NBS MONOGRAPH 25—SECTION 19

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

Standard X-ray Diffraction Powder Patterns

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Standard X-ray Diffraction Powder Patterns Section 19 — Data for 51 Substances

Marlene C. Morris, Howard F. McMurdie, Eloise H. Evans,
Boris Paretzkin, Harry S. Parker, and Nikos P. Pyrros

International Centre for Diffraction Data
1601 Park Lane
Swarthmore, PA 19081

and

Camden R. Hubbard

National Measurement Laboratory
National Bureau of Standards
Washington, DC 20234

JCPDS®

International Centre for
Diffraction Data

U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, Secretary
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director

Issued December 1982

Library of Congress Catalog Card Number: 53-61386

National Bureau of Standards Monograph 25
Section 19—Data for 51 Substances
Natl. Bur. Stand. (U.S.), Monogr. 25—Sec. 19, 118 pages (Dec. 1982)
CODEN: NBSMA6

U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON: 1982

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402
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Publications Available

Previous work has been published as a book entitled Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976) (obtainable from the publisher: JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, price furnished on request). The volume is sold with an accompanying search manual, and contains 949 card images of patterns of experimental data, published originally as Circular 539 (vols. 1-10) and Monograph 25, Sections 1-12, and most of Section 13.

Individual copies of the Circular and Monograph are still available and may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161. If a publication listed below is identified with a number, use this number in ordering. All are available in photocopy or microfiche; the price is not fixed and will be furnished on request.

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ERRATA

Circular 539

Volume 8, p. 67: A least squares refinement of the d's gives results: a=6.8837(2), c=6.0197(5). Several of the hkℓ's need to be changed for angles higher than 100°.

Monograph 25

Section 11, p. 18: Density should be 2.197.

p. 56: Density should be 2.733.

Section 17, p. 3: The correct formula for σ_i^2 is: $\sigma_i^2 = \frac{1}{n-1} \sum_{k=1}^{n} \left(I_i^{rel}(k) - \langle I \rangle_i \right)^2$

p. 32: Z should be 4.

p. 34: Density should be 1.608.

Section 18, p. 3: Figure 2 is upside down.

p. 9: The value c/b should be 0.3548, and the calculated density should be 3.876.

p. 10: Add to the sample description "A final heating was made at 1350 °C for 2 days."

p. 35: The value c/b should be 0.5356.

p. 63: In the reference to Bouaziz, delete the volume number 7.

p. 63: In the table, at d=1.5509, the intensity should be 14.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 19 --- Data for 51 Substances

by

Marlene C. Morris, Howard F. McMurdie, Eloise H. Evans,
Boris Paretzkin, Harry S. Parker, and Nikos P. Pyrros
JCPDS--International Centre for Diffraction Data

and

Camden R. Hubbard
National Bureau of Standards

Standard x-ray powder diffraction patterns are presented for 51 substances. These patterns, useful for identification, were obtained by manual or automated diffractometer methods, or were calculated from published crystal structure data. The lattice constants from the experimental work were refined by least-squares methods, and reflections were assigned Miller indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

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

INTRODUCTION

The Powder Diffraction File (PDF) is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the JCPDS--International Centre for Diffraction Data[1], the PDF 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 or improved data to the PDF. Our work also aids in the development of diffraction techniques. This report presents information for one calculated and 50 experimental patterns, and is the twenty-ninth of the series of Standard X-ray Diffraction Powder Patterns[2].

EXPERIMENTAL POWDER PATTERNS

Names. The nomenclature follows the current practice of the PDF. A mineral name in ( ) indicates a synthetic sample.

CAS registry number. The Chemical Abstracts Service Registry Number is included, when available, to help identify the sample. This number forms the basis for computer aided searching of Chemical Abstracts. [Chemical Abstracts Service Registry Handbook-Number Section, 1974]

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 samples improved the quality of many of the patterns. A check of phase purity was provided by indexing the x-ray pattern and by optical examination.

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 1.40 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors are selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. All spacing determinations were made using an internal standard mixed with the sample, packed in a shallow holder. 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. The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in Table 1; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Standard Reference Material 640, Si powder (a=5.43088Å), was used for many patterns. This SRM is now out of stock and has been replaced by SRM 640a (a=5.430825Å), [1982; Hubbard, 1982a]. The SRM 640a lattice constant for Si was refined from multiple powder data measurements made with tungsten and silver as internal standards. Single crystal cell parameter data were also collected. The lattice parameters from the two methods agreed within three parts in 10^5. D-spacing results using SRM 640a will be in agreement with patterns recorded in this series of Monographs since 1966.

[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.

A second internal standard, fluorophlogopite (FP), is available as Standard Reference Material 675 [1982]. The d(001) spacing was refined from multiple powder data measurements using SRM 640a (Si), and tungsten as internal standards [Hubbard, 1982b]. The calculated 2θ values of the d(00ℓ) lines are given in Table 2.

Table 1

Calculated 2θ Angles, $CuK\alpha_1$ λ = 1.540598Å			
hkℓ	W a=3.16524Å ±.00004	Ag a=4.08651Å ±.00002	Si a=5.430825Å ±.000011 (SRM 640a)*
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.304
310	100.632		
311		77.390	56.124
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.132
331		110.499	76.378
420		114.914	
422		134.871	88.033
511/333		156.737	94.955
440			106.712
531			114.096
620			127.550
533			136.900
444			158.644

*Data for SRM 640 can be found in previous monographs of this series.

Table 2

SRM 675, Fluorophlogopite (FP) d_{001} = 9.98104Å ± 0.00007 Calculated 2θ Angles, $CuK\alpha_1$ λ = 1.540598Å	
00ℓ	2θ
1	8.853
2	17.759
3	26.774
4	35.962
5	45.397
6	55.169
7	65.399
8	76.255
10	101.025
11	116.193
12	135.674

All data were collected at 25 ± 1 °C on a diffractometer equipped with a focusing graphite crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. The data were collected using copper radiation: $\lambda(CuK\alpha_1$, peak) = 1.540598Å [Deslattes and Henins, 1973].

Due to a transition from strip chart to digital recording the majority of the patterns reported in this monograph were measured both manually and automatically.

Manual patterns were measured on a diffractometer equipped with a strip chart recorder. 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. This avoided errors associated with aberrations at the very top of the peaks. The $K\alpha_2$ peaks were occasionally read to assist in establishing a $K\alpha_1$ peak position, but $K\alpha_2$ peaks are not reported.

Automatic patterns were measured with a computer controlled diffractometer. Digital data were measured on one of two diffractometers controlled by the AUTO program. [Snyder et al., 1981]. All the patterns were measured in step-scan mode with a step width of 0.01 degrees and counting times at each point greater than or equal to 3 sec.

The data were processed with the JCPDS-NBS POWPAT82 system of processing programs. First the raw data were processed by the program POWDER.PATTERN that locates peaks with the second derivative algorithm of Savitzky and Golay [1964]. A three point Newton-Gregory interpolation [Daniels, 1978] was used to locate the derivative minimum. For some patterns, weak peaks were located with the interactive graphics program PLOT.PATTERN/INT. This program displays the spectrum on a Tektronix graphic terminal. The user can locate peaks by positioning a cursor at the peak. The peak position is defined either as the position of the cursor or as the minimum of the second derivative nearest to the cursor.

All patterns were plotted on paper with the plot program PLOT.PATTERN/HRD on a scale of one degree per inch and were visually inspected. The program POWDER.REFLEC was used to calculate a polynominal correction curve from the expected and observed 2θ peak positions of the internal standard reflections and to correct the observed 2θ values of the sample. The program POWDER.EDTPKS was used to flag reflections to be used in the least-squares cell parameter refinement. Reflections due to $CuK\alpha_2$ radiation were excluded from the refinement.

Comparisons between the two sets of 2θ peak positions of patterns that were processed both manually and automatically showed agreement within the estimated standard deviations. In most cases the results of the digital processing are reported.

At low angles, $K\alpha_1$ and $K\alpha_2$ peaks were unresolved for both the sample and the internal standard. 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. For the manual patterns, if the internal standard correction varied along the length of the pattern, linear interpolations were used.

Structure, lattice constants. The space group symbols are given in the short Hermann-Mauguin notation. Also given are the space group numbers listed in the International Tables for X-ray Crystallography, Vol. I [1965]. When the space group symbol is not known, the lattice centering symbol or the diffraction aspect for the Laue class may be given [Donnay and Kennard, 1964; Mighell et al., 1981].

Orthorhombic cell dimensions are arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants are transformed if necessary in order to follow the convention of Crystal Data [1973]. The lattice constant ratios, a/b, c/b, and c/a, also follow the conventions used for the determinative ratios in Crystal Data [1973].

In most cases, preliminary lattice constants were available in the literature, and were used for the initial indexing and refinement. In cases where such data were not available, other methods were tried. If suitable single crystals were available, the lattice constants were obtained by use of a four-circle diffractometer. Axial ratios and densities from Groth [1908] were sometimes useful. Cell constants were also found in some instances by use of the Visser computer program [1969].

A least squares program [Evans et al., 1963] assigned hkℓ's and refined the lattice constants. Cell refinement was based only upon 2θ values which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{obs}-\theta_{calc})^2$. Generally, when two or more calculated 2θ's were within 0.04 degrees of the observed 2θ, unique indices were not assigned. The possible multiple indices are reported. A plus sign (+) indicates more than 2 possible indices. In indexing cubic patterns, for a given reflection multiple hkℓ's were not utilized or reported. Instead, a single appropriate index was used.

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 published in this series of NBS publications prior to 1973. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

For each d-value, the number of significant figures was derived from the average error in $|2\theta_{obs} - 2\theta_{calc}|$ and the equation $\Delta d/d = -(\cot\theta)\Delta\theta$. With these conditions, the rounded value of d agrees with its appropriate 2θ within the average error in 2θ. The value of Δθ varies with the symmetry and crystallinity of each sample.

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and 1977 atomic weights published by the International Union of Pure and Applied Chemistry [1979].

Figure of merit. Several figures of merit ratings are available for assessing indexed powder data. M_{20} [de Wolff, 1968] is a criterion for the reliability of the unit cell and indexing. A value of $M_{20} > 10$ will guarantee the essential correctness of the indexing provided there are not more than 2 spurious lines ($X_{20} \leq 2$) [de Wolff, 1968]. In general, patterns reported in this publication had $M_{20} > 20$ and $X_{20} = 0$. M_{20} is reported if a cell was derived only through computer indexing from powder data, without further confirmation.

The accuracy and completeness of measured interplanar spacings is conveniently reported using the format:

$$F = \text{overall value } (\overline{|\Delta 2\theta|}, N_{poss}) \quad .$$

The "overall" value is the figure of merit of Smith and Snyder [1979] defined by:

$$\frac{1}{\overline{|\Delta 2\theta|}} \cdot \frac{N}{N_{poss}} \quad .$$

N, the number of observed reflections was chosen as 30, or as the maximum number of lines of the pattern if the pattern had fewer than 30 lines. $\overline{|\Delta 2\theta|}$ is the average absolute magnitude of discrepancy between observed and calculated 2θ values for each reported hkℓ. When multiple indices are reported for an observed reflection, then each possible Δ2θ is included in the $\overline{|\Delta 2\theta|}$. N_{poss} is the number of diffraction lines allowed in the space group, up to the N^{th} observed and indexed line. Co-positional lines such as the cubic 221 and 300 are counted as one possible line.

Intensity measurements. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentage of the strongest line. It has been found that samples which give satisfactory intensity patterns usually have 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.

Figure 1.

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 (see Figure 2).

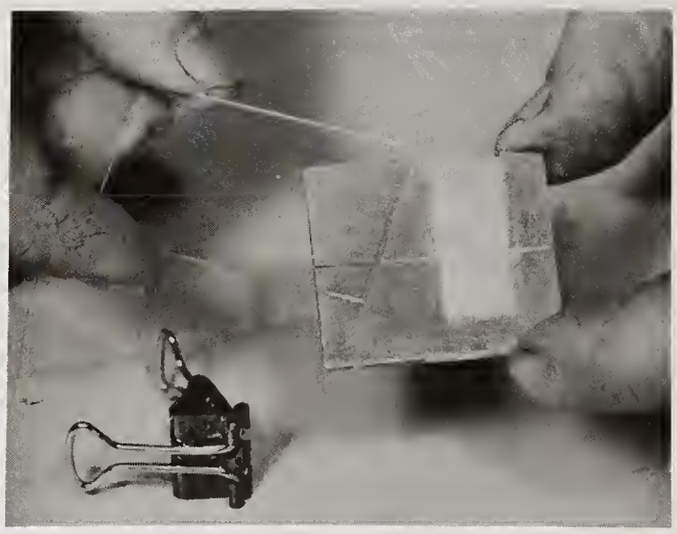

Figure 2.

As a general practice, approximately 50 volume percent of finely ground silica-gel was added as a diluent. Occasionally, a rotating sample holder was used.

As a check on reproducibility, each sample was mounted at least 3 times. The intensity values were determined for each of the mountings. The reported I^{rel} value for each observed spacing is the average of 3 or more observations and is rounded to the nearest integer. Theta-compensating (variable divergence) slits were sometimes used to gather the intensity data. In that case, the average I(comp) for each spacing was converted to an equivalent fixed slit value, using the approximate equation:

$$I(\text{fixed}) = \frac{I(\text{comp})}{\sin\theta}$$

The estimated standard deviation, σ, in the relative intensity values was calculated from the values of the five strongest lines, excluding the line with I^{rel}=100.

$$\sigma_i^2 = \frac{1}{n-1} \sum_{k=1}^{n} \left(I_i^{rel}(k) - \langle I \rangle_i\right)^2$$

and

$$\sigma = \left\{\frac{1}{m} \sum_{i=1}^{m} \sigma_i^2\right\}^{\frac{1}{2}}$$

where

m is the number of strong lines (usually 5), and
n is the number of independent observations i, per line.

Where conversion of intensities for effects of theta-compensating slits was required, each σ_i was multiplied by the conversion factor

$$f = \frac{I(\text{comp})}{I(\text{fixed})}$$

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 113 (hexagonal) reflection of corundum (α-Al_2O_3) [Visser and de Wolff, 1964]. In this publication the ratios I/I_c are tabulated for copper $K\alpha_1$ radiation, for a 1:1 mixture by weight of the sample and corundum. I/I_c was determined only for very common phases.

A 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 ($X_s = 1-X_c$), the intensities for reflection $\underline{h}_1$ of the sample and $\underline{h}_2$ of corundum were measured for several combinations of $\underline{h}_1$ and $\underline{h}_2$ 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

$$\frac{I(h_o)}{I_c(113)} = \frac{X_c}{X_s} \cdot \frac{I_c^{rel}(\underline{h}_2)}{I^{rel}(\underline{h}_1)} \cdot \frac{I(\underline{h}_1)}{I_c(\underline{h}_2)}$$

where (h_o) indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection (h_o) 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 yielded the tabulated average $\langle I/I_c \rangle$. From these data, the standard deviation, σ, was obtained from

$$\sigma^2 = \frac{\sum_{i=1}^{n} \left((I/I_c)_i - \langle I/I_c \rangle\right)^2}{n(n-1)}$$

where n was the number of measurements of the reference intensity ratio. The standard deviation in the least significant figures is given in parentheses.

Format of tables. The printing of the data has been computerized. Superimposed reflections are treated in one of two ways. If a d-spacing has only two possible indices, an M is added to the d-spacing which is repeated on the next line, but with the second index. However, if there are more than two possible indices, a plus sign is used in like manner. In both cases, the composite intensity is printed only once and aligned with the first reflection. The symbol "1L" in the intensity column is used to indicate "less than 1".

UNITS

In this publication the Ångström unit (1Å = 100 pm) was selected for presentation of the d-spacings and lattice parameters. This maintained consistency with (a) the earlier publications of Standard X-ray Diffraction Powder Patterns [1982] (b) the publications of the International Union of Crystallography, and (c) the continuing publication of cards and search manuals of the PDF (now consisting of over 40,000 entries). The PDF search manuals are based on the d-spacings in Å of the 3 strongest lines. Consistent with the choice of the Å unit for length, the volume of the unit cell is expressed in $Å^3$ ($1Å^3 = 1 \times 10^{-30}$ m^3). Densities are reported in g/cm^3 ($1\ gm/cm^3 = 10^3\ kg/m^3$).

ACKNOWLEDGMENTS

We would like to thank Carolyn Wingo and Donna Gladhill of the JCPDS Associateship for their assistance, particularly for keyboarding the data and helping with the proofreading of this manuscript. Appreciation is also expressed to the Text Editing Facility of the National Measurement Laboratory of NBS for typing the manuscript.

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Aluminum Yttrium Oxide, $AlYO_3$

Synonym
Yttrium aluminate

CAS registry no.
12003-86-0

Sample
The sample was prepared at NBS. Calculated amounts of Al_2O_3 and Y_2O_3 were mixed and heated at 1675 °C for 1 day. The composition was adjusted to approach the 1:1 phase, and the mixture was reheated at 1600 °C for 4 days and at 1675 °C for 3 days. The compound was ground daily during the process.

Color
Yellowish white

Structure
Orthorhombic, Pnma (62), Z = 4, isostructural with $GdFeO_3$ and $YFeO_3$ (Geller and Wood, 1956). The structure of $GdFeO_3$ was determined by Geller (1956). Coppens and Eibschütz (1965) refined the centric structure of $GdFeO_3$ and $YFeO_3$. The latter was refined also in the alternative non-centrosymmetric space group $Pn2_1a$ (33), and that refinement showed small, possibly real, deviations from a centric structure.

Lattice constants of this sample
a = 5.3286(4)Å
b = 7.3706(5)
c = 5.1796(3)

a/b = 0.7230
c/b = 0.7027

Volume
203.43 Å^3

Density
(calculated) 5.351 g/cm^3

Polymorphism
Bertaut and Mareschal (1963) reported a hexagonal form that occurred at temperatures of 900 to 950 °C. Their powder pattern appears on PDF card 16-219.

Figure of merit
F_{30} = 92.6(0.010,33)

Additional patterns
PDF card 11-662 (Roth, 1957)

PDF card 28-37 (Abell et al., 1972). The pattern appears to contain 2nd phase lines.

