_2Sm

Structure
Cubic, Fd3m(227), Z=8, isostructural with Cu_2Mg, from powder data [Harris et al., 1965].

Atom positions
16(d) 16 cobalt
8(a) 8 samarium
origin at $\bar{4}3m$

Lattice constants
a = 7.2627 Å
(published value, a = 7.2476 kX [Harris et al., 1965])

Volume
383.08 $Å^3$

Density
(calculated) 9.301 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0 [Cromer and Mann, 1968]
Sm^0 [International Tables, 1974].

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

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(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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	3 3 1	55.08
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 3 1	77.72
1.1483	5	6 2 0	84.26
1.1075	5	5 3 3	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

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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	3 3 3	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 3 1	109.11
.9455	5	5 5 3	109.11
.9078	5	8 0 0	116.10
.8559	5	6 6 0	128.31
.8559	5	8 2 2	128.31
.8386	10	7 5 1	133.42
.8386	1	5 5 5	133.42
.8331	5	6 6 2	135.23
.7972	1	7 5 3	150.15
.7972	1	9 1 1	150.15

Cobalt Tin Vanadium, Co_2SnV

Structure
Cubic, Fm3m(225), Z = 4, a Heusler alloy isostructural with $AlCu_2Mn$, from powder data [Kripyakevich and Markiv, 1963].

Atom positions
8(c) 8 cobalt
4(a) 4 tin
4(b) 4 vanadium

Lattice constant
a = 5.994 Å [ibid.]

Volume
215.35 $Å^3$

Density
(calculated) 8.867 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Sn^0, V^0 [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. A24, 321.
Kripyakevich. P. I. and Markiv, V.Ya. (1963). Dopov. Akad. Nauk Ukr. RSR 12, 1606.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.458	15	1 1 1	25.74
2.996	5	2 0 0	29.80
2.119	100	2 2 0	42.64
1.807	5	3 1 1	50.46
1.730	1	2 2 2	52.88
1.499	15	4 0 0	61.86
1.375	1	3 3 1	68.14
1.340	1	4 2 0	70.16
1.223	20	4 2 2	78.04
1.153	1	5 1 1+	83.80
1.060	5	4 4 0	93.26
1.013	1	5 3 1	98.98
.948	10	6 2 0	108.74
.865	1	4 4 4	125.84
.839	1	7 1 1+	133.20
.801	15	6 4 2	148.18

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.461	15	1 1 1	25.72
2.997	5	2 0 0	29.79
2.119	100	2 2 0	42.63
1.807	5	3 1 1	50.46
1.730	1	2 2 2	52.87
1.499	15	4 0 0	61.87
1.375	5	3 3 1	68.14
1.340	1	4 2 0	70.16
1.224	25	4 2 2	78.04
1.154	1	5 1 1	83.79
1.060	5	4 4 0	93.27
1.013	1	5 3 1	98.98
.948	10	6 2 0	108.74
.914	1	5 3 3	114.85
.865	5	4 4 4	125.84
.839	1	5 5 1	133.20
.839	1	7 1 1	133.20
.801	30	6 4 2	148.18

Cobalt Tin Zirconium, Co_2SnZr

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy, isostructural with $AlCu_2Mn$, from x-ray and neutron powder data [Ziebeck and Webster, 1974].

Atom positions
8(c) 8 cobalt
4(a) 4 tin
4(b) 4 zirconium

Lattice constant
a = 6.249 Å [Ziebeck and Webster, 1974]

Volume
244.0 $Å^3$

Density
(calculated) 8.921 g/cm^3
(measured) 8.90 g/cm^3 [Ziebeck and Webster, 1974]

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Sn^0, Zr^0 [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 Crystallogr. A24, 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 (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.607	1	1 1 1	24.66
3.123	15	2 0 0	28.56
2.209	100	2 2 0	40.82
1.884	1	3 1 1	48.26
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 (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.608	1	1 1 1	24.66
3.124	15	2 0 0	28.55
2.209	100	2 2 0	40.81
1.884	1	3 1 1	48.26
1.804	5	2 2 2	50.56
1.562	15	4 0 0	59.09
1.397	5	4 2 0	66.91
1.276	25	4 2 2	74.30
1.1047	5	4 4 0	88.42
1.0415	1	4 4 2	95.40
.9881	10	6 2 0	102.45
.9421	1	6 2 2	109.70
.9020	5	4 4 4	117.30
.8666	1	6 4 0	125.47
.8351	20	6 4 2	134.57

Cobalt Vanadium Silicide, Co_2VSi

Structure
Cubic, Fm3m(225), Z=4, a Heusler alloy, isostructural with $AlCu_2Mn$, 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 $Å^3$

Density
(calculated) 7.216 g/cm^3

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. A24, 321.
Gladyshevs'kii, E. I. (1962). Porosh. Met. 2, 46.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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	3 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	1	4 4 4	141.14

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.267	5	1 1 1	27.27
2.829	10	2 0 0	31.60
2.001	100	2 2 0	45.29
1.7063	1	3 1 1	53.67
1.6336	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 2 2	83.65
1.0004	5	4 4 0	100.71
.8948	10	6 2 0	118.83
.8168	5	4 4 4	141.14
.7848	1	6 4 0	157.97

Metharbital, $C_9H_{14}N_2O_3$

Synonyms
1-Methyl-5,5-diethylbarbituric acid
N-Methylbarbital
Gemonil

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The structure was determined by Wunderlich [1973].