Geller and Wood (1956)

Keith and Roy (1954). The pattern in table 4 labeled $3Y_2O_3 \cdot 5Al_2O_3$, $YCrO_3$ type, seems to be the phase reported here.

References

Abell, J. S., Harris, I. R., and Cockayne, B. (1972). J. Mater. Sci. 7, 1088.

Bertaut, F. and Mareschal, J. (1963). C. R. Hebd. Séances Acad. Sci. 257, 867.

Coppens, P. and Eibschütz, M. (1965). Acta Crystallogr. 19, 524.

Geller, S. (1956). J. Chem. Phys. 24, 1236.

Geller, S. and Wood, E. A. (1956). Acta Crystallogr. 9, 563.

Keith, M. L. and Roy, R. (1954). Am. Mineral. 39, 1.

Roth, R. (1957). J. Res. Natl. Bur. Stand. 58, 75.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
4.233	1	0 1 1	20.97
3.711	29	1 0 1	23.96
3.685	16	0 2 0	24.13
3.317	19	1 1 1	26.86
2.664	22	2 0 0	33.62
2.617	100	1 2 1	34.24
2.589	24	0 0 2	34.62
2.505	11	2 1 0	35.82
2.368	1L	2 0 1	37.97
2.329	1	1 0 2	38.63
2.255	1	2 1 1	39.94
2.220M	9	1 1 2	40.60
2.220M		0 3 1	40.60
2.1588	23	2 2 0	41.81
2.1192	25	0 2 2	42.63
2.0483	8	1 3 1	44.18
1.9923	2	2 2 1	45.49
1.9686	2	1 2 2	46.07
1.8565	31	2 0 2	49.03
1.8424	18	0 4 0	49.43
1.8051	9	2 3 0	50.52
1.8005	15	2 1 2	50.66
1.7055	1L	2 3 1	53.70
1.6904	1	1 3 2	54.22
1.6579	3	2 2 2	55.37
1.6505	6	1 4 1	55.64
1.6424	6	1 0 3	55.94
1.6381	17	3 1 1	56.10
1.6030	3	1 1 3	57.44
1.5286	10	3 2 1	60.52

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
1.5155	9	2 4 0	61.10
1.5006M	32	0 4 2	61.77
1.5006M		1 2 3	61.77
1.4814	4	2 3 2	62.66
1.4492	1	2 0 3	64.22
1.4368	1L	3 1 2	64.84
1.4181	1L	0 5 1	65.80
1.3869	8	3 3 1	67.48
1.3701	1	1 5 1	68.42
1.3655	1L	1 3 3	68.68
1.3320	2	4 0 0	70.66
1.3108	6	4 1 0	71.98
1.3082	17	2 4 2	72.15
1.2950	5	0 0 4	73.00
1.2901M	3	4 0 1	73.32
1.2901M		2 5 0	73.32
1.2581M	1	1 0 4	75.51
1.2581M		3 3 2	75.51
1.2517	1L	2 5 1	75.96
1.2456	1L	1 5 2	76.40
1.2403	1	1 1 4	76.79
1.2281	2	0 6 0	77.69
1.2260	4	1 4 3	77.85
1.2209	6	3 1 3	78.24
1.1845	1	4 0 2	81.13
1.1734	3	3 2 3	82.06
1.1696	7	4 1 2	82.39
1.1663	11	1 6 1	82.67
1.1645	5	2 0 4	82.83
1.1547	4	2 5 2	83.69
1.1503	3	2 1 4	84.08
1.1391	1L	2 4 3	85.10
1.1200	1	1 3 4	86.91
1.1155	2	2 6 0	87.35
1.1102M	3	2 2 4	87.87
1.1102M		0 6 2	87.87
1.1080	5	3 5 1	88.09
1.1056	8	3 3 3	88.33
1.0970	1	1 5 3	89.20
1.0796	1	4 4 0	91.04
1.0671	5	4 3 2	92.42
1.0596	4	0 4 4	93.27
1.0524	2	2 3 4	94.10
1.0439M	1L	4 1 3	95.11
1.0439M		5 0 1	95.11

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
1.0335M	4	5 1 1	96.37
1.0335M		2 5 3	96.37
1.0278	1L	3 4 3	97.09
1.0247	1	2 6 2	97.48
1.0170	1	1 0 5	98.48
1.0141	1	4 2 3	98.86
1.0129	1	1 7 1	99.02
1.0067	1L	3 2 4	99.84
.9966	1	4 4 2	101.24
.9918	2	3 6 1	101.91
.9885	3	4 5 0	102.38
.9842	6	2 4 4	103.01

Aluminum Yttrium Oxide, $Al_2Y_4O_9$

Synonym
Yttrium Aluminate

Sample
The sample was made from stoichiometric amounts of Y_2O_3 and Al_2O_3. The mixture was heated at 1600 °C for 2 days, ground and reheated at 1675 °C for 3-½ days. After adjusting the composition, the material was ground and heated periodically, 11 days at 1600 °C and finally in two stages at 1675 °C.

Color
Very pale yellowish white

Structure
Monoclinic, $P2_1/a$ (14), Z = 4 (Reed and Chase, 1962).

Comment
Reed and Chase (1962) report that due to the complexity of the monoclinic calculated pattern, they found it virtually impossible to index the powder pattern.

Lattice constants of this sample
a = 11.1156(16)Å
b = 10.4689(16)
c = 7.3791(9)
β = 108.61(1)°

a/b = 1.0618
c/b = 0.7049

Volume
813.79 Å^3

Density
(calculated) 4.518 g/cm^3

Figure of merit
F_{30} = 22.9(0.015,86)

Additional patterns
PDF card 22-987 (Schneider et al. 1961)

Warshaw and Roy (1959)

Abell et al. (1974)

References
Abell, J. S., Harris, I. R., Cockayne, B., and Lent, B. (1974). J. Mater. Sci. 9, 527.

Reed, J. W. and Chase, A. B. (1962). Acta Crystallogr. 15, 812.

Schneider, S. J., Roth, R. S., and Waring, J. L. (1961). J. Res. Natl. Bur. Stand. A65, 345.

Warshaw, I. and Roy, R. (1959). J. Am. Ceram. Soc. 42, 434.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
7.41	17	1 1 0	11.93
6.99	1	0 0 1	12.66
5.264	3	2 0 0	16.83
5.046	1	-2 0 1	17.56
4.701	23	2 1 0	18.86
4.551	4	-2 1 1	19.49
4.188	2	0 2 1	21.20
3.713	6	2 2 0	23.95
3.682	4	2 0 1	24.15
3.494	2	0 0 2	25.47
3.470M	2	2 1 1	25.65
3.470M		-2 0 2	25.65
3.330	24	3 1 0	26.75
3.017	100	-1 2 2	29.59
2.919M	78	1 1 2	30.60
2.919M		3 2 0	30.60
2.892	9	-2 2 2	30.90
2.615	18	0 4 0	34.26
2.561	13	2 0 2	35.01
2.538M	8	1 4 0	35.34
2.538M		-1 3 2	35.34
2.527	12	-4 0 2	35.49
2.487	5	2 1 2	36.09
2.470M	7	0 3 2	36.34
2.470M		3 2 1	36.34
2.458M	6	-2 3 2	36.53
2.458M		-4 1 2	36.53
2.352	1L	4 2 0	38.23
2.325	2	-2 4 1	38.69
2.292	7	1 3 2	39.27
2.276+	6	-4 2 2	39.57
2.276+		0 1 3	39.57
2.256	2	-3 1 3	39.93
2.210	2	-2 2 3	40.79
2.174	2	-5 1 1	41.51
2.133M	1	-1 4 2	42.33
2.133M		2 4 1	42.33
2.129	2	0 2 3	42.43
2.095M	2	0 4 2	43.15
2.095M		1 1 3	43.15
2.088M	2	-2 4 2	43.29
2.088M		-5 1 2	43.29
2.066	18	5 1 0	43.78
2.053	5	1 5 0	44.07
2.047M	9	-4 3 2	44.22
2.047M		-5 2 1	44.22
1.984	3	1 4 2	45.69
1.973M	2	-3 4 2	45.97
1.973M		-5 2 2	45.97
1.955	1	5 2 0	46.41

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
1.946	2	2 5 0	46.64
1.939M	1	0 3 3	46.82
1.939M		1 5 1	46.82
1.904	2	-4 4 1	47.74
1.885M	1	2 1 3	48.23
1.885M		4 3 1	48.23
1.875	2	-5 3 1	48.52
1.856	4	4 4 0	49.03
1.845	19	-2 0 4	49.36
1.831M	17	5 1 1	49.75
1.831M		2 4 2	49.75
1.818+	17	-5 3 2	50.15
1.818+		-4 4 2	50.15
1.7998	4	2 2 3	50.68
1.7929M	4	-2 5 2	50.89
1.7929M		-6 1 2	50.89
1.7798	1L	-5 2 3	51.29
1.7562	1	6 0 0	52.03
1.7522	1L	5 2 1	52.16
1.7450	2	0 6 0	52.39
1.7410	1	0 4 3	52.52
1.7324M	6	-3 4 3	52.80
1.7324M		6 1 0	52.80
1.7248M	10	1 5 2	53.05
1.7248M		0 1 4	53.05
1.7200	10	-1 2 4	53.21
1.7180M	10	-6 2 2	53.28
1.7180M		-3 5 2	53.28
1.6930M	1L	0 6 1	54.13
1.6930M		-1 6 1	54.13
1.6843M	1	3 1 3	54.43
1.6843M		-6 0 3	54.43
1.6643+	1L	3 4 2	55.14
1.6643+		6 2 0	55.14
1.6588	1	0 2 4	55.34
1.6566	2	2 6 0	55.42
1.6516M	2	-5 4 2	55.60
1.6516M		1 6 1	55.60
1.6462	1	-4 2 4	55.80
1.6386	2	4 5 0	56.08

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
1.6285	4	4 3 2	56.46
1.6235	4	3 2 3	56.65
1.6133	3	-6 3 2	57.04
1.6046	2	-5 1 4	57.38
1.5889	1L	-2 5 3	58.00
1.5772M	9	-1 6 2	58.47
1.5772M		2 6 1	58.47
1.5670	9	1 2 4	58.89
1.5631M	12	0 3 4	59.05
1.5631M		3 6 0	59.05
1.5607M	8	0 6 2	59.15
1.5607M		-7 1 1	59.15
1.5512M	8	-3 5 3	59.55
1.5512M		-5 2 4	59.55
1.5293	2	4 5 1	60.49
1.5249	2	5 2 2	60.68
1.5159	2	5 4 1	61.08
1.5110	3	-7 2 1	61.30
1.5072	4	-2 4 4	61.47
1.5015	3	-6 0 4	61.73
1.4896	2	7 1 0	62.28
1.4859+	3	-7 1 3	62.45
1.4859+		1 3 4	62.45
1.4812M	3	3 6 1	62.67
1.4812M		1 7 0	62.67
1.4589	2	-2 1 5	63.74
1.4548	3	4 6 0	63.94
1.4386M	4	2 7 0	64.75
1.4386M		-7 3 1	64.75

Aluminum Yttrium Oxide, $Al_5Y_3O_{12}$

Synonyms
Yttrium aluminate
Yttrogarnet

CAS registry no.
12005-21-9

Sample
The sample was prepared at NBS. Stoichiometric amounts of the constituent oxides were blended and calcined at 1650 °C for two hours. After grinding, the resultant product was placed in an iridium crucible, fused in an induction heater and several single crystal boules grown using the Czochralski technique.

Color
Colorless

Structure
Cubic, Ia3d (230), Z = 8. The structure was studied by Yoder and Keith (1951). It has the garnet structure type.

Lattice constant of this sample
a = 12.0089(3)Å

Volume
1731.85 Å^3

Density
(calculated) 4.552 g/cm^3

Polymorphism
Yoder and Keith (1951) reported that yttrogarnet inverts to a high temperature form, yttroalumite, at 1970° ± 50 °C.

Figure of merit
F_{30} = 91.8(0.011,30)

Additional patterns
PDF card 8-178 (Keith and Roy, 1954)

PDF card 30-51 (Abell et al., 1974)

References
Abell, J. S., Harris, I. R., Cockayne, B., and Lent, B. (1974). J. Mater. Sci. 9, 527.

Keith, M. L. and Roy, R. (1954). Am. Mineral. 39, 1.

Yoder, H. S. and Keith, M. L. (1951). Am. Mineral. 36, 519.

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

d(Å)	I^{rel} σ = ±2	hkℓ			2θ(°)
4.905	27	2	1	1	18.07
4.247	7	2	2	0	20.90
3.210	19	3	2	1	27.77
3.002	27	4	0	0	29.74
2.687	100	4	2	0	33.32
2.561	1L	3	3	2	35.01
2.452	20	4	2	2	36.62
2.355	6	4	3	1	38.18
2.192	23	5	2	1	41.15
2.122	5	4	4	0	42.56
1.9474	26	5	3	2	46.60
1.8994	1L	6	2	0	47.85
1.8536	1L	5	4	1	49.11
1.7705	2	6	3	1	51.58
1.7330	17	4	4	4	52.78
1.6988	1L	5	4	3	53.93
1.6652	31	6	4	0	55.11
1.6338	9	7	2	1	56.26
1.6046	28	6	4	2	57.38
1.5247	4	6	5	1	60.69
1.5006	10	8	0	0	61.77
1.4780	1L	7	4	1	62.82
1.4561	1L	8	2	0	63.88
1.4352	1	6	5	3	64.92
1.4157	1	6	6	0	65.93
1.3962	1L	7	4	3	66.97
1.3598	1L	7	5	2	69.01
1.3423	7	8	4	0	70.04
1.3102	17	8	4	2	72.02
1.2949	2	7	6	1	73.01
1.2800	6	6	6	4	74.00
1.2656	1	8	5	1	74.98
1.2388	2	9	3	2	76.90
1.2257	1L	8	4	4	77.87
1.2128	1L	9	4	1	78.86
1.2011	1L	8	6	0	79.78
1.1889	1L	10	1	1	80.77
1.1776	2	10	2	0	81.71
1.1665	1L	9	4	3	82.65
1.1451	3	10	3	1	84.55
1.1249	1L	8	7	1	86.44
1.1151	14	10	4	0	87.39
1.1056	2	9	6	1	88.33
1.0964	6	10	4	2	89.27
1.0874	1L	9	5	4	90.21

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ			2θ(°)
1.0698	3	10	5	1	92.12
1.0616	6	8	8	0	93.04
1.0373	2	9	7	2	95.91
1.0298	1	10	6	0	96.84
1.0223	1L	11	4	1	97.79
1.0150	1L	10	6	2	98.74
1.0077	1L	9	6	5	99.71
1.0007	1	12	0	0	100.66
.9939	1L	9	7	4	101.62
.9872	3	12	2	0	102.58
.9805	2	11	5	2	103.55
.9741	6	10	6	4	104.51
.9676	1L	12	3	1	105.51

Ammonium Cadmium Phosphate Hydrate, $NH_4CdPO_4 \cdot H_2O$

Sample
The sample was prepared at NBS. Water solutions of $CdCl_2$ and $(NH_4)_2HPO_4$ were mixed. NH_4OH was added to the mixture dropwise, until the pH reached 9.

Color
Colorless

Structure
Orthorhombic, $Pmn2_1$ (31), Z = 2. (Tranqui et al., 1968).

Lattice constants of this sample
a = 5.8173(10)Å
b = 8.8797(8)
c = 5.0134(8)

a/b = 0.6551
c/b = 0.5646

Volume
258.97 Å^3

Density
(calculated) 3.122 g/cm^3

Figure of merit
F_{30} = 98.2(0.009,34)

Additional patterns
PDF card 14-397 (Ropp et al., 1961)

Ropp and Mooney (1960)

References

Ropp, R. C. and Mooney, R. W. (1960). J. Am. Chem. Soc. 82, 4848.

Ropp, R. C., Mooney, R. W., and Hoffman, C. W. W. (1961). Anal. Chem. 33, 1687.

Tranqui, D., Durif, A., Guitel, J. C., and Averbuch-Pouchot, M. T. (1968). Bull. Soc. Chim. Fr., 1759.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
8.87	100	0 1 0	9.96
4.868	4	1 1 0	18.21
4.436	11	0 2 0	20.00
4.367	13	0 1 1	20.32
3.799	13	1 0 1	23.40
3.528	7	1 2 0	25.22
3.493	38	1 1 1	25.48
3.324	3	0 2 1	26.80
2.957	1L	0 3 0	30.20
2.908	36	2 0 0	30.72
2.885	63	1 2 1	30.97
2.764	10	2 1 0	32.37
2.637	3	1 3 0	33.97
2.549	5	0 3 1	35.18
2.506	6	0 0 2	35.80
2.433	7	2 2 0	36.92
2.420	8	2 1 1	37.12
2.413	7	0 1 2	37.24
2.334	18	1 3 1	38.54
2.2187	2	0 4 0	40.63
2.1883	9	2 2 1	41.22
2.1822	10	0 2 2	41.34
2.0738M	8	2 3 0	43.61
2.0738M		1 4 0	43.61
2.0435	2	1 2 2	44.29
2.0300	1	0 4 1	44.60
1.9164M	13	2 3 1	47.40
1.9164M		1 4 1	47.40
1.9122	10	0 3 2	47.51
1.8991	7	2 0 2	47.86
1.8568	8	2 1 2	49.02
1.8169	3	1 3 2	50.17
1.7753	7	0 5 0	51.43
1.7456	5	2 2 2	52.37
1.6982	3	1 5 0	53.95
1.6744M	8	3 2 1	54.78
1.6744M		0 5 1	54.78
1.6624	3	0 4 2	55.21
1.6224	2	3 3 0	56.69
1.5984M	5	2 3 2	57.62
1.5984M		1 4 2	57.62
1.5809	3	1 1 3	58.32
1.5434	3	3 3 1	59.88
1.5161	3	2 5 0	61.07
1.4802	1L	0 6 0	62.72
1.4599	1	3 4 0	63.69
1.4508	4	2 5 1	64.14
1.4344	2	1 6 0	64.96
1.4193	2	0 6 1	65.74
1.4070	1	1 5 2	66.39
1.4019	2	3 4 1	66.66
1.3789	3	1 6 1	67.92
1.3196	1L	2 6 0	71.43
1.3097	1L	3 5 0	72.05
1.2978	2	2 5 2	72.82
1.2760	2	2 6 1	74.27

Barium Aluminum Titanium Oxide, $BaAl_6TiO_{12}$

Synonym
Barium aluminum titanate

CAS registry no.
58834-02-9

Sample
The sample was synthesized by melting, then very slowly cooling, stoichiometric amounts of $BaTiO_3$, Al_2O_3, and TiO_2. After heating at 1275 °C for 16.5 days, the sample was reheated at 1350 °C for 23 days. The material was ground every 24 hours.

Color
Colorless

Structure
Orthorhombic, Pn*n, Z = 2. The structure studied by Roth et al. (1981) was based on single crystal precession data.

Lattice constants of this sample
a = 7.1375(3) Å
b = 13.5978(8)
c = 4.8651(2)

a/b = 0.5249
c/b = 0.3578

Volume
472.18 Å^3

Density
(calculated) 3.792 g/cm^3

Figure of merit
F_{30} = 152.7(0.006,36)

Additional pattern
PDF card 29-147 (Guha et al., 1976)

References
Guha, J. P., Kolar, D., and Volavšek, B. (1976). J. Solid State Chem. 16, 49.

Roth, R. S., Parker, H. S., and Koob, M. M. (1981). 12th Intl. Congress of Cryst. Ottawa, C-167.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.799	22	0 2 0	13.01
6.316	2	1 1 0	14.01
4.581	15	0 1 1	19.36
4.021	2	1 0 1	22.09
3.828	15	1 3 0	23.22
3.570	9	2 0 0	24.92
3.462	82	1 2 1	25.71
3.401	4	0 4 0	26.18
3.318	51	0 3 1	26.85
3.161	100	2 2 0	28.21
2.8152	50	2 1 1	31.76
2.6506	2	2 2 1	33.79
2.5954	80	1 4 1	34.53
2.5412	17	1 5 0	35.29
2.4610	3	2 4 0	36.48
2.4333	24	0 0 2	36.91
2.3738	2	0 5 1	37.87
2.3440	11	3 1 0	38.37
2.3025	8	1 0 2	39.09
2.2901	6	0 2 2	39.31
2.2702	22	1 1 2	39.67
2.2663	22	0 6 0	39.74
2.2527	17	1 5 1	39.99
2.1965	10	2 4 1	41.06
2.1373	11	3 0 1	42.25
2.1064	8	3 3 0	42.90
2.0532	5	1 3 2	44.07
2.0391	6	3 2 1	44.39
2.0103	12	2 0 2	45.06
1.9886	6	2 1 2	45.58
1.9763	24	2 5 1	45.88
1.9743	24	1 6 1	45.93
1.9275	33	2 2 2	47.11
1.8748	5	1 7 0	48.52
1.8095	39	3 4 1	50.39
1.7906	6	3 5 0	50.96
1.7844	9	4 0 0	51.15
1.7798	7	2 6 1	51.29
1.7569	11	1 5 2	52.01
1.7300	4	2 4 2	52.88
1.7258	4	4 2 0	53.02
1.6996	2	0 8 0	53.90
1.6875	1	3 1 2	54.32
1.6627	5	4 1 1	55.20
1.6579	11	0 6 2	55.37
1.6267	1	4 2 1	56.53
1.6154	1	1 6 2	56.96
1.6100M	3	0 1 3	57.17
1.6100M		2 7 1	57.17
1.5924	11	3 3 2	57.86
1.5799	2	4 4 0	58.36
1.5716M	6	1 1 3	58.70
1.5716M		4 3 1	58.70
1.5655	6	1 8 1	58.95
1.5550	24	3 6 1	59.39
1.5404	7	1 2 3	60.01
1.5346	16	2 8 0	60.26
1.5268	6	0 3 3	60.60
1.5046M	2	3 7 0	61.59
1.5046M		2 6 2	61.59

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.5028	1	4 4 1	61.67
1.4844	2	1 7 2	62.52
1.4678	5	2 1 3	63.31
1.4428+	6	0 9 1	64.54
1.4428+		2 2 3	64.54
1.4388	15	4 0 2	64.74
1.4337	20	1 4 3	65.00
1.4260	8	4 5 1	65.39
1.4195	2	5 1 0	65.73
1.4077	4	4 2 2	66.35
1.4040	4	2 3 3	66.55
1.4015	4	4 6 0	66.68
1.3929M	4	0 8 2	67.15
1.3929M		0 5 3	67.15
1.3711	2	4 3 2	68.36
1.3696	2	5 0 1	68.45
1.3598M	5	3 6 2	69.01
1.3598M		0 10 0	69.01
1.3428	7	5 2 1	70.01
1.3252	2	4 4 2	71.08
1.3146	3	3 2 3	71.74
1.2978M	18	2 8 2	72.82
1.2978M		2 5 3	72.82
1.2880	2	1 10 1	73.46
1.2797	3	3 7 2	74.02
1.2754	3	3 9 0	74.31
1.2706M	9	2 10 0	74.64
1.2706M		5 4 1	74.64
1.2639	2	5 5 0	75.10
1.2466	3	3 4 3	76.33
1.2307M	1	5 0 2	77.50
1.2307M		4 8 0	77.50
1.2235	2	5 5 1	78.04
1.2162	3	0 0 4	78.60
1.2148	4	4 6 2	78.71
1.2079	1L	2 9 2	79.24
1.1991	1L	1 0 4	79.94
1.1956	2	4 1 3	80.22
1.1942	1L	1 1 4	80.34
1.1896	3	6 0 0	80.71
1.1869	3	0 10 2	80.93
1.1721M	3	5 6 1	82.17
1.1721M		6 2 0	82.17
1.1602	3	4 3 3	83.20
1.1576M	2	1 8 3	83.43
1.1576M		5 4 2	83.43
1.1533	2	3 6 3	83.81
1.1514M	3	6 1 1	83.98
1.1514M		2 0 4	83.98
1.1473M	2	3 10 1	84.35
1.1473M		2 1 4	84.35

Barium Aluminum Titanium Oxide, $Ba_3Al_{10}TiO_{20}$

Synonym
Barium aluminum titanate

CAS registry no.
58834-01-8

Sample
The sample was synthesized by melting together, then very slowly cooling stoichiometric amounts of $BaTiO_3$, Al_2O_3, and TiO_2. The sample was heated at 1000 °C for 20 hours, then at 1275 °C for 14 days and finally at 1350 °C for 23 days. The material was ground after each 24 hour period.

Color
Colorless

Structure
Monoclinic, I*/*, Z = 2. The structure studied by Roth et al. (1981) was based on single crystal precession data.

Lattice constants of this sample
a = 14.8884(12)Å
b = 11.3676(13)
c = 4.9781(5)
β = 90.84(1)°

a/b = 1.3097
c/b = 0.4379

Volume
842.43 Å^3

Density
(calculated) 4.138 g/cm^3

Figure of merit
F_{30} = 53.24(0.010,55)

Additional pattern
PDF card 29-148 (Guha et al., 1976)

References
Guha, J. P., Kolar, D., and Volavšek, B. (1976). J. Solid State Chem. 16, 49.

Roth, R. S., Parker, H. S., and Koob, M. M. (1981). 12th Intl. Congress of Cryst. Ottawa, C-167.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
5.683	23	0 2 0	15.58
4.741	2	-1 0 1	18.70
4.560	34	0 1 1	19.45
3.912	1	-2 1 1	22.71
3.869	1	2 1 1	22.97
3.723	5	4 0 0	23.88
3.673	5	1 3 0	24.21
3.642	5	-1 2 1	24.42
3.541	6	-3 0 1	25.13
3.490	8	3 0 1	25.50
3.113	57	4 2 0	28.65
3.015M	100	0 3 1	29.61
3.015M		3 3 0	29.61
2.974	38	3 2 1	30.02
2.903	30	-4 1 1	30.77
2.882	14	5 1 0	31.01
2.865	28	4 1 1	31.19
2.842	8	0 4 0	31.45
2.805	22	-2 3 1	31.88
2.787	9	2 3 1	32.09
2.572	2	-5 0 1	34.86
2.538	1L	5 0 1	35.33
2.489	25	0 0 2	36.05
2.432	7	1 4 1	36.93
2.404	8	-1 1 2	37.37
2.352M	17	-4 3 1	38.24
2.352M		2 0 2	38.24
2.334	1L	4 3 1	38.55
2.280	9	0 2 2	39.49
2.259	7	4 4 0	39.88
2.204	20	3 4 1	40.91
2.1707M	7	2 2 2	41.57
2.1707M		3 1 2	41.57
2.0906	20	7 1 0	43.24
2.0824	11	-4 0 2	43.42
2.0675M	18	0 5 1	43.75
2.0675M		3 5 0	43.75
1.9948	2	-2 5 1	45.43
1.9903	3	2 5 1	45.54
1.9670	8	-7 0 1	46.11
1.9562	13	-4 2 2	46.38
1.9455	4	7 0 1	46.65
1.9326	8	4 2 2	46.98
1.9271	7	-3 3 2	47.12
1.9100	7	3 3 2	47.57
1.8942M	12	0 6 0	47.99
1.8942M		5 4 1	47.99
1.8719	6	0 4 2	48.60
1.8697M	5	5 1 2	48.66
1.8697M		6 4 0	48.66
1.8600	8	8 0 0	48.93
1.8572	7	-7 2 1	49.01
1.8547	8	7 3 0	49.08
1.8403	7	7 2 1	49.49
1.8125	10	-4 5 1	50.30
1.8031	3	4 5 1	50.58
1.7692M	1	-6 0 2	51.62
1.7692M		8 2 0	51.62
1.7591	1L	-1 6 1	51.94
1.7444	3	6 0 2	52.41

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.7309	1	-8 1 1	52.85
1.6950	1L	5 3 2	54.06
1.6881	5	4 6 0	54.30
1.6798	5	-4 4 2	54.59
1.6702M	5	-3 6 1	54.93
1.6702M		-1 5 2	54.93
1.6652M	6	4 4 2	55.11
1.6652M		3 6 1	55.11
1.6416	2	0 1 3	55.97
1.6367	2	9 1 0	56.15
1.6167	19	-7 4 1	56.91
1.6051	16	7 4 1	57.36
1.5949	5	-3 5 2	57.76
1.5894M	8	-8 3 1	57.98
1.5894M		7 1 2	57.98
1.5854M	9	-1 2 3	58.14
1.5854M		3 5 2	58.14
1.5807M	3	1 2 3	58.33
1.5807M		-3 0 3	58.33
1.5665	2	3 0 3	58.91
1.5531	1	7 5 0	59.47
1.5436M	3	0 7 1	59.87
1.5436M		3 7 0	59.87
1.5225	3	-3 2 3	60.79
1.5193+	8	0 3 3	60.93
1.5193+		-9 2 1	60.93
1.5101+	11	2 7 1	61.34
1.5101+		-4 1 3	61.34
1.5070M	11	0 6 2	61.48
1.5070M		9 2 1	61.48
1.5006	5	-8 0 2	61.77
1.4965	5	-7 3 2	61.96
1.4935M	8	4 1 3	62.10
1.4935M		-2 3 3	62.10
1.4800M	5	-2 6 2	62.73
1.4800M		8 0 2	62.73
1.4783	5	7 3 2	62.81
1.4514	1	-8 2 2	64.11
1.4402M	2	5 0 3	64.67
1.4402M		10 2 0	64.67
1.4282M	8	-4 7 1	65.28
1.4282M		-1 4 3	65.28
1.4245M	9	1 4 3	65.47
1.4245M		4 7 1	65.47
1.4206M	9	0 8 0	65.67
1.4206M		-10 1 1	65.67
1.4096	2	10 1 1	66.25
1.4015	2	-4 6 2	66.68
1.3931	1	4 6 2	67.14
1.3770	1L	-9 1 2	68.03
1.3720	2	3 4 3	68.31
1.3641	2	-7 6 1	68.76
1.3608	1	-1 8 1	68.95

Barium Boride, BaB_6

Synonym
Barium hexaboride

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA.

Color
Very dark gray

Structure
Cubic, Pm3m (221), Z = 1, isostructural with CaB_6. The structure was determined by Stackelberg and Neumann (1932). Keissling (1950) and Bertaut and Blum (1954) studied the hexaborides.

Lattice constant of this sample
a = 4.2624(1)Å

Volume
77.44 Å^3

Density
(calculated) 4.336 g/cm^3

Figure of merit
F_{24} = 106.1(0.009,24)

Additional pattern
PDF card 11-213 (Amendola, Polytechnic Inst. of Brooklyn, N.Y., 1959)

References

Bertaut, F. and Blum, P. (1954). Acta Crystallogr. 7, 81.

Kiessling, R. (1950). Acta. Chem. Scand. 4, 209.

Stackelberg, M. V. and Neumann, F. (1932). Z. Phys. Chem. B, 19, 314.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å
W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
4.261	54	1 0 0	20.83
3.014	100	1 1 0	29.62
2.462	45	1 1 1	36.47
2.1311	21	2 0 0	42.38
1.9069	48	2 1 0	47.65
1.7404	24	2 1 1	52.54
1.5072	9	2 2 0	61.47
1.4206	25	3 0 0	65.67
1.3480	20	3 1 0	69.70
1.2850	11	3 1 1	73.66
1.2304	2	2 2 2	77.52
1.1822	7	3 2 0	81.32
1.1393	13	3 2 1	85.08
1.0657	2	4 0 0	92.57
1.0338	10	4 1 0	96.34
1.0047	9	3 3 0	100.12
.9780	3	3 3 1	103.93
.9532	5	4 2 0	107.82
.9301	12	4 2 1	111.83
.9088	4	3 3 2	115.91
.8701	2	4 2 2	124.58
.8524	3	5 0 0	129.28
.8359	13	5 1 0	134.31
.8203	6	5 1 1	139.79

Barium Neodymium Titanium Oxide, $BaNd_2Ti_5O_{14}$

Synonym
Barium neodymium titanate

Sample
The sample was prepared at NBS from a mixture of BaO, Nd_2O_3, and TiO_2 (rutile). The mixture was heated at 1250 °C for 1 day. After being ground, the sample was heated further at 1350 °C for 4 days, ground, and heated at 1365 °C for 6 days.

Two known phases, rutile and $Ba_2Ti_9O_{20}$, were present as impurities. Corrections were made for the overlap of intensities.

Color
Colorless

Structure
Orthorhombic, Pbam (55) or Pba2 (32). The space group symmetry was determined from a single crystal by Kolar et al. (1981). Z = 4 is consistent with the density of 5.44, measured by Kolar et al. (1981).

Lattice constants of this sample
a = 12.1983(13)Å
b = 22.347(3)
c = 3.8403(6)

a/b = 0.5459
c/b = 0.1718

Volume
1046.8 Å^3

Density
(calculated) 5.643 g/cm^3
(measured) 5.44 g/cm^3 (Kolar et al., 1981)

Figure of merit
F_{30} = 50.1(0.012,50)

Additional pattern
Kolar et al. (1981)

Reference
Kolar, D., Gaberščvek, S., Volavšek, B., Parker, H. S., and Roth, R. S. (1981). J. Solid State Chem. 2, 89.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
11.20	12	0 2 0	7.89
10.73	5	1 1 0	8.23
8.25	1L	1 2 0	10.71
6.36	3	1 3 0	13.91
6.10	1	2 0 0	14.51
5.359	3	2 2 0	16.53
5.081	18	1 4 0	17.44
4.719	4	2 3 0	18.79
4.197	12	1 5 0	21.15
4.003	7	3 1 0	22.19
3.842	15	0 0 1	23.13
3.821	11	3 2 0	23.26
3.635	4	0 2 1	24.47
3.607	4	2 5 0	24.66
3.565M	1	3 3 0	24.96
3.565M		1 6 0	24.96
3.484	6	1 2 1	25.55
3.250	14	2 0 1	27.42
3.214	6	2 1 1	27.73
3.179	16	2 6 0	28.05
3.089	12	1 7 0	28.88
3.063	44	1 4 1	29.13
2.980	12	2 3 1	29.96
2.942	20	4 2 0	30.36
2.832	100	1 5 1	31.57
2.826	85	2 7 0	31.63
2.771	28	3 1 1	32.28
2.708	58	3 2 1	33.05
2.676M	13	4 4 0	33.46
2.676M		0 6 1	33.46
2.628	18	2 5 1	34.09
2.613M	27	3 3 1	34.29
2.613M		1 6 1	34.29
2.540	4	2 8 0	35.31
2.518	3	4 5 0	35.63
2.497	3	3 4 1	35.93
2.384	1	5 2 0	37.71
2.376	1L	4 1 1	37.84
2.336	6	4 2 1	38.51
2.300	8	2 9 0	39.14
2.276M	26	2 7 1	39.56
2.276M		4 3 1	39.56
2.258	1	0 8 1	39.90
2.221	4	1 8 1	40.59
2.195	11	4 4 1	41.08
2.142	6	5 5 0	42.15
2.118M	10	3 9 0	42.65
2.118M		2 8 1	42.65
2.098	18	2 10 0	43.08
2.033	1L	6 0 0	44.53
2.003	8	1 11 0	45.24
1.999	7	6 2 0	45.32
1.9730	3	2 9 1	45.96
1.9605	9	6 3 0	46.27
1.9380	8	5 7 0	46.84

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
1.9195	40	0 0 2	47.32
1.9103	16	6 4 0	47.56
1.8701M	4	5 5 1	48.65
1.8701M		1 2 2	48.65
1.8501	5	6 5 0	49.21
1.8410M	2	2 10 1	49.47
1.8410M		1 12 0	49.47
1.8309	1L	2 0 2	49.76
1.8172	3	3 11 0	50.16
1.7965M	5	6 0 1	50.78
1.7965M		1 4 2	50.78
1.7750	14	6 2 1	51.44
1.7463M	5	6 3 1	52.35
1.7463M		1 5 2	52.35
1.7306M	17	3 1 2	52.86
1.7306M		5 7 1	52.86
1.7215+	9	7 2 0	53.16
1.7215+		4 9 1	53.16
1.7167	7	3 2 2	53.32
1.7108	1L	6 4 1	53.52
1.6959M	2	7 3 0	54.03
1.6959M		2 5 2	54.03
1.6758	6	0 12 1	54.73
1.6599	6	1 12 1	55.30
1.6437+	5	6 8 0	55.89
1.6437+		2 6 2	55.89
1.6309M	2	4 10 1	56.37
1.6309M		1 7 2	56.37
1.6240M	3	4 0 2	56.63
1.6240M		7 5 0	56.63
1.6079	6	4 2 2	57.25
1.5874	30	4 3 2	58.06
1.5841M	33	5 9 1	58.19
1.5841M		3 13 0	58.19
1.5706	11	7 2 1	58.74
1.5602M	4	5 11 0	59.17
1.5602M		4 4 2	59.17
1.5564	5	1 13 1	59.33
1.5526	4	7 3 1	59.49
1.5316	1	2 8 2	60.39
1.5279	1	4 5 2	60.55
1.5249M	1L	3 7 2	60.68
1.5249M		8 0 0	60.68
1.5039	1L	6 10 0	61.62
1.4937	1	8 3 0	62.09

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
1.4859	3	3 14 0	62.45
1.4741+	3	0 14 1	63.01
1.4741+		2 9 2	63.01
1.4686	3	4 12 1	63.27
1.4559+	1	0 10 2	63.89
1.4559+		6 9 1	63.89
1.4429	1L	8 5 0	64.53
1.4293	1	5 5 2	65.22
1.4235	1	3 9 2	65.52
1.3962M	2	0 16 0	66.97
1.3962M		6 0 2	66.97
1.3856M	8	3 14 1	67.55
1.3856M		6 2 2	67.55
1.3761	4	8 7 0	68.08
1.3722	6	6 3 2	68.30
1.3640	4	5 7 2	68.77

Barium Tungsten Oxide, Ba_3WO_6

Synonyms
Barium tungstate
Tribarium tungstate

Sample
The sample was prepared at NBS by T. Negas from spectrographic grade $BaCO_3$ and WO_3 (73:27 mol ratio). It was heated in a Au crucible in air at 950 °C for 48 hours. This sample is approximately 2 mol % richer in WO_3 than the true 3:1 oxide.