Atom positions
All atoms are in general positions 4(e) [ibid.].

Lattice constants
a = 6.798(2) Å
b = 11.398(3)
c = 13.191(3)
β = 90.29(1)°

(published values: a = 6.798(2)Å, b = 11.397(3), c = 13.190(3), β = 90.29(1)° [Wunderlich, 1973])

CD cell: a = 13.191(3)Å, b = 11.398(3), c = 6.798(2), β = 90.29(1)°; sp. gp. $P2_1/a$; a/b = 1.1573; c/b = 0.5964

Volume
1022.07 $Å^3$

Density
(calculated) 1.288 g/cm^3
(measured) 1.273 g/cm^3 [Wunderlich, 1973]

Thermal parameters
For hydrogen atoms: isotropic B's [Wunderlich, 1973]. For other atoms isotropic B_i were estimated from β_{11}, β_{22}, β_{33} for each atom.

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.503 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 0.601

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Wunderlich, H. (1973). Acta Crystallogr. B29, 168.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.61	100	0 1 1	10.26
6.79	36	1 0 0	13.02
6.59	90	0 0 2	13.42
5.83	16	1 1 0	15.18
5.70	94	0 2 0+	15.54
5.33	97	1 1 1+	16.62
5.23	21	0 2 1	16.94
4.74	4	-1 0 2	18.70
4.380	31	-1 1 2	20.26
4.312	8	0 2 2	20.58
4.141	10	1 2 1	21.44
4.100	12	0 1 3	21.66
3.642	14	-1 2 2+	24.42
3.480	63	0 2 3	25.58
3.399	3	2 0 0	26.20
3.293	25	0 3 2	27.06
3.213	4	1 3 1	27.74
3.164	20	-2 1 1	28.18
3.093	15	1 2 3+	28.84
3.014	3	2 0 2	29.62
2.961	3	-1 3 2+	30.16
2.915	14	2 1 2+	30.64
2.873	29	0 3 3	31.10
2.852	12	-2 2 1+	31.34
2.665	3	2 2 2	33.60
2.651	3	-1 3 3	33.78
2.617	9	0 4 2+	34.24
2.570	3	0 1 5	34.88
2.486	2	2 3 1+	36.10
2.439	3	1 4 2	36.82
2.408	3	-1 1 5	37.32
2.400	5	1 1 5	37.44
2.393	4	0 4 3	37.56
2.372	2	-2 0 4	37.90
2.368	2	-2 3 2	37.96
2.335	3	1 3 4	38.52
2.253	8	1 4 3	39.98
2.192	9	-3 1 1+	41.14
2.167	5	0 3 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
2.024	3	0 5 3	44.74
2.005	2	2 3 4	45.18
1.988	1	-3 1 3	45.60
1.961	1	1 2 6+	46.26

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.954	1	2	4	3	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	3	3	2	48.82
1.860	2	1	4	5+	48.94
1.850	2	-2	0	6	49.20
1.823	3	-2	4	4+	49.98
1.819	3	2	4	4	50.12
1.806	1	1	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	0	5	5	53.06
1.700	1	4	0	0	53.90
1.679	1	-3	3	4+	54.60
1.658	1	2	6	0	55.36
1.645	1	-2	6	1+	55.84
1.628	1	2	1	7+	56.48
1.583	2	0	5	6+	58.24
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 (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
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	16.56
5.33	83	1	1	1	16.62
5.23	18	0	2	1	16.93
4.75	4	-1	0	2	18.68
4.72	1	1	0	2	18.78
4.381	32	-1	1	2	20.25
4.367	3	1	2	0	20.32
4.362	1	1	1	2	20.34
4.312	7	0	2	2	20.58
4.142	10	1	2	1	21.44
4.102	13	0	1	3	21.65
3.651	1	0	3	1	24.36
3.647	12	-1	2	2	24.39
3.636	5	1	2	2	24.46
3.520	2	-1	1	3	25.28
3.505	8	1	1	3	25.39
3.481	72	0	2	3	25.57
3.399	2	2	0	0	26.20
3.316	7	1	3	0	26.86
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	3	0	2	4	31.31
2.853	7	-2	2	1	31.33
2.848	3	2	2	1	31.39
2.665	3	2	2	2	33.60
2.651	2	-1	3	3	33.79
2.628	6	1	4	0	34.09
2.623	2	-2	1	3	34.15
2.616	7	0	4	2	34.25
2.611	2	2	1	3	34.31
2.570	3	0	1	5	34.88
2.486	1	2	3	1	36.10
2.440	4	1	4	2	36.81
2.408	3	-1	1	5	37.31
2.400	4	1	1	5	37.44
2.391	3	0	4	3	37.58
2.373	2	-2	0	4	37.89
2.368	1	-2	3	2	37.97
2.336	3	1	3	4	38.51
2.266	1	3	0	0	39.75
2.254	10	1	4	3	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	-3	2	1	43.45
2.067	1	-1	3	5	43.76
2.062	1	1	3	5	43.87
2.060	1	-1	1	6	43.91
2.024	3	0	5	3	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