Color
Colorless

Structure
Cubic, Fm3m (225), Z = 32. Negas (private communication, 1982).

Lattice constants of this sample
a = 17.1765(5)Å

Comment
There are 4 lines with $I_{rel} \approx 1$ that do not index satisfactorily on this unit cell. Several unit cells have been reported in the literature for Ba_3WO_6; Kreidler (1972), Kovba et al. (1971), and Steward and Rooksby (1951). None of the unit cell values reported by these authors will adequately index their data. Some of these patterns appear to be mixed with the off stoichiometric phase reported here. Structural data for the true 3:1 oxide have not been published.

Volume
5067.6 Å^3

Density
(calculated) 7.254 g/cm^3 (based on 3:1 ratio)

Figure of merit
F_{30} = 68.2(0.012,38)

Additional patterns
PDF card 25-82 (Kreidler, 1972)

PDF card 26-195 (Kovba et al., 1971)

Chang et al., (1966)

References
Chang, L. L. Y., Scroger, M. G., and Phillips, B. (1966). J. Am. Ceram. Soc. 49, No. 7.

Kovba, L. M., Lykova, L. N., and Shevchenko, N. N. (1971). Russ. J. Inorg. Chem. 16, 1150.

Kreidler, E. (1972). J. Am. Chem. Soc. 55, No. 10.

Steward, E. G. and Rooksby, H. P. (1951). Acta Crystallogr. 4, 503.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.40388 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
9.89	2	1 1 1	8.93
6.075	2	2 2 0	14.57
4.962	9	2 2 2	17.86
4.296	5	4 0 0	20.66
3.942	3	3 3 1	22.54
3.509	5	4 2 2	25.36
3.307	25	5 1 1	26.94
3.036	100	4 4 0	29.40
2.905	1	5 3 1	30.75
2.863	3	6 0 0	31.22
2.716	1	6 2 0	32.95
2.620	2	5 3 3	34.20
2.590	8	6 2 2	34.60
2.405	3	5 5 1	37.36
2.236	14	7 3 1	40.30
2.146	17	8 0 0	42.07
2.084	1L	6 4 4	43.39
2.024	3	6 6 0	44.73
1.9841	5	7 5 1	45.69
1.9694	5	6 6 2	46.05
1.9206	4	8 4 0	47.29
1.8850	1	7 5 3	48.24
1.8737	2	8 4 2	48.55
1.8306	1L	6 6 4	49.77
1.8005	4	9 3 1	50.66
1.7522	21	8 4 4	52.16
1.7261	1	7 7 1	53.01
1.6840	2	10 2 0	54.44
1.6602	9	9 5 1	55.29
1.6522	6	10 2 2	55.58
1.6018	1	9 5 3	57.49
1.5949	1L	10 4 0	57.76
1.5486	1L	7 7 5	59.66
1.5179	7	8 8 0	60.99
1.5009	1	9 5 5	61.76
1.4952	1L	10 4 4	62.02
1.4567	3	9 7 3	63.85
1.4516	7	10 6 2	64.10
1.4313	2	12 0 0	65.12
1.4166	1	11 5 1	65.88
1.3934	3	10 6 4	67.12
1.3797	1L	11 5 3	67.88
1.3457	7	9 9 1	69.84
1.3415	1L	10 8 0	70.09
1.3134	2	13 1 1	71.82

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.3097	2	10 6 6	72.05
1.2840	1	13 3 1	73.73
1.2665	1	12 6 2	74.92
1.2564	2	13 3 3	75.63
1.2397	2	8 8 8	76.83
1.2301	1	13 5 1	77.54
1.2145	1L	10 10 0	78.73
1.2055	1	13 5 3	79.43
1.2024	4	10 10 2	79.68
1.1908	1	12 8 0	80.61
1.1826	2	11 9 3	81.29
1.1797	1	14 4 0	81.53
1.1687	1	14 4 2	82.46
1.1607	1	13 7 1	83.16
1.1476	3	12 8 4	84.32
1.1401	2	15 1 1	85.01
1.1277	1	14 6 0	86.17
1.1181	4	14 6 2	87.09

Beryllium Carbide, Be_2C

CAS registry no.
506-66-1

Sample
The compound was obtained from Alfa Products, Thiokol/Ventron Division, Beverly, MA.

Color
Grayish yellow brown

Structure
Cubic, Fm3m (225), Z = 4. The structure was determined qualitatively by Stachelberg and Quantran (1934).

Lattice constant of this sample
a = 4.3422(1) Å

Volume
81.872 Å^3

Density
(calculated) 2.437 g/cm^3

Figure of merit
F_{10} = 152.3(0.007,10)

Additional pattern
PDF card 9-196 (Staritzky, 1956)

References
Stachelberg, M. v. and Quantran, F. (1934). Z. Phys. Chem. Leipzig B27, 50.

Staritzky, E. (1956). Anal. Chem. 28, 915.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
2.5069	100	1 1 1	35.79
2.1712	1L	2 0 0	41.56
1.5355	75	2 2 0	60.22
1.3092	12	3 1 1	72.08
1.2537	1L	2 2 2	75.82
1.0856	10	4 0 0	90.40
.9961	6	3 3 1	101.30
.9709	1L	4 2 0	105.00
.8864	31	4 2 2	120.69
.8356	7	5 1 1	134.39

Cadmium Iodide, α-CdI_2

CAS registry no.
7790-80-9

Sample
The sample was obtained from J. T. Baker Chemical Co., Phillipsburg, N.J.

Color
Colorless

Structure
Hexagonal, $P6_3mc$ (186), Z = 2. The structure was qualitatively done by Mitchell (1965). This is the 4H polytype encountered most frequently.

Lattice constants of this sample
a = 4.2481(3)Å
c = 13.7265(8)

c/a = 3.2312

Volume
214.53 Å^3

Density
(calculated) 5.669 g/cm^3

Polymorphism
Mitchell (1965) reports the existence of 32 polytypes. Structural data have been reported for 10 polytypes from 2H to 14H where the number indicates the number of iodine layers within the repeat distance above the c axis.

Figure of merit
F_{30} = 26.2(0.012,92)

Additional patterns
PDF card 3-470 (Dow Chemical Co., Midland, MI)

PDF card 12-573 (Institute of Physics, University College, Cardiff, Wales, 1962)

Reference
Mitchell, R. S. (1965). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 108, 296.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
6.87	100	0 0 2	12.88
3.433	40	0 0 4	25.93
3.245	38	1 0 2	27.46
2.868	16	1 0 3	31.16
2.287	7	0 0 6	39.36
2.201	7	1 0 5	40.97
2.124	91	1 1 0	42.52
2.030	16	1 1 2	44.61
1.9435	3	1 0 6	46.70
1.8061	15	1 1 4	50.49
1.7779	8	2 0 2	51.35
1.7159	19	0 0 8	53.35
1.5564	3	1 1 6	59.33
1.3725	2	0 0 10	68.28
1.3622	5	2 1 2	68.87
1.3347	20	1 1 8	70.50
1.2859	1L	1 0 10	73.60
1.2263	6	3 0 0	77.83
1.1820	2	1 0 11	81.34
1.1530	2	1 1 10	83.84
1.1441	1L	0 0 12	84.64
1.0621	3	2 2 0	92.98
1.0146	1	2 2 4	98.79
1.0070	3	1 1 12	99.80
.9977	4	3 0 8	101.08
.9806	1L	0 0 14	103.54
.9780	1L	3 1 4	103.93
.9474	1L	1 0 14	108.79
.9030	2	2 2 8	117.09
.8578	1L	0 0 16	127.79

Calcium Aluminum Oxide Hydrate, $Ca_4Al_6O_{13}\cdot 3H_2O$

Synonym
Tetracalcium trialuminate trihydrate

CAS registry no.
12355-68-9

Sample
The sample was made by J. Waring by hydrothermal reaction in an autoclave at 375 °C for 4 days. It had a few percent of impurity; therefore, the intensities may be slightly in error.

Color
Colorless

Structure
Orthorhombic, Ab2a (41), Z = 4. (Percival and Taylor, 1961).

Lattice constants of this sample
a = 12.422(3)Å
b = 12.803(3)
c = 8.862(2)

a/b = 0.9702
c/b = 0.6922

Volume
1409.45 Å^3

Density
(calculated) 2.753 g/cm^3

Figure of merit
F_{30} = 52.8(0.014,41)

Additional patterns
PDF card 14-464 (Pistorius, 1962)

PDF card 16-49 (Percival and Taylor, 1961)

PDF card 24-178 (Ponomarer et al., 1970)

Johnson and Thorvaldson, (1943)

References
Johnson, H. and Thorvaldson, T. (1943). Can. J. Res. B21, 236.

Percival, A. and Taylor, H. F. W. (1961). Acta Crystallogr. 14, 324.

Pistorius, C. W. F. T. (1962). Amer. J. Sci. 260, 221.

Ponomarer, V. I., Litvin, B. N., and Belov, N. V. (1970). Inorg. Mater. Engl. Transl. 6, 1459.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
4.432	5	0 0 2	20.02
3.639	38	0 2 2	24.44
3.602M	100	2 0 2	24.70
3.602M		3 1 1	24.70
3.493	17	1 2 2	25.48
3.270	86	2 3 1	27.25
3.199	2	0 4 0	27.87
3.141	14	2 2 2	28.39
3.103	1	4 0 0	28.75
3.028	44	3 0 2	29.48
2.846	46	2 4 0	31.41
2.820	72	3 3 1	31.70
2.805	83	1 1 3	31.88
2.797	81	4 2 0	31.97
2.734	4	3 2 2	32.73
2.612	21	2 1 3	34.31
2.594	13	0 4 2	34.55
2.541M	31	4 0 2	35.29
2.541M		1 4 2	35.29
2.416	15	4 3 1	37.18
2.392	11	2 4 2	37.57
2.383	11	1 3 3	37.72
2.364	8	4 2 2	38.04
2.351	8	5 1 1	38.25
2.287	38	2 5 1	39.36
2.261	2	2 3 3	39.83
2.229	33	4 4 0	40.44
2.216	9	0 0 4	40.69
2.199	1	3 4 2	41.02
2.181	7	1 0 4	41.36
2.167	14	5 0 2	41.64
2.133	5	0 6 0	42.33
2.115	2	3 5 1	42.72
2.094M	38	3 3 3	43.17
2.094M		0 2 4	43.17
2.087M	44	5 3 1	43.32
2.087M		2 0 4	43.32
2.069	16	6 0 0	43.71
2.065	17	1 2 4	43.80
2.019	1L	2 6 0	44.85
1.985	4	2 2 4	45.67
1.970	3	6 2 0	46.03
1.928	6	4 5 1	47.11
1.913M	11	4 3 3	47.49
1.913M		1 5 3	47.49

Calcium Aluminum Oxide Hydrate, $Ca_4Al_6O_{13}\cdot 3H_2O$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 4$	hkℓ	2θ(°)
1.875	1	6 0 2	48.51
1.8368	5	2 6 2	49.59
1.8237	1	6 3 1	49.97
1.8005	9	5 4 2	50.66
1.7737	2	1 7 1	51.48
1.7435	8	3 6 2	52.44
1.7395M	11	6 4 0	52.57
1.7395M		1 1 5	52.57
1.7245	2	7 1 1	53.06

Calcium Aluminum Silicate Hydrate, Chabazite, $Ca_2Al_4Si_8O_{24}\cdot 12H_2O$

Synonym
Calcium aluminosilicate hexahydrate

CAS registry no.
12251-32-0

Sample
The sample, a natural mineral, from Wasson's Bluff, Nova Scotia, Canada, was obtained from F. G. Gardinier.

Chemical Analysis (wt. %)
Ca 6.12%, Al 9.67%, Si 22.17%, Na 0.55%, K 0.86%, Sr 0.10%, Fe 0.043%, H_2O 22.48%

Color
Colorless to salmon pink

Structure
Rhombohedral, $R\bar{3}m$ (166) (Calligaris et al., 1982). Single crystal studies (Himes and Mighell, 1981) were carried out on a clear single crystal selected from the sample. A primitive cell was determined with lattice parameters: a = 9.3799(14)Å, b = 9.3926(14), c = 3918(14), α = 94.263(12)°, β = 94.408(12), γ = 94.469(12). This cell differs only slightly from the reduced form of the hexagonal cell given below.

Lattice constants of this sample
Hexagonal axes
a = 13.784(2)Å
c = 14.993(3)

c/a = 1.0877
Z = 3

Volume
2467.0 Å^3

Density
(calculated) 2.045 g/cm^3
(observed) 2.05(2) (Himes and Mighell, 1981)

Figure of merit
F_{30} = 65.0(0.012,38)

Additional pattern
PDF card 19-208 (Gude and Sheppard, 1966)

References
Calligaris, M., Nardin, G., Randaccio, L., and Chiaramonti, P. C. (1982). Acta Crystallogr. B38, 602.

Gude, A. J. and Sheppard, R. A. (1966). Amer. Mineral. 51, 909.

Himes, V. and Mighell, A. (1981). Private communication.

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

d(Å)	I^{rel} σ = ±3	hkℓ			2θ(°)
9.34	54	1	0	1	9.46
6.89	13	1	1	0	12.83
6.36	7	0	1	2	13.92
5.552	26	0	2	1	15.95
5.001	29	0	0	3	17.72
4.667	6	2	0	2	19.00
4.323	100	2	1	1	20.53
4.053	2	1	1	3	21.91
3.978	4	3	0	0	22.33
3.865	21	1	2	2	22.99
3.576	42	1	0	4	24.88
3.446	19	2	2	0	25.83
3.236	5	1	3	1	27.54
3.176	11	0	2	4	28.07
2.927	93	4	0	1	30.52
2.908	21	0	1	5	30.72
2.882	45	2	1	4	31.01
2.838	6	2	2	3	31.50
2.775	4	0	4	2	32.23
2.693	4	3	2	1	33.24
2.678	9	2	0	5	33.43
2.606	20	4	1	0	34.39
2.572	4	2	3	2	34.85
2.497M	21	0	0	6	35.94
2.497M		1	2	5	35.94
2.351	3	1	1	6	38.26
2.310	4	4	1	3	38.96
2.298	5	3	3	0	39.17
2.275	3	5	0	2	39.58
2.231	1L	2	4	1	40.40
2.159	2	4	2	2	41.80
2.122	1	5	1	1	42.57
2.087	9	3	3	3	43.33
2.060	1	1	5	2	43.91
2.013	1	0	5	4	44.99
1.9455	1L	4	3	1	46.65
1.9126	2	5	2	0	47.50
1.8664	9	5	0	5	48.75
1.8515	4	0	1	8	49.17
1.8035M	18	4	1	6	50.57
1.8035M		4	2	5	50.57
1.7857	2	5	2	3	51.11
1.7689	3	6	1	2	51.63
1.7306	6	1	2	8	52.86
1.7236	10	4	4	0	53.09

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.6921	4	3 3 6	54.16
1.6660	4	0 0 9	55.08
1.6454	7	6 2 1	55.83
1.5864	2	0 4 8	58.10
1.5559M	7	6 0 6	59.35
1.5559M		6 1 5	59.35
1.5204	3	5 4 1	60.88
1.5155	4	5 1 7	61.10

Calcium Silicate (Larnite), β-Ca_2SiO_4

Synonyms
Beta dicalcium silicate
Belite

CAS registry no.
10034-77-2

Sample
The sample was made at the Portland Cement Association Laboratory. $CaCO_3$ and SiO_2 with 0.5% B_2O_3 were heated at 900 °C for 20 minutes, raised to 1450 °C over 45 minutes, heated for 20 minutes and air quenched. PCA #102381-1.

Chemical analysis
Wt%: SiO_2, 34.56; Al_2O_3, 0.17; Fe_2O_3, 0.03; CaO, 64.24; SO_3, 0.18; Na_2O, 0.33; K_2O, 0.01; TiO_2, 0.01; B_2O_3, 0.18.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure of β-Ca_2SiO_4 was determined by Midgley (1952).

Lattice constants of this sample
a = 9.310(2)Å
b = 6.7565(10)
c = 5.5059(11)
β = 94.46(2)°

a/b = 1.3779
c/b = 0.8149

Volume
345.29 Å^3

Density
(calculated) 3.313 g/cm^3

Polymorphism
There are a number of forms of Ca_2SiO_4. The beta form is unstable when it is pure. The present sample was stabilized by 0.18% B_2O_3.

Figure of merit
F_{30} = 54.5(0.013,43)

Additional patterns
PDF card 9-351 (Yannaquis, 1955)

PDF card 29-371 (Smith and Fausey, 1977) (calculated)

Brownmiller and Bogue, (1930)

References

Brownmiller, T. and Bogue, R. H. (1930). Amer. J. Sci. 20, 241.

Midgley, C. (1952). Acta Crystallogr. 5, 307.

Smith, D. and Fausey, (1977). Annual Report to the Joint Committee on Powder Diffraction Standards.

Yannaquis, N. (1955). Rev. Mater. Constr. Trav. Publics 1955, 213.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
4.892	3	-1 0 1	18.12
4.641	9	2 0 0	19.11
3.824	5	2 1 0	23.24
3.786	5	1 1 1	23.48
3.378	7	0 2 0	26.36
3.241	6	-2 1 1	27.50
3.176	5	1 2 0	28.07
3.049	9	2 1 1	29.27
2.877	21	0 2 1	31.06
2.814	22	3 1 0	31.77
2.790	97	-3 0 1	32.05
2.783	100	-1 2 1	32.14
2.745	83	0 0 2	32.59
2.718	30	1 2 1	32.93
2.610	42	3 0 1	34.33
2.545	9	0 1 2	35.24
2.448	12	-2 0 2	36.68
2.433	9	3 1 1	36.91
2.410	13	1 1 2	37.28
2.403	18	2 2 1	37.40
2.323	2	4 0 0	38.74
2.301	4	-2 1 2	39.12
2.281	22	3 2 0	39.48
2.189	51	1 3 0	41.21
2.165	13	2 1 2	41.69
2.129	7	0 2 2	42.42
2.103	1	-1 2 2	42.97
2.091	6	-4 1 1	43.24
2.083	6	0 3 1	43.40
2.050	14	1 2 2	44.15
2.037	9	-3 1 2	44.43
2.027	15	2 3 0	44.68
2.020	15	1 3 1	44.83
1.987	20	4 1 1	45.61
1.982	24	-2 2 2	45.75
1.9115	6	4 2 0	47.53
1.8979	9	3 1 2	47.89
1.8935	11	2 2 2	48.01
1.8441	4	-4 0 2	49.38
1.8441M		-4 2 1	49.38
1.8210	3	3 3 0	50.05
1.8051	9	-3 2 2	50.52
1.8018	9	-5 0 1	50.62
1.7899	7	5 1 0	50.98
1.7657	1	0 1 3	51.73

Calcium Silicate, (Larnite), β-Ca_2SiO_4 - (continued)

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
1.7270	5	-1 3 2	52.98
1.7067	10	3 2 2	53.66
1.6964	5	1 3 2	54.01
1.6889	5	0 4 0	54.27
1.6282	12	5 2 0	56.47
1.6146	8	0 4 1	56.99
1.6110	10	2 1 3	57.13
1.6040M	11	2 3 2	57.40
1.6040M		-1 2 3	57.40
1.5874	6	2 4 0	58.06
1.5839	7	1 4 1	58.20
1.5738	5	-4 3 1	58.61

Calcium Silicon Fluoride Hydrate, $CaSiF_6 \cdot 2H_2O$

Synonym
Calcium fluorosilicate dihydrate

CAS registry no.
16961-80-1

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The cell was obtained by using the Visser program (1969). The space group was assumed by a study of the extinctions.

Lattice constants of this sample
a = 10.477(2)Å
b = 9.1771(13)
c = 5.7281(13)
β = 98.98(2)°

a/b = 1.1416
c/b = 0.6242

Volume
543.99 Å^3

Density
(calculated) 2.664 g/cm^3

Figure of merit
F_{30} = 47.1(0.013,49)
M_{20} = 29.4

Additional pattern
PDF card 1-227 (Hanawalt et al., 1938)

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

Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.85	16	1 1 0	12.91
5.323	43	-1 0 1	16.64
5.166	5	2 0 0	17.15
4.810	23	0 1 1	18.43
4.598M	16	-1 1 1	19.29
4.598M		0 2 0	19.29
4.503	9	2 1 0	19.70
4.195	27	1 2 0	21.16
4.160	21	1 1 1	21.34
3.783	19	-2 1 1	23.50
3.432	100	2 2 0	25.94
3.311	41	2 1 1	26.91
3.271	13	1 2 1	27.24
3.228	3	3 1 0	27.61
3.172	17	-3 0 1	28.11
3.079	12	-2 2 1	28.98
3.000	13	-3 1 1	29.76
2.932	4	1 3 0	30.46
2.757M	5	3 0 1	32.45
2.757M		3 2 0	32.45
2.717	9	-1 1 2	32.94
2.703	11	0 1 2	33.11
2.690	10	0 3 1	33.28
2.652	10	-1 3 1	33.77
2.633	3	2 3 0	34.02
2.559M	2	1 3 1	35.04
2.559M		-2 1 2	35.04
2.491	4	4 1 0	36.03
2.417M	6	-1 2 2	37.17
2.417M		-4 1 1	37.17
2.334	7	2 0 2	38.55
2.318	6	2 3 1	38.82
2.303M	15	-2 2 2	39.08
2.303M		-3 1 2	39.08
2.293	14	0 4 0	39.25
2.279	6	1 2 2	39.51
2.261	20	2 1 2	39.83
2.252	14	4 2 0	40.00
2.239	23	1 4 0	40.24
2.199	8	-4 2 1	41.01
2.164	1	4 1 1	41.71
2.127	4	0 4 1	42.47
2.110	24	-3 2 2	42.83
2.084	2	-1 3 2	43.39
2.079M	3	2 2 2	43.50
2.079M		-4 0 2	43.50
2.060	3	1 4 1	43.92
2.049M	13	-5 0 1	44.16
2.049M		3 3 1	44.16
2.020	4	5 1 0	44.84
2.009M	13	-2 3 2	45.09
2.009M		-2 4 1	45.09
1.992	13	1 3 2	45.50
1.976	15	4 3 0	45.89
1.9103	26	3 4 0	47.56

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.8865	17	5 2 0	48.20
1.8777	13	-3 3 2	48.44
1.8711	11	-5 2 1	48.62
1.8614	9	3 2 2	48.89
1.8565	4	2 3 2	49.03
1.7998	19	4 3 1	50.68
1.7860	2	-1 4 2	51.10
1.7760+	10	-5 1 2	51.41
1.7760+		4 0 2	51.41
1.7638	6	3 4 1	51.79
1.7438+	13	0 2 3	52.43
1.7438+		4 1 2	52.43
1.7285	11	1 4 2	52.93
1.7144	9	5 3 0	53.40
1.7034	6	-5 3 1	53.77
1.6944M	16	3 3 2	54.08
1.6944M		6 1 0	54.08
1.6921	14	-4 4 1	54.16
1.6566M	1	4 2 2	55.42
1.6566M		-3 2 3	55.42
1.6312	3	2 5 1	56.36
1.5947	2	-2 3 3	57.77
1.5849M	5	2 2 3	58.16
1.5849M		5 3 1	58.16
1.5597	5	6 1 1	59.19
1.5554M	3	3 0 3	59.37
1.5554M		1 3 3	59.37
1.5288M	4	-5 4 1	60.51
1.5288M		3 5 1	60.51
1.5117	3	-2 5 2	61.27
1.4998	1	-6 2 2	61.81
1.4424	5	2 5 2	64.56
1.4354	4	-2 6 1	64.91
1.4145M	5	-1 1 4	65.99
1.4145M		0 0 4	65.99
1.4045+	1	2 6 1	66.52
1.4045+		4 4 2	66.52
1.3871M	3	-7 1 2	67.47
1.3871M		3 3 3	67.47
1.3756	3	-4 5 2	68.11
1.3638M	3	3 5 2	68.78
1.3638M		7 1 1	68.78

Cesium Iodide, CsI_3

Synonym
Cesium triiodide

CAS registry no.
12527-22-9

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA. The sample decomposed slowly in the open air.

Color
Unground: dark purplish blue.
Ground: dark grayish reddish brown.

Structure
Orthorhombic, Pbnm (62), Z = 4. The structure was determined by Tasman and Boswijk (1955).

Lattice constants of this sample
a = 10.0289(9)Å
b = 11.0869(9)
c = 6.8457(8)

a/b = 0.9062
c/b = 0.6186

Volume
761.17 Å^3

Density
(calculated) 4.482 g/cm^3

Figure of merit
F_{30} = 83.5(0.007,50)

Reference
Tasman, H. A. and Boswijk, K. W. (1955). Acta Crystallogr. 8, 59.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
5.658	5	1 0 1	15.65
5.542	4	0 2 0	15.98
5.035	7	1 1 1	17.60
3.959	36	1 2 1	22.44
3.800	43	2 1 1	23.39
3.720	15	2 2 0	23.90
3.468	20	1 3 0	25.67
3.423	79	0 0 2	26.01
3.268	100	2 2 1	27.27
3.093	10	1 3 1	28.84
3.004	10	3 0 1	29.72
2.899	11	3 1 1	30.82
2.863	14	3 2 0	31.22
2.826	4	2 0 2	31.63
2.772	12	0 4 0	32.27
2.729	30	2 3 1	32.79
2.671	9	1 4 0	33.52
2.5687	5	0 4 1	34.90
2.5185	9	2 2 2	35.62
2.4781	1	3 3 0	36.22
2.4461	13	4 1 0	36.71
2.4372	12	1 3 2	36.85
2.4264	5	2 4 0	37.02
2.3312	4	3 3 1	38.59
2.3036	2	4 1 1	39.07
2.2846M	2	2 4 1	39.41
2.2846M		4 2 0	39.41
2.1960	10	3 2 2	41.07
2.1662M	10	4 2 1	41.66
2.1662M		1 5 0	41.66
2.1544	10	0 4 2	41.90
2.1339	5	3 4 0	42.32
2.1060	8	1 4 2	42.91
2.0751	5	4 3 0	43.58
2.0652M	6	1 2 3	43.80
2.0652M		1 5 1	43.80
2.0417	7	2 1 3	44.33
2.0231	2	4 0 2	44.76
2.0082	1	3 3 2	45.11
1.9898	12	4 1 2	45.55
1.9853	11	4 3 1	45.66
1.9796	5	2 4 2	45.80
1.9451M	17	2 2 3	46.66
1.9451M		2 5 1	46.66
1.9248	5	5 0 1	47.18
1.9054	3	1 3 3	47.69
1.9002	4	4 2 2	47.83
1.8957	4	5 1 1	47.95
1.8850M	5	5 2 0	48.24
1.8850M		3 0 3	48.24
1.8575	3	3 1 3	49.00
1.8476M	1	3 5 0	49.28
1.8476M		0 6 0	49.28
1.8295	6	1 5 2	49.80
1.8172M	5	5 2 1	50.16
1.8172M		1 6 0	50.16
1.8105M	10	3 4 2	50.36
1.8105M		2 3 3	50.36
1.7945	11	4 4 1	50.84
1.7847M	5	3 2 3	51.14
1.7847M		3 5 1	51.14
1.7737	3	4 3 2	51.48
1.7566	7	1 6 1	52.02
1.7336	2	2 6 0	52.76
1.7111	8	0 0 4	53.51

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.6607	2	4 5 0	55.27
1.6524M	4	6 1 0	55.57
1.6524M		5 2 2	55.57
1.6144+	2	4 2 3	57.00
1.6144+		4 5 1	57.00
1.6064	3	6 1 1	57.31
1.5809	2	5 4 1	58.32
1.5465	2	2 6 2	59.75
1.5346M	2	4 3 3	60.26
1.5346M		1 3 4	60.26
1.5247	2	1 7 1	60.69
1.5068	2	5 0 3	61.49
1.4945	3	4 5 2	62.05
1.4881+	4	6 1 2	62.35
1.4881+		5 5 0	62.35
1.4753	1	2 7 1	62.95
1.4688	2	3 2 4	63.26
1.4561	2	0 4 4	63.88
1.4530M	1	5 5 1	64.03
1.4530M		4 6 1	64.03
1.4500	1	6 2 2	64.18
1.4416M	5	4 4 3	64.60
1.4416M		1 4 4	64.60
1.4360M	6	3 5 3	64.88
1.4360M		0 6 3	64.88
1.4212M	3	1 6 3	65.64
1.4212M		7 1 0	65.64
1.4015M	4	4 1 4	66.68
1.4015M		3 7 1	66.68

Cesium Molybdenum Oxide, $Cs_2Mo_3O_{10}$

Synonyms
Cesium molybdate
Dicesium trimolybdate

Sample
The sample was prepared using cesium carbonate and molybdic anhydride. Appropriate amounts were blended by grinding in an agate mortar under acetone. The dried mixture was heated at 500 °C for a total of 16 hours with periodic grinding. After the last heating, the sample was ground to pass a 100 mesh sieve, and the resulting powder was annealed at 240 °C for 19 hours.

Color
Colorless

Structure
Monoclinic, C2/c (15), Z = 4, isostructural with $K_2Mo_3O_{10}$. The structure of $K_2Mo_3O_{10}$ was determined by Gatehouse and Leverett (1968).

Lattice constants of this sample
a = 14.469(2)Å
b = 8.4022(9)
c = 9.4609(14)
β = 97.73(1)°

a/b = 1.7220
c/b = 1.1260

Volume
1139.7 Å^3

Density
(calculated) 4.159 g/cm^3

Figure of merit
F_{30} = 94.2(0.008,42)

Additional pattern
PDF card 24-277 (Salmon and Caillet, 1969)

References
Gatehouse, B. M. and Leverett, P. (1968). J. Chem. Soc. A, 1398.

Salmon, R. and Caillet, P. (1969). Bull. Soc. Chim. Fr., 1569.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
7.237	17	1 1 0	12.22
5.933	18	-1 1 1	14.92
5.552	19	1 1 1	15.95
4.199	47	0 2 0	21.14
4.155	18	3 1 0	21.37
4.064	8	-1 1 2	21.85
3.975	13	-3 1 1	22.35
3.823	100	1 1 2	23.25
3.699	34	2 0 2	24.04
3.644	88	3 1 1	24.41
3.625	35	2 2 0	24.54
3.586	15	4 0 0	24.81
3.462	93	-2 2 1	25.71
3.306M	14	-3 1 2	26.95
3.306M		2 2 1	26.95
3.127	19	0 2 2	28.52
3.052	50	-4 0 2	29.24
2.966	45	-2 2 2	30.11
2.942M	41	-1 1 3	30.36
2.942M		3 1 2	30.36
2.801	2	1 1 3	31.93
2.778	2	2 2 2	32.20
2.749	5	1 3 0	32.55
2.727	18	4 2 0	32.82
2.715	32	5 1 0	32.97
2.694	4	-4 2 1	33.23
2.657	3	-1 3 1	33.71
2.620	11	1 3 1	34.20
2.548	3	4 2 1	35.20
2.470	7	-4 2 2	36.35
2.451	4	-2 2 3	36.64
2.416	1	3 3 0	37.18
2.3903	5	6 0 0	37.60
2.3031	20	3 3 1	39.08
2.2762	25	-1 1 4	39.56
2.2565	12	-6 0 2	39.92
2.2287	5	5 1 2	40.44
2.1909	1L	-5 1 3	41.17
2.1868	2	1 1 4	41.25
2.1677	13	-4 2 3	41.63
2.1514	6	-3 1 4	41.96
2.1456	8	2 0 4	42.08
2.0902M	6	-1 3 3	43.25
2.0902M		3 3 2	43.25
2.0801	7	-6 2 1	43.47

d(Å)	I^{rel}	hkℓ	2θ(°)
	σ = ±4		
2.0497	11	0 4 1	44.15
2.0457	3	0 2 4	44.24
2.0382	29	1 3 3	44.41
2.0223	10	6 0 2	44.78
2.0167	6	2 4 0	44.91
1.9994M	19	-7 1 1	45.32
1.9994M		-5 3 1	45.32
1.9861M	10	-6 2 2	45.64
1.9861M		-2 4 1	45.64
1.9562	8	2 4 1	46.38
1.9463	6	3 1 4	46.63
1.9310	7	5 1 3	47.02
1.9225	11	5 3 1	47.24
1.8972M	4	-5 1 4	47.91
1.8972M		7 1 1	47.91
1.8773	3	-2 4 2	48.45
1.8515M	8	3 3 3	49.17
1.8515M		4 0 4	49.17
1.8312	2	-6 2 3	49.75
1.8268	2	2 4 2	49.88
1.8122	1L	4 4 0	50.31
1.7978	4	-6 0 4	50.74
1.7873M	7	-7 1 3	51.06
1.7873M		1 1 5	51.06
1.7644	1	-5 3 3	51.77
1.7622	1	1 3 4	51.84
1.7512	3	7 1 2	52.19
1.7129M	1L	-2 2 5	53.45
1.7129M		0 2 5	53.45
1.6938	4	4 2 4	54.10
1.6596M	8	-7 3 1	55.31
1.6596M		-8 2 1	55.31
1.6538M	11	-6 2 4	55.52
1.6538M		7 3 0	55.52
1.6489M	9	8 2 0	55.70
1.6489M		-1 5 1	55.70
1.6435M	5	6 2 3	55.90
1.6435M		-5 1 5	55.90
1.6193M	7	-8 2 2	56.81
1.6193M		5 3 3	56.81
1.6162	15	-4 4 3	56.93
1.5987M	8	-5 3 4	57.61
1.5987M		7 3 1	57.61
1.5896	4	8 2 1	57.97
1.5854	4	3 5 0	58.14
1.5787M	6	-6 4 1	58.41
1.5787M		-9 1 1	58.41
1.5643M	7	1 5 2	59.00
1.5643M		0 4 4	59.00
1.5516	6	3 5 1	59.53

d(Å)	I^{rel}	hkℓ	2θ(°)
	σ = ±4		
1.5476	5	-9 1 2	59.70
1.5385	6	-8 2 3	60.09
1.5332M	10	6 4 1	60.32
1.5332M		-3 3 5	60.32
1.5227+	5	-3 5 2	60.78
1.5227+		-3 1 6	60.78
1.5114	2	9 1 1	61.28
1.4982	1	8 2 2	61.88
1.4853	3	2 0 6	62.48
1.4816M	5	-1 5 3	62.65
1.4816M		3 5 2	62.65
1.4718M	1L	-2 2 6	63.12
1.4718M		6 2 4	63.12
1.4634M	4	-7 1 5	63.52
1.4634M		1 5 3	63.52
1.4612	4	-6 4 3	63.63
1.4496	1L	5 5 0	64.20
1.4398	1	-3 5 3	64.69

Chromium Boride, CrB_2

Synonym
Chromium diboride

CAS registry no.
12007-16-8

Sample
The sample was obtained from the Metallurgy group at NBS. A small admixture of Cr was removed by sieving.