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.873	1	2	5	1	48.56
1.864	2	3	3	2	48.81
1.850	2	-2	0	6	49.20
1.824	1	2	3	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	3	52.53
1.741	2	0	4	6	52.53
1.725	2	0	5	5	53.05
1.699	1	4	0	0	53.91
1.663	1	-2	3	6	55.17
1.658	1	2	6	0	55.36
1.628	1	2	1	7	56.49
1.582	1	0	5	6	58.26
1.572	1	1	7	1	58.68
1.565	1	-3	4	4	58.99

Silicon Oxide (Low Cristobalite), SiO_2

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 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 $Å^3$

Density

(calculated) 2.335 g/cm^3

Thermal parameters

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

Scattering factors

Si^{3+} [International Tables, 1962]
O^- [Cromer and Mann, 1968]
The silicon factors were corrected for dispersion [Cromer and Liberman, 1970].

Scale factors (integrated intensities)

$\gamma = 2.152 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 4.64

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

Additional patterns

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

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Calculated Pattern (Peak heights)

d(Å)	I	hkl	2θ(°) λ = 1.540598Å
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
2.117	3	2 1 1	42.68
2.092	1	1 0 3	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
1.572	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	70.60
1.2990	2	3 1 3	72.74
1.2809	2	3 2 2	73.94
1.2328	1	2 2 4	77.34
1.2232	1	4 0 1	78.06
1.2087	1	2 0 5	79.18
1.2057	1	4 1 0	79.42
1.1878	1	4 1 1	80.86
1.1834	1	3 2 3	81.22
1.1746	1	2 1 5	81.96
1.1718	1	3 3 0	82.20
1.1694	1	4 0 2	82.40
1.1632	1	3 1 4	82.94

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.1552	1	3 3 1	83.64
1.1385	1	4 1 2	85.16
1.1097	1	3 3 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	3 2 4	91.20
1.0685	1	4 1 3	92.26
1.0583	1	4 2 2	93.42
1.0446	1	3 3 3	95.02
1.0387	1	3 1 5	95.74
1.0013	1	4 2 3	100.58
.9941	1	4 3 0	101.58
.9891	1	4 1 4	102.30
.9841	1	4 3 1	103.02
.9766	1	3 2 5	104.14
.9747	1	5 1 0	104.42
.9700	1	3 3 4	105.14
.9694	1	1 0 7	105.24
.9654	1	5 1 1	105.86

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.037	100	1 0 1	22.00
4.037	100	-1 0 -1	22.00
3.515	1	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 0 3	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
1.611	5	3 0 1	57.11
1.611	5	-3 0 -1	57.11
1.600	1	2 1 3	57.54
1.600	1	-2 -1 -3	57.54
1.572	1	3 1 0	58.68
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	3 0 2	62.06
1.494	4	-3 0 -2	62.06
1.431	3	3 1 2	65.13
1.431	3	-3 -1 -2	65.13
1.420	2	2 0 4	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	3	2 1 4	68.71
1.365	3	-2 -1 -4	68.71
1.352	1	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
1.333	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	3 2 2	73.95
1.2807	3	-3 -2 -2	73.95
1.2428	1	4 0 0	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
1.1877	1	4 1 1	80.86
1.1877	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	81.95
1.1717	1	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

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
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
1.0956	2	1 1 6	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	3 2 4	91.21
1.0781	1	-3 -2 -4	91.21
1.0684	1	4 1 3	92.27
1.0684	1	-4 -1 -3	92.27
1.0583	1	4 2 2	93.42
1.0583	1	-4 -2 -2	93.42
1.0446	1	3 3 3	95.03
1.0446	1	-3 -3 -3	95.03
1.0386	1	3 1 5	95.75
1.0386	1	-3 -1 -5	95.75
1.0013	1	4 2 3	100.58
1.0013	1	-4 -2 -3	100.58
.9942	1	4 3 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	3 2 5	104.14
.9766	1	-3 -2 -5	104.14
.9749	1	5 1 0	104.40
.9749	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

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.

*Natural mineral

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Standard x-ray diffraction patterns are presented for 112 substances. Fifty-four 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.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)* Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

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