Color
Olive gray

Structure
Hexagonal, P6/mmm (191), Z = 1, (PDF card 8-119).

Lattice constants of this sample
a = 2.9730(13)Å
c = 3.0709(2)

c/a = 1.0329

Volume
23.506 $Å^3$

Density
(calculated) 5.200 g/cm^3

Figure of merit
F_{20} = 94.4(0.011,20)

Additional pattern
PDF card 8-119 (Paretzkin, 1956, Polytechnic Institute of Brooklyn, Brooklyn, NY.)

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
3.071	20	0 0 1	29.05
2.574	57	1 0 0	34.82
1.9730	100	1 0 1	45.96
1.5355	10	0 0 2	60.22
1.4866	25	1 1 0	62.42
1.3380	14	1 1 1	70.30
1.3191	15	1 0 2	71.46
1.2871	7	2 0 0	73.52
1.1874	16	2 0 1	80.89
1.0682	16	1 1 2	92.29
1.0238	1	0 0 3	97.60
.9865	8	2 0 2	102.67
.9732	6	2 1 0	104.65
.9512	9	1 0 3	108.15
.9277	20	2 1 1	112.26
.8582	7	3 0 0	127.67
.8430	4	1 1 3	132.05
.8265	4	3 0 1	137.50
.8220	11	2 1 2	139.15
.8012	8	2 0 3	148.09

Chromium Niobium Oxide, $CrNbO_4$

Synonyms
Niobium chromium oxide
Chromium niobate

CAS registry no.
58500-35-9

Sample
Made by heating Cr_2O_3 and Nb_2O_5 at 1000 °C for 24 hours. The sample contained some Cr_2O_3.

Color
Gray olive

Structure
Tetragonal, $P4_2/mnm$ (136), Z = 1. Rutile structure (Brandt, 1943). The structure of $CrNbO_4$ is discussed by Khazai et al. (1981).

Lattice constants of this sample
a = 4.6443(2) Å
c = 3.0125(3)

c/a = 0.6486

Volume
64.977 $Å^3$

Density
(calculated) 5.338 g/cm^3

Figure of merit
F_{28} = 60.94(0.013,36)

Additional patterns
PDF card 20-311 (Young, Battelle Mem. Inst., 1964)

PDF card 31-927 (Ben-Dor and Shimony, 1978). The composition of this phase is $Cr_{0.4}Nb_{0.6}O_2$.

References
Ben-Dor, L. and Shimony, Y. (1978). J. Cryst. Growth 34, 1.

Brandt, K. (1943). Ark. Kemi Mineral. Geol. 17A, 15.

Khazai, B., Kershaw, R., Dwight, K., and Wold, A. (1981). J. Solid State Chem. 39, 395.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å			
d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
3.283	100	1 1 0	27.14
2.528	65	1 0 1	35.48
2.322	15	2 0 0	38.75
2.220	11	1 1 1	40.60
2.077	4	2 1 0	43.54
1.7102	62	2 1 1	53.54
1.6421	18	2 2 0	55.95
1.5066	7	0 0 2	61.50
1.4690	13	3 1 0	63.25
1.4419	1L	2 2 1	64.58
1.3772	17	3 0 1	68.02
1.3696	12	1 1 2	68.45
1.3204	1	3 1 1	71.38
1.2638	3	2 0 2	75.11
1.2190	1	2 1 2	78.38
1.1845	6	3 2 1	81.13
1.1614	2	4 0 0	83.10
1.1100	6	2 2 2	87.89
1.0945	3	3 3 0	89.46
1.0551	7	4 1 1	93.79
1.0516	8	3 1 2	94.19
1.0384	3	4 2 0	95.77
.9816M	2	4 2 1	103.39
.9816M		1 0 3	103.39
.9289	1	4 3 0	112.05
.9108	1L	5 1 0	115.51
.9039	3	2 1 3	116.90
.8875	4	4 3 1	120.43
.8854	4	3 3 2	120.91

Cobalt Arsenate Hydrate (Erythrite), $Co_3(AsO_4)_2 \cdot 8H_2O$

Synonym
Cobalt orthoarsenate octahydrate

CAS registry no.
54496-59-2

Sample
The sample was made by slowly adding 2 grams of $Na_2HAsO_4 \cdot 7H_2O$ dissolved in 1 liter of H_2O to 2 grams of $CoSO_4$ in 3 liters of H_2O. The liquid was kept at about 70 °C for 40 days.

Spectrographic analysis
Major impurities

0.02	to	0.1%	Ni
0.01	to	0.05%	Cu,Si
0.005	to	0.025%	Al,Fe
0.002	to	0.01%	Mn,Sn,Zn
		<0.005%	Ag,Mg

Color
Medium purplish pink

Structure
Monoclinic, I2/m (12), Z = 2. Vivianite structure (Wolfe, 1940). The structure of vivianite, $Fe_3(PO_4)_2 \cdot 8H_2O$, was discussed by Mori and Ito (1950).

Lattice constants of this sample
a = 10.118(5) Å
b = 13.433(4)
c = 4.762(2)
β = 101.90(3)°

a/b = 0.7532
c/b = 0.3545

Volume
633.32 Å^3

Density
(calculated) 3.140 g/cm^3

Comment
Note the similarity between the data above, and the data for the phase $Zn_3(AsO_4)_2 \cdot 8H_2O$, also appearing in this Monograph.

Figure of merit
F_{30} = 43.0(0.013,53)

Additional pattern
PDF card 11-626 (U.S. Bureau of Mines, Albany, OR)

References
Mori, H. and Ito, T. (1950). Acta Crystallogr. 3, 1.

Wolfe, C. W. (1940). Am. Mineral. 25, 787.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
7.96	26	1 1 0	11.11
6.72	100	0 2 0	13.17
4.951	9	2 0 0	17.90
4.602	2	-1 0 1	19.27
4.403	19	0 1 1	20.15
4.081	5	1 3 0	21.76
3.978	7	2 2 0	22.33
3.916	12	1 0 1	22.69
3.787	2	-1 2 1	23.47
3.663	7	-2 1 1	24.28
3.381	3	1 2 1	26.34
3.357	4	0 4 0	26.53
3.227	42	0 3 1	27.62
3.003	47	-3 0 1	29.73
2.779	9	2 4 0	32.18
2.740	30	-3 2 1	32.66
2.712	24	-1 4 1	33.00
2.658	14	3 3 0	33.69
2.593	1	1 5 0	34.56
2.549	9	1 4 1	35.18
2.463	18	3 0 1	36.45
2.327	17	0 5 1	38.66
2.238M	3	0 6 0	40.26
2.238M		-3 4 1	40.26
2.196	9	-2 5 1	41.06
2.094	7	-3 1 2	43.17
2.083	9	3 5 0	43.41
2.040	2	2 6 0	44.36
2.012	3	-1 6 1	45.02
1.987	5	3 4 1	45.61
1.954	7	1 3 2	46.44
1.9172	8	-3 3 2	47.38

Cobalt Phosphate Hydrate, $Co_3(PO_4)_2 \cdot 8H_2O$

Synonym
Cobalt orthophosphate octahydrate

CAS registry no.
10294-50-5

Sample
The sample was prepared by dissolving stoichiometric amounts of $CoSO_4$ and Na_2HPO_4 in water and letting the solution partly evaporate at room temperature.

Color
Unground: deep red
Ground: moderate pale red

Structure
Monoclinic, I2/m (12), Z = 2. The pattern was indexed by analogy with the pattern of the corresponding iron compound vivianite. The structure of vivianite was discussed by Mori and Ito (1950).

Lattice constants of this sample
a = 9.9265(14) Å
b = 13.3360(14)
c = 4.6786(7)
β = 102.310(12)°

a/b = 0.7443
c/b = 0.3508

Volume
605.11 Å^3

Density
(calculated) 2.804 g/cm^3

Figure of merit
F_{30} = 97.0(0.007,43)

Additional pattern
PDF card 1-0121 (Hanawalt et al., 1938)

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

Mori, H. and Ito, T. (1950). Acta Crystallogr. 3, 1.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
7.852	23	1 1 0	11.26
6.667	100	0 2 0	13.27
4.849	25	2 0 0	18.28
4.521	15	-1 0 1	19.62
4.323	6	0 1 1	20.53
4.042	15	1 3 0	21.97
3.832	23	1 0 1	23.19
3.609	5	-2 1 1	24.65
3.320	5	1 2 1	26.83
3.187	31	0 3 1	27.97
3.141	4	3 1 0	28.39
2.946	32	2 1 1	30.31
2.866	2	-2 3 1	31.18
2.749	5	2 4 0	32.55
2.698	27	-3 2 1	33.18
2.683	23	-1 4 1	33.37
2.615	11	3 3 0	34.27
2.572	5	1 5 0	34.86
2.5150	18	1 4 1	35.67
2.4981	8	2 3 1	35.92
2.4082	17	3 0 1	37.31
2.3036M	13	0 5 1	39.07
2.3036M		-1 1 2	39.07
2.2647	4	3 2 1	39.77
2.2104	12	-3 4 1	40.79
2.1727	11	-2 5 1	41.53
2.1628	6	0 2 2	41.73
2.1417	3	-2 2 2	42.16
2.0985	1	1 1 2	43.07
2.0842	2	-4 3 1	43.38
2.0576	8	3 5 0	43.97
2.0214	1	2 6 0	44.80
1.9953	3	-1 6 1	45.42
1.9530	3	4 1 1	46.46
1.9222	8	1 6 1	47.25
1.9176	11	1 3 2	47.37
1.8909	7	-3 3 2	48.08
1.8701	5	1 7 0	48.65
1.8632	2	-5 2 1	48.84
1.8424	1	2 2 2	49.43
1.8051M	3	4 3 1	50.52
1.8051M		-4 2 2	50.52
1.7785	2	5 3 0	51.33
1.7686	5	-4 5 1	51.64
1.7581M	5	0 7 1	51.97
1.7581M		-1 5 2	51.97
1.6671	9	0 8 0	55.04
1.6635M	11	5 0 1	55.17
1.6635M		1 5 2	55.17
1.6440	8	-3 5 2	55.88
1.6154	2	6 0 0	56.96
1.5904	5	3 3 2	57.94
1.5866	5	4 5 1	58.09
1.5765	2	2 8 0	58.50
1.5706	7	6 2 0	58.74

Cobalt Phosphate Hydrate, $Co_3(PO_4)_2 \cdot 8H_2O$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ			2θ(°)
1.5694	7	5	5	0	58.79
1.5645	5	-1	8	1	58.99
1.5581	2	-5	3	2	59.26
1.5367	3	-6	3	1	60.17
1.5281	3	1	8	1	60.54
1.5103	4	4	0	2	61.33
1.5079	4	-3	0	3	61.44
1.4883	2	5	4	1	62.34
1.4766	6	-6	0	2	62.89
1.4728	4	4	2	2	63.07
1.4647	3	-2	3	3	63.46
1.4518	3	2	6	2	64.09
1.4418M	2	-6	2	2	64.59
1.4418M		0	3	3	64.59
1.4352	1L	3	5	2	64.92
1.4247	2	1	2	3	65.46
1.4187	1	1	7	2	65.77
1.4115M	3	-7	0	1	66.15
1.4115M		-5	5	2	66.15
1.4094	3	0	9	1	66.26
1.3958	2	-6	5	1	66.99
1.3711M	2	4	7	1	68.36
1.3711M		3	8	1	68.36
1.3465M	1	3	9	0	69.79
1.3465M		0	8	2	69.79
1.3406	3	-2	5	3	70.14
1.3334	4	0	10	0	70.58
1.3299	4	2	9	1	70.79
1.3233M	3	0	5	3	71.20
1.3233M		7	3	0	71.20

Erbium Iron, $ErFe_2$

Synonym
Erbium diiron

CAS registry no.
12060-15-4

Sample
The sample was obtained from the Solid State Physics Division at NBS.

Color
Dark grayish olive

Structure
Cubic, Fd3m (227), Z = 8. The structure was determined by Wernick and Geller (1960).

Lattice constant of this sample
a = 7.2777(2) Å

Volume
385.46 $Å^3$

Density
(calculated) 9.614 g/cm^3

Figure of merit
F_{23} = 63.8(0.014,26)

Additional pattern
PDF card 17-32 Dwight, Met. Div., Argonne Nat. Lab., Argonne, IL.

Reference
Wernick, J. H. and Geller, S. (1960). Trans. AIME 218, 866.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
4.201	9	1 1 1	21.13
2.572	54	2 2 0	34.85
2.193	100	3 1 1	41.13
2.101	18	2 2 2	43.01
1.8193	1L	4 0 0	50.10
1.6699	5	3 3 1	54.94
1.4861	26	4 2 2	62.44
1.4006	32	5 1 1	66.73
1.2862	20	4 4 0	73.58
1.2305	3	5 3 1	77.51
1.1509	13	6 2 0	84.03
1.1098	12	5 3 3	87.91
1.0971	6	6 2 2	89.19
1.0504	1L	4 4 4	94.33
1.0190	2	5 5 1	98.21
.9726	12	6 4 2	104.74
.9476	20	7 3 1	108.76
.9096	6	8 0 0	115.75
.8892	1L	7 3 3	120.06
.8576	8	6 6 0	127.85
.8403	12	7 5 1	132.89
.8349	4	6 6 2	134.63
.7988	2	9 1 1	149.28

Ethylenediamine Hydrochloride, $C_2H_8N_2 \cdot 2HCl$

Synonyms
1,2-Ethanediamine dihydrochloride
1,2-Diaminoethane dihydrochloride
Ethylene diammonium chloride

CAS registry no.
20273-40-9

Sample
The sample was obtained from Sigma Chemical Co., St. Louis, MO. It was recrystallized from water.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14), Z = 2. The structure was determined by Ashida and Hirokawa (1963).

Lattice constants of this sample
a = 9.9683(13)Å
b = 6.8913(12)
c = 4.4293(6)
β = 91.311(12)°

a/b = 1.4465
c/b = 0.6427

Volume
304.19 Å^3

Density
(calculated) 1.452 g/cm^3

Figure of merit
F_{30} = 57.8(0.011,49)

Additional patterns
PDF card 9-580 (Brock and Hannum, 1955)

PDF card 20-1692 (Gatte, Penn. State Univ., 1967)

References
Ashida, T. and Hirokawa, S. (1963). Acta Crystallogr. 16, 841.

Brock, M. J. and Hannum, M. J. (1955). Anal. Chem. 27, 1374.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
5.669	1	1 1 0	15.62
4.427	5	0 0 1	20.04
3.725	15	0 1 1	23.87
3.466	100	1 1 1	25.68
3.350	89	-2 0 1	26.59
3.256	59	1 2 0	27.37
3.012	47	-2 1 1	29.64
2.993	86	3 1 0	29.83
2.956	59	2 1 1	30.21
2.836	25	2 2 0	31.52
2.719	47	0 2 1	32.91
2.633	10	-1 2 1	34.02
2.504	9	-3 1 1	35.83
2.491	8	4 0 0	36.03
2.458	17	3 1 1	36.53
2.401	15	-2 2 1	37.43
2.373	1L	2 2 1	37.88
2.343	20	4 1 0	38.38
2.215	6	0 0 2	40.71
2.151	9	4 0 1	41.96
2.118	6	-3 2 1	42.65
2.107	6	0 1 2	42.89
2.086	25	2 3 0	43.34
2.0715	8	-1 1 2	43.66
2.0541M	17	1 1 2	44.05
2.0541M		4 1 1	44.05
2.0404M	10	-2 0 2	44.36
2.0404M		0 3 1	44.36
2.0066	5	2 0 2	45.15
1.9577	2	-2 1 2	46.34
1.9145	3	5 1 0	47.45
1.8799	13	2 3 1	48.38
1.8504	3	-4 2 1	49.20
1.8375	4	-1 2 2	49.57
1.8244M	5	1 2 2	49.95
1.8244M		4 2 1	49.95
1.7972	2	-3 1 2	50.76
1.7721	13	-5 1 1	51.53
1.7252	4	5 2 0	53.04
1.6982	6	1 4 0	53.95
1.6881	6	4 3 0	54.30
1.6750	1L	-4 0 2	54.76
1.6610	4	6 0 0	55.26
1.6381	11	-3 2 2	56.10
1.6264	3	-4 1 2	56.54
1.6118	7	3 2 2	57.10
1.5969	16	5 2 1	57.68
1.5934	17	0 3 2	57.82
1.5859	18	-4 3 1	58.12
1.5691M	4	1 3 2	58.80
1.5691M		4 3 1	58.80
1.5665	3	-6 0 1	58.91
1.5436	4	6 0 1	59.87
1.5284	1	-6 1 1	60.53
1.5249M	2	-2 3 2	60.68

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.5249M		2 4 1	60.68
1.5117	3	2 3 2	61.27
1.5061+	5	6 1 1	61.52
1.5061+		-4 2 2	61.52
1.4958	1	6 2 0	61.99
1.4776	2	4 2 2	62.84
1.4643	1	-5 1 2	63.48
1.4502	1	-3 4 1	64.17
1.4434	2	0 1 3	64.51
1.4414	3	3 4 1	64.61
1.4327+	2	-1 1 3	65.05
1.4327+		-5 3 1	65.05
1.4235M	1	-2 0 3	65.52
1.4235M		1 1 3	65.52

Ethylenediaminetetraacetic Acid, $C_{10}H_{16}N_2O_8$

Synonyms
N,N'-1,2-Ethanediylbis[N-(carboxymethyl) glycine]
Edetic Acid
EDTA
Versene

CAS registry no.
60-00-4

Sample
The sample was prepared at NBS and recrystallized from water.

Color
Colorless

Structure
Monoclinic, A2/a (15), Z = 4. The structure was determined by Lu and Shao (1962).

Lattice constants of this sample
a = 16.112(3)Å
b = 5.5774(15)
c = 13.287(3)
β = 96.30(2)°

a/b = 2.8890
c/b = 2.3825

Volume
1186.8 Å^3

Density
(calculated) 1.636 g/cm^3

Figure of merit
F_{30} = 47.7(0.013,50)

Additional pattern
PDF card 27-1927 (Wang, P., Polytechnic Institute of Brooklyn, Brooklyn, N.Y.)

Reference
Lu, Y. T. and Shao, M. C. (1962). Sci. Sin. 9, 469.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
8.01	17	2 0 0	11.04
6.59	23	0 0 2	13.42
5.394	13	-2 0 2	16.42
5.142	12	0 1 1	17.23
4.960	40	-1 1 1	17.87
4.847M	4	2 0 2	18.29
4.847M		1 1 1	18.29
4.412	32	-2 1 1	20.11
4.003	100	4 0 0	22.19
3.783	12	-3 1 1	23.50
3.603	81	-4 0 2	24.69
3.443	21	-1 1 3	25.86
3.323	25	1 1 3	26.81
3.276	9	-2 1 3	27.20
3.180	11	-2 0 4	28.04
3.079	22	2 1 3	28.98
3.021	22	-3 1 3	29.54
2.940	7	2 0 4	30.38
2.773	24	-5 1 1	32.26
2.696	9	-4 0 4	33.20
2.669M	5	6 0 0	33.55
2.669M		5 1 1	33.55
2.632	4	2 2 0	34.04
2.574	8	-6 0 2	34.82
2.518	4	1 2 2	35.62
2.511	4	4 1 3	35.73
2.477	7	-2 2 2	36.24
2.456	2	-5 1 3	36.55
2.416	23	2 2 2	37.18
2.398	9	-1 1 5	37.48
2.385	8	6 0 2	37.68
2.353M	1	-3 2 2	38.21
2.353M		-2 1 5	38.21
2.328	1	1 1 5	38.65
2.288	2	4 2 0	39.35
2.227	5	2 1 5	40.48
2.201	12	0 0 6	40.97
2.131M	6	-1 2 4	42.38
2.131M		0 2 4	42.38
2.125	4	-7 1 1	42.51
2.093	6	1 2 4	43.20
2.065	7	2 0 6	43.81
2.024M	2	-4 0 6	44.73
2.024M		2 2 4	44.73
2.012	4	-5 1 5	45.03
1.977	4	-8 0 2	45.87
1.973	4	6 0 4	45.95
1.964	6	5 2 2	46.18
1.929	4	6 2 0	47.07
1.8593	1	8 0 2	48.95
1.8389	4	8 1 1	49.53
1.8025	7	-8 0 4	50.60

Synonym
Hafnium mononitride

CAS registry no.
25817-87-2

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA.

Color
Dark olive brown

Structure
Cubic, Fm3m (225), Z = 4. Glaser et al. (1953).

Lattice constant of this sample
$a = 4.5253(4)$ Å

Volume
92.67 Å^3

Density
(calculated) 13.797 g/cm^3

Figure of merit
$F_{10} = 63.3(0.016,10)$

Additional pattern
PDF card 25-1410 (Fiala, Central Research Institute, Skoda, Czechoslovakia, 1973).

Reference
Glaser, F. W., Moscowitz, D., and Post, B. (1953). J. Metals 5, 1119.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
2.612	100	1 1 1	34.31
2.262	62	2 0 0	39.82
1.6002	37	2 2 0	57.55
1.3641	33	3 1 1	68.76
1.3061	9	2 2 2	72.28
1.1314	4	4 0 0	85.82
1.0379	8	3 3 1	95.84
1.0120	10	4 2 0	99.13
.9237	7	4 2 2	113.01
.8710	7	5 1 1	124.36

p-Iodobenzoic Acid, $C_7H_5IO_2$

CAS registry no.
691-58-9

Sample
The sample was obtained from Eastman Organic Chemicals, Rochester, NY. It was recrystallized from ethanol.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure was determined qualitatively by Toussaint (1950, 1952).

Lattice constants of this sample

a = 30.087(5) Å
b = 6.0346(12)
c = 4.1563(9)
β = 90.55(2)°

a/b = 4.9857
c/b = 0.6887

Volume
754.60 Å^3

Density
(calculated) 2.183 g/cm^3

Figure of merit
F_{30} = 42.1(0.010,69)

Additional pattern
PDF card 11-828 (Cherin, Polytechnic Institute of Brooklyn, 1960)

References
Toussaint, J. (1950). Congr. Nat. Sci. Bruxelles Radiologie, p. 169.

Toussaint, J. (1952). Mem. Soc. Roy. Sci. Liège 12, 1.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
15.07	100	2 0 0	5.86
7.53	8	4 0 0	11.75
5.604	8	2 1 0	15.80
5.175	3	3 1 0	17.12
4.706	57	4 1 0	18.84
4.261	4	5 1 0	20.83
4.124	8	-1 0 1	21.53
3.855M	61	6 1 0	23.05
3.855M		-3 0 1	23.05
3.764	7	8 0 0	23.62
3.501	4	7 1 0	25.42
3.399	36	1 1 1	26.20
3.334	5	2 1 1	26.72
3.228	15	3 1 1	27.61
3.191	25	8 1 0	27.94
3.109	3	4 1 1	28.69
3.009	16	10 0 0	29.67
2.974	18	7 0 1	30.02
2.964	19	5 1 1	30.13
2.892	2	3 2 0	30.90
2.801	3	4 2 0	31.93
2.690	8	-7 1 1	33.28
2.667	3	7 1 1	33.58
2.593	5	9 0 1	34.56
2.507	4	12 0 0	35.79
2.433	5	1 2 1	36.92
2.401	7	-9 1 1	37.43
2.382	6	9 1 1	37.73
2.374	6	-3 2 1	37.86
2.295	2	-11 0 1	39.23
2.267	4	-5 2 1	39.72
2.257	3	5 2 1	39.92
2.241	1	9 2 0	40.20
2.1480	6	14 0 0	42.03
2.1301M	8	10 2 0	42.40
2.1301M		11 1 1	42.40
2.1168	4	7 2 1	42.68
2.0257M	3	11 2 0	44.70
2.0257M		14 1 0	44.70
2.0142	3	13 0 1	44.97
2.0074M	3	-4 0 2	45.13
2.0074M		1 3 0	45.13
1.9650M	6	9 2 1	46.16
1.9650M		0 1 2	46.16
1.9498	5	-2 1 2	46.54
1.9435	6	4 3 0	46.70
1.9252+	5	-6 0 2	47.17
1.9252+		3 1 2	47.17
1.9134	4	6 0 2	47.48
1.8806	1L	16 0 0	48.36
1.8737	1L	-5 1 2	48.55
1.8672	2	6 3 0	48.73
1.8632	2	5 1 2	48.84
1.8213	2	7 3 0	50.04
1.8166	3	11 2 1	50.18
1.8122M	3	-15 0 1	50.31
1.8122M		8 0 2	50.31
1.7952	2	16 1 0	50.82
1.7737	1	8 3 0	51.48
1.7503	1	14 2 0	52.22
1.7478	1	-8 1 2	52.30
1.7255	2	15 1 1	53.03

Iron Aluminum Oxide (Hercynite), $FeAl_2O_4$

Synonym
Iron aluminate

CAS registry no.
12068-49-4

Sample
The sample was prepared by grinding under acetone stoichiometric amounts of α-Fe_2O_3 and γ-Al_2O_3 in an agate mortar. After drying, the mixture was transferred to an iron crucible for heat treatment in controlled atmosphere. The sample was heated at 1200 °C for 8 hours in an oxygen pressure $\leq 10^{-16}$ atm. followed by grinding and reheating for 8 hours at 1300 °C for 8 hours in an oxygen pressure $\leq 10^{-16}$ atm.

Color
Greenish gray

Structure
Cubic, Fd3m (227), Z = 8. Isostructural with spinel (Holgersson, 1927). The structure of spinel was determined by Bragg (1915) and Nishikawa (1915).

Lattice constant of this sample
a = 8.1534(1)Å

Volume
542.03 Å^3

Density
(calculated) 4.260 g/cm^3

Figure of merit
F_{27} = 112.33(0.008,32)

Additional patterns
PDF card 3-894 (Dow Chemical Co., Midland, MI)

Clark, et al. (1931)

Fischer and Hoffmann (1955)

Krause and Thiel (1932)

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
4.709	3	1 1 1	18.83
2.883	58	2 2 0	30.99
2.460	100	3 1 1	36.50
2.0382	17	4 0 0	44.41
1.8711	5	3 3 1	48.62
1.6649	16	4 2 2	55.12
1.5691	36	5 1 1	58.80
1.4414	42	4 4 0	64.61
1.2892	5	6 2 0	73.38
1.2434	8	5 3 3	76.56
1.2293	3	6 2 2	77.60
1.1769	2	4 4 4	81.77
1.1417	1	5 5 1	84.86
1.0897	5	6 4 2	89.97
1.0614	10	7 3 1	93.06
1.0191	5	8 0 0	98.20
.9962	1L	7 3 3	101.29
.9608	3	6 6 0	106.59
.9415	5	7 5 1	109.81
.9353	1	6 6 2	110.89
.9116	3	8 4 0	115.35
.8949	2	9 1 1	118.80
.8691	2	6 6 4	124.82
.8547	5	9 3 1	128.64
.8321	10	8 4 4	135.55
.8195	1	7 7 1	140.10
.7995	3	10 2 0	148.93

References

Bragg, W. H. (1915). Nature London 95, 561.

Clark, G. L., Ally, A., and Badger, A. E. (1931). Am. J. Sci. 22, 539.

Fischer, W. A. and Hoffmann, A. (1955). Arch. Eisenhuettenw 26, 43.

Holgersson, S. (1927). Lunds Univ. Årsskr. Avd. 2, 23 No. 9.

Krause, O. and Thiel, W. (1932). Z. Anorg. Allgem. Chem. 203, 120.

Nishikawa, S. (1915). Proc. Tokyo Math. Phys. Soc. 8, 199.

Iron Antimony Oxide, $FeSbO_4$

Synonym
Iron antimonate

Sample
The sample was prepared at NBS.

Chemical analysis
Chemical analysis showed 22.94 weight percent Fe, 49.47 weight percent Sb, and by difference, 27.59 weight percent oxygen. On this basis, the composition most nearly corresponds to the formula $FeSbO_4$.

Color
Medium yellowish brown

Structure
Tetragonal, $P4_2/mnm$ (136), Z = 1, isostructural with rutile (Brandt, 1943).

Lattice constants of this sample
a = 4.6352(2) Å
c = 3.0733(2)

c/a = 0.6630

Volume
66.030 $Å^3$

Density
(calculated) 6.076 g/cm^3

Figure of merit
F_{30} = 61.2(0.011,43)

Comment
PDF card 7-349 (Mason and Vitaliano, 1953) requires the value of c = 9.14 only because of its first reflection. The pattern may be a mixture of the rutile and trirutile phases of $Fe_xSb_yO_4$.

References
Brandt, K. (1943). Ark. Kemi Mineral. Geol. 17A, 15.

Mason, B. and Vitaliano, C. J. (1953). Mineral. Mag. 30, 100.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
3.279	100	1 1 0	27.17
2.562	71	1 0 1	34.99
2.318	17	2 0 0	38.82
2.242	8	1 1 1	40.19
2.0720	3	2 1 0	43.65
1.7185	56	2 1 1	53.26
1.6386	14	2 2 0	56.08
1.5367	6	0 0 2	60.17
1.4655	10	3 1 0	63.42
1.3912	12	1 1 2	67.24
1.3802	14	3 0 1	67.85
1.3231	1L	3 1 1	71.21
1.2806	4	2 0 2	73.96
1.2344	1L	2 1 2	77.22
1.1858	7	3 2 1	81.02
1.1585	3	4 0 0	83.35
1.1211	4	2 2 2	86.80
1.0925	3	3 3 0	89.67
1.0606	5	3 1 2	93.15
1.0559	5	4 1 1	93.69
1.0364	2	4 2 0	96.02
1.0004	2	1 0 3	100.71
.9253	2	4 0 2	112.71
.9183	4	2 1 3	114.03
.9091	2	5 1 0	115.84
.8903	3	3 3 2	119.82
.8877	5	4 3 1	120.40
.8593	3	4 2 2	127.38
.8538	2	3 0 3	128.89
.8288	4	5 2 1	136.68
.8194	1L	4 4 0	140.11
.8012	2	3 2 3	148.06

Iron Chromium Oxide (Chromite), $FeCr_2O_4$

Synonym
Iron chromite

CAS registry no.
12068-77-8

Sample
The sample was prepared from a 1:2 molar ratio of Fe_2O_3 and Cr_2O_3 in a controlled atmosphere furnace. The procedure adopted from Katsura and Muan (1964) was followed.

Color
Dark reddish brown

Structure
Cubic, Fd3m (227), Z = 8. Isostructural with spinel, Holgersson (1927).

Lattice constant of this sample
a = 8.3790(2)Å

Volume
588.27 $Å^3$

Density
(calculated) 5.055 g/cm^3

Polymorphism
Francombe (1958) reports a distorted tetragonal polymorph that exists below -90 °C.

Figure of merit
F_{27} = 87.8(0.009,34)

Additional patterns
PDF card 3-873 (Clark and Ally, 1932)

Holgersson (1927)

Hilty, et al. (1955)

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

d(Å)	I^{rel} σ = ±3	hkℓ			2θ(°)
4.839	13	1	1	1	18.32
2.962	33	2	2	0	30.15
2.526	100	3	1	1	35.51
2.418	7	2	2	2	37.15
2.0943	22	4	0	0	43.16
1.7105	11	4	2	2	53.53
1.6125	39	5	1	1	57.07
1.4812	48	4	4	0	62.67
1.4162	2	5	3	1	65.90
1.3247	3	6	2	0	71.11
1.2777	10	5	3	3	74.15
1.2632	5	6	2	2	75.15
1.2095	3	4	4	4	79.12
1.1734	1	7	1	1	82.06
1.1197	4	6	4	2	86.94
1.0907	12	7	3	1	89.86
1.0476	5	8	0	0	94.67
.9873	2	8	2	2	102.56
.9675	10	7	5	1	105.53
.9612	2	6	6	2	106.53
.9367	2	8	4	0	110.64
.8931	1	6	6	4	119.19
.8783	5	9	3	1	122.58
.8552	12	8	4	4	128.50
.8217	1	10	2	0	139.27
.8101	7	9	5	1	143.95
.8063	1L	10	2	2	145.65

References
Clark, G. L. and Ally, A. (1932). Am. Mineral. 17, 66.

Francombe, M. H. (1958). XVIéme Congr. internation. Chim. pure appl., Paris, 1957, Mém. Sect. Chim. Minér., Sedes, Paris, 129.

Hilty, D. C., Forgeng, W. D., and Folkman, R. L. (1955). J. Metals, N.Y. 7, 253.

Holgersson, S. (1927). Lunds Univ. Årsskr., Avd. 2, 23, No. 9.

Katsura, T. and Muan, A. (1964). Trans. AIME 230, 77.

Lithium Zirconium Oxide, Li_2ZrO_3

Synonyms
Lithium zirconate
Dilithium zirconium trioxide

CAS registry no.
12031-83-3

Sample
The sample was prepared by L. Martel at NBS. Equimolar amounts of Li_2CO_3 and ZrO_2 were calcined at 700 °C for one day, then heated to 1000 °C for 16 hours and finally heated to 1400 °C for several hours in a tightly covered platinum crucible.

Color
Colorless

Structure
Monoclinic, C2/c (15), Z = 4. The structure was determined by Dittrich and Hoppe (1969) and redetermined by Hodeau et al. (1982).

Lattice constants of this sample
a = 5.4266(5)Å
b = 9.0310(8)
c = 5.4227(7)
β = 112.720(8)°

a/b = 0.6009
c/b = 0.6005

Volume
245.13 Å^3

Density
(calculated) 4.148 g/cm^3

Figure of merit
F_{30} = 62.6(0.011,43)

Additional pattern
PDF card 23-372 (Dittrich and Hoppe, 1969)

References
Dittrich, G. and Hoppe, R. R. O. (1969). Z. Anorg. Allg. Chem., 371, 306.

Hodeau, J. L., Marezio, M., Santoro, A., and Roth, R. S. (1982). Accepted for publication in the J. Solid State Chem., October 1982.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
4.512	18	0 2 0	19.66
4.377	100	1 1 0	20.27
4.037	39	-1 1 1	22.00
3.351	56	0 2 1	26.58
2.852	13	1 1 1	31.34
2.580M	23	1 3 0	34.74
2.580M		-1 1 2	34.74
2.504+	24	-1 3 1	35.84
2.504+		2 0 0	35.84
2.313	19	-2 2 1	38.90
2.258M	33	-2 0 2	39.90
2.258M		0 4 0	39.90
2.189M	7	2 2 0	41.21
2.189M		0 2 2	41.21
2.127	46	1 3 1	42.46
2.0590	17	0 4 1	43.94
2.0197	4	-2 2 2	44.84
2.0070	1L	-1 3 2	45.14
1.9115	12	1 1 2	47.53
1.7952	9	2 2 1	50.82
1.7702M	5	-3 1 1	51.59
1.7702M		-1 1 3	51.59
1.7300	4	-2 4 1	52.88
1.6991M	20	-3 1 2	53.92
1.6991M		1 5 0	53.92
1.6764+	10	-1 5 1	54.71
1.6764+		2 4 0	54.71
1.6408M	8	3 1 0	56.00
1.6408M		1 3 2	56.00
1.6151	13	-2 2 3	56.97
1.5969	3	-2 4 2	57.68
1.5643	7	0 2 3	59.00
1.5481+	32	-3 3 1	59.68
1.5481+		1 5 1	59.68
1.5048	10	0 6 0	61.58
1.5019	13	2 0 2	61.71
1.4998M	10	-3 3 2	61.81
1.4998M		-1 5 2	61.81
1.4849	2	-3 1 3	62.50
1.4785	5	2 4 1	62.80
1.4414	1L	0 6 1	64.61
1.4257	1	2 2 2	65.41
1.4081M	3	3 1 1	66.33
1.4081M		1 1 3	66.33
1.3727	5	-2 4 3	68.27

d(Å)	I^{rel} $\sigma = \pm 4$	hkℓ			2θ(°)
1.3463M	5	-3	3	3	69.80
1.3463M		-4	0	2	69.80
1.3413	4	0	4	3	70.10
1.3268M	8	1	5	2	70.98
1.3268M		-1	1	4	70.98
1.3138	1L	-2	6	1	71.79
1.2889M	9	3	3	1	73.40
1.2889M		1	3	3	73.40
1.2867	8	-4	2	1	73.55
1.2766M	1	-3	5	1	74.23
1.2766M		-1	5	3	74.23
1.2526	15	-2	6	2	75.90
1.2492+	13	-3	5	2	76.14
1.2492+		1	7	0	76.14
1.2405	2	-1	7	1	76.77
1.2257	3	3	5	0	77.87
1.2153	2	-4	2	3	78.67
1.2059	1	4	2	0	79.40
1.1854	2	1	7	1	81.06
1.1814	3	3	1	2	81.39
1.1632M	1	-3	3	4	82.94
1.1632M		-1	7	2	82.94
1.1564M	3	-3	5	3	83.54
1.1564M		-4	4	2	83.54
1.1535	4	-4	4	1	83.79
1.1521	4	2	2	3	83.92

Magnesium Arsenate Hydrate (Hoernesite), $Mg_3(AsO_4)_2 \cdot 8H_2O$

Synonym
Magnesium arsenate octahydrate

CAS registry no.
37541-75-6

Sample
A dilute solution of Na_2HAsO_4 was dropped into a dilute solution of $MgSO_4$ with a small amount of NaOH. The precipitate was left in the mother liquor for 3 days at about 80 °C. It was then filtered and washed with ethanol.

Color
Colorless

Structure
Monoclinic, I2/m (12), Z = 2. Isostructural with vivianite. (Wolfe, 1940) The structure of vivianite, $Fe_3(PO_4)_2 \cdot 8H_2O$, is discussed by Mori and Ito (1950).

Lattice constants of this sample

a = 10.137(2)Å
b = 13.455(2)
c = 4.7542(10)
β = 101.73(2)°

a/b = 0.7530
c/b = 0.3533

Volume
634.9 Å^3

Density
(calculated) 2.589 g/cm^3

Figure of merit
F_{30} = 32.0(0.019,45)

Additional pattern
PDF card 19-752 (Koritnij and Süsse, 1966)

References

Koritnij, S. and Süsse, P. (1966). Neues Jahrb. Mineral. Monatsh. 349.

Mori, H. and Ito, T. (1950). Acta Crystallogr. 3, 1.

Wolfe, C. W. (1940). Am. Mineral. 25, 787.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
7.97	31	1 1 0	11.09
6.73	100	0 2 0	13.14
4.399	48	0 1 1	20.17
3.992	26	2 2 0	22.25
3.916	16	1 0 1	22.69
3.786	17	-1 2 1	23.48
3.655	17	-2 1 1	24.33
3.367	13	0 4 0	26.45
3.212	50	3 1 0	27.75
3.002	58	-3 0 1	29.74
2.784	11	2 4 0	32.13
2.740	42	-3 2 1	32.65
2.714	30	-1 4 1	32.98
2.664	14	3 3 0	33.61
2.596	3	1 5 0	34.52
2.554	19	1 4 1	35.11
2.480	18	4 0 0	36.19
2.468	21	3 0 1	36.38
2.341	17	-1 1 2	38.42
2.331M	14	0 5 1	38.60
2.331M		4 2 0	38.60
2.295	5	-2 0 2	39.23
2.244	5	0 6 0	40.16
2.238	4	-3 4 1	40.26
2.199M	7	0 2 2	41.02
2.199M		-2 5 1	41.02
2.170	2	-2 2 2	41.58
2.090	17	-3 1 2	43.26
2.042	4	2 6 0	44.32
2.030	4	2 5 1	44.59
2.015	7	-1 6 1	44.96
1.992	7	3 4 1	45.50
1.964	9	5 1 0	46.19
1.955	7	1 3 2	46.42
1.916M	11	-3 3 2	47.42
1.916M		0 4 2	47.42
1.882	1	2 2 2	48.32
1.846	3	4 3 1	49.32
1.796	1	-3 6 1	50.81
1.792	1	-4 5 1	50.92
1.776	3	0 7 1	51.41
1.730	2	3 1 2	52.88
1.704M	4	5 0 1	53.74
1.704M		-5 4 1	53.74
1.688	10	1 5 2	54.29
1.683	11	0 8 0	54.48
1.660	15	3 6 1	55.29
1.657	16	-6 1 1	55.39
1.6180	4	4 5 1	56.86
1.6154	5	0 6 2	56.96
1.6071	4	6 2 0	57.28
1.5643M	4	-6 3 1	59.00
1.5643M		-2 1 3	59.00
1.5457	4	1 8 1	59.78
1.5413M	4	0 1 3	59.97
1.5413M		-1 2 3	59.97
1.5297	2	-3 0 3	60.47
1.5204	5	5 4 1	60.88
1.4995	8	-6 0 2	61.82
1.4939	5	-1 7 2	62.08

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.4855	5	-2 3 3	62.47
1.4659	7	0 3 3	63.40
1.4502	4	-4 6 2	64.17
1.4476	4	-4 1 3	64.30
1.4305	4	-5 5 2	65.16
1.4191	3	-6 5 1	65.75
1.3909M	5	-2 9 1	67.26
1.3909M		3 8 1	67.26
1.3811	1	5 7 0	67.80
1.3694	2	-6 4 2	68.46
1.3577	4	5 6 1	69.13
1.3516	4	7 3 0	69.49
1.3457	5	0 10 0	69.84
1.3440	5	0 5 3	69.94

Magnesium Phosphate (Farringtonite), $Mg_3(PO_4)_2$

Synonyms
Magnesium orthophosphate
Trimagnesium biphosphate

CAS registry no.
10043-83-1

Sample
The sample was obtained from the Research Organic/Inorganic Chemical Corp., Sun Valley, CA. It was heated at NBS at 800 °C for 18 hours.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 2. The structure of $Mg_3(PO_4)_3$ was determined by Nord and Kierkegaard (1968).

Lattice constants of this sample
a = 7.5995(8) Å
b = 8.2355(8)
c = 5.0762(5)
β = 94.062(9)°

a/b = 0.9228
c/b = 0.6164

Volume
317.42 $Å^3$

Density
(calculated) 2.750 g/cm^3

Polymorphism
Berak (1958) suggests a second form of $Mg_3(PO_4)_2$ stable above about 1000 °C.

Figure of merit
F_{30} = 57.0(0.011,47)

Additional patterns
PDF card 13-554 (Du Fresne and Roy, 1961)

PDF card 25-1373 (Nord and Kierkegaard, 1968)

References
Berak, J. (1958). Rocz. Chem. 32, 19.

Du Fresne, E. R. and Roy, S. K. (1961). Geochim. Cosmochim. Acta 24, 198.

Nord, A. G. and Kierkegaard, P. (1968). Acta Chem. Scand. 22, 1466.

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

d(Å)	I^{rel} σ = ±1	hkℓ			2θ(°)
5.576	10	1	1	0	15.88
4.356	30	-1	0	1	20.37
4.312	24	0	1	1	20.58
4.118	30	0	2	0	21.56
4.077	28	1	0	1	21.78
3.852	84	-1	1	1	23.07
3.792	6	2	0	0	23.44
3.657	28	1	1	1	24.32
3.619	6	1	2	0	24.58
3.443	100	2	1	0	25.86
3.195	14	0	2	1	27.90
2.992	21	-1	2	1	29.84
2.896	4	1	2	1	30.85
2.790	16	2	2	0	32.05
2.764	3	2	1	1	32.36
2.533	22	0	0	2	35.41
2.498	23	-2	2	1	35.92
2.414M	32	3	1	0	37.22
2.414M		0	3	1	37.22
2.322	8	-1	3	1	38.75
2.240	5	-3	1	1	40.22
2.222	4	2	3	0	40.57
2.177	3	-2	0	2	41.45
2.158	1L	0	2	2	41.83
2.125	22	3	1	1	42.51
2.108	9	-1	2	2	42.87
2.0679	10	-2	3	1	43.74
2.0599	8	0	4	0	43.92
2.0417	13	1	2	2	44.33
1.9866	2	1	4	0	45.63
1.9256	3	-2	2	2	47.16
1.9077	2	0	4	1	47.63
1.8950	7	4	0	0	47.97
1.8597	7	3	3	0	48.94
1.8275	9	2	2	2	49.86
1.8108	1L	-3	1	2	50.35
1.7860	3	1	3	2	51.10
1.7753	8	-3	3	1	51.43
1.7224M	7	-2	4	1	53.13
1.7224M		4	2	0	53.13
1.6976	4	4	1	1	53.97
1.6918M	10	-3	2	2	54.17
1.6918M		3	1	2	54.17
1.6860	1L	2	4	1	54.37
1.6727	1L	-1	0	3	54.84

Magnesium Phosphate (Farringtonite), $Mg_3(PO_4)_2$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
1.6394	7	-1 1 3	56.05
1.6094	3	1 5 0	57.19
1.5982	1L	4 2 1	57.63
1.5619	10	0 2 3	59.10
1.5502M	1L	-1 2 3	59.59
1.5502M		1 4 2	59.59
1.5373	11	-3 3 2	60.14
1.5103M	6	2 5 0	61.33
1.5103M		1 2 3	61.33
1.5026	6	3 4 1	61.68
1.4911	2	5 1 0	62.21
1.4780M	2	-2 2 3	62.82
1.4780M		2 1 3	62.82
1.4674M	1	-4 2 2	63.33
1.4674M		4 0 2	63.33
1.4587M	1	-2 5 1	63.75
1.4587M		-5 1 1	63.75
1.4488	3	2 4 2	64.24
1.4366	4	2 5 1	64.85
1.4249	1	5 0 1	65.45
1.4043	1L	5 1 1	66.53
1.3947M	1	4 4 0	67.05
1.3947M		-5 2 1	67.05
1.3798	1	3 5 0	67.87
1.3724M	1	0 6 0	68.29
1.3724M	1	-2 3 3	68.29
1.3638	1	-4 3 2	68.78
1.3509	1	1 6 0	69.53
1.3270M	1	5 3 0	70.97
1.3270M		4 4 1	70.97
1.3181M	1	3 5 1	71.52
1.3181M		2 3 3	71.52
1.2770	1L	-5 2 2	74.20
1.2745	3	1 4 3	74.37
1.2513	3	0 1 4	75.99
1.2066+	1	0 6 2	79.35
1.2066+		-5 3 2	79.35
1.1854	1	1 6 2	81.06
1.1683	1	4 2 3	82.50
1.1582	1	-5 1 3	83.38

Manganese Tartrate, $C_4H_4MnO_6$

Sample
The sample was prepared at NBS. It contained a very small amount of tartaric acid as a second phase which did not interfere with measurements.

Color
Pale greenish yellow

Structure
Orthorhombic, possibly Pnnm (58), Z assumed to be 4. The cell constants were determined by use of the Visser (1969) program. Absent reflections suggested the space group assignment which was used for the data analysis that follows.

Lattice constants of this sample
a = 9.4388(8)Å
b = 11.6925(13)
c = 5.0706(4)

a/b = 0.8073
c/b = 0.4337

Volume
559.61 $Å^3$

Density
(calculated) 2.410 g/cm^3, assuming Z = 4.

Figures of merit
F_{30} = 57.1(0.011,49)
M_{20} = 40.5

Additional pattern
PDF card 1-343 (Hanawalt et al., 1938)

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

Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
7.34	14	1 1 0	12.04
5.843	65	0 2 0	15.15
4.716	12	2 0 0	18.80
4.653	53	0 1 1	19.06
4.467	100	1 0 1	19.86
3.673	57	2 2 0	24.21
3.604	20	1 3 0	24.68
3.549	98	1 2 1	25.07
3.313	18	2 1 1	26.89
3.092	3	0 3 1	28.85
3.008	1L	2 3 0	29.68
2.923	8	0 4 0	30.56
2.794	1L	1 4 0	32.01
2.673	27	3 0 1	33.50
2.585	49	2 3 1	34.67
2.536	4	0 0 2	35.36
2.485	16	2 4 0	36.12
2.446M	72	3 3 0	36.71
2.446M		1 4 1	36.71
2.430	31	3 2 1	36.96
2.398	5	1 1 2	37.48
2.359	1L	4 0 0	38.12
2.327	2	0 2 2	38.66
2.270	11	1 5 0	39.68
2.233M	16	2 0 2	40.36
2.233M		2 4 1	40.36
2.188	5	4 2 0	41.23
2.124	3	0 5 1	42.52
2.105	10	4 1 1	42.94
2.086	29	2 2 2	43.34
2.0733M	14	1 3 2	43.62
2.0733M		1 5 1	43.62
1.9727	8	3 4 1	45.97
1.9466	13	3 1 2	46.62
1.9361	19	2 5 1	46.89
1.9153	14	0 4 2	47.43
1.8755M	12	3 5 0	48.50
1.8755M		4 3 1	48.50
1.8361	7	4 4 0	49.61
1.7857	1	1 6 1	51.11
1.7744	3	2 4 2	51.46
1.7699	3	5 0 1	51.60
1.7606M	6	3 3 2	51.89
1.7606M		3 5 1	51.89
1.7273M	16	4 0 2	52.97
1.7273M		4 4 1	52.97
1.6985	10	5 3 0	53.94
1.6927	14	5 2 1	54.14
1.6638	3	1 0 3	55.16
1.6563M	4	3 6 0	55.43
1.6563M		4 2 2	55.43
1.6446	8	1 7 0	55.86
1.6000	7	1 2 3	57.56
1.5861M	7	0 7 1	58.11
1.5861M		5 4 0	58.11
1.5780	6	4 5 1	58.44
1.5735	5	6 0 0	58.62
1.5509	2	0 3 3	59.56
1.5450	1L	0 6 2	59.81
1.5191	4	6 2 0	60.94

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.5128	7	5 4 1	61.22
1.5090	8	3 5 2	61.39
1.5037	6	2 7 1	61.63
1.4904	2	6 1 1	62.24
1.4891	3	3 0 3	62.30
1.4732	5	2 3 3	63.05
1.4688M	4	5 5 0	63.26
1.4688M		2 6 2	63.26
1.4460	4	1 4 3	64.38
1.4021	3	6 3 1	66.65
1.3887M	3	4 5 2	67.38
1.3887M		1 8 1	67.38
1.3852	2	6 4 0	67.57
1.3697	2	0 5 3	68.44
1.3396	2	7 1 0	70.20
1.3265	1L	3 4 3	71.00
1.3160M	5	4 7 1	71.65
1.3160M		2 5 3	71.65
1.3033M	5	7 0 1	72.46
1.3033M		6 2 2	72.46
1.2927	1L	4 6 2	73.15
1.2870	1L	1 9 0	73.53
1.2746M	7	3 7 2	74.36
1.2746M		7 3 0	74.36
1.2711	4	5 5 2	74.60
1.2675	3	0 0 4	74.85
1.2642M	2	6 3 2	75.08
1.2642M		6 5 1	75.08
1.2589M	4	5 0 3	75.45
1.2589M		0 9 1	75.45
1.2388	2	0 2 4	76.90
1.2308	3	5 2 3	77.49
1.2155M	3	2 9 1	78.65
1.2155M		6 4 2	78.65

Molybdenum Silicide, Mo_5Si_3

CAS registry no.
12033-40-8

Sample
Stoichiometric amounts of Mo and Si_3N_4 were mixed, pelleted and heated in a crucible to 1600 °C for 1 hour while lying on a pellet of previously made Mo_5Si_3 which was put on a piece of Mo.

Color
Olive black

Structure
Tetragonal I4/mcm (140), Z = 4. The structure was determined qualitatively by Aronsson (1955).

Lattice constants of this sample
a = 9.6483(6) Å
c = 4.9135(5)

c/a = 0.5093

Volume
457.40 Å^3

Density
(calculated) 8.190 g/cm^3

Figure of merit
F_{30} = 98.6(0.009,35)

Additional patterns
PDF card 8-429 (Schachner et al. 1954)

Nowotny et al. (1956)

References
Aronsson, B. (1955). Acta Chem. Scand. 9, 1107.

Nowotny, H., Lux, B., and Kudielka, H. (1956) Monatsh. Chem. 87, 462.

Schachner, H., Cerwenka, E., and Nowotny, H. (1954). Monatsh. Chem. 85, 245.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.820	1	1 1 0	12.97
4.826	2	2 0 0	18.37
3.413	5	2 2 0	26.09
3.242	25	2 1 1	27.49
3.052	21	3 1 0	29.24
2.457	25	0 0 2	36.54
2.412	16	4 0 0	37.25
2.351	71	3 2 1	38.26
2.311	12	1 1 2	38.94
2.2740	10	3 3 0	39.60
2.1903	38	2 0 2	41.18
2.1578	59	4 2 0	41.83
2.1130	100	4 1 1	42.76
1.9940	57	2 2 2	45.45
1.7955	2	4 3 1	50.81
1.7209	2	4 0 2	53.18
1.6835	8	5 2 1	54.46
1.6544	1	5 3 0	55.50
1.6087	2	6 0 0	57.22
1.5314	4	2 1 3	60.40
1.5254	10	6 2 0	60.66
1.5103	1L	6 1 1	61.33
1.4991	11	5 1 2	61.84
1.4406	11	5 4 1	64.65
1.4012	11	4 4 2	66.70
1.3971	18	3 2 3	66.92
1.3804	12	6 3 1	67.84
1.3724	11	5 3 2	68.29
1.3643	17	7 1 0	68.75
1.3453	24	6 0 2	69.86
1.3418	33	4 1 3	70.07
1.2797	2	7 2 1	74.02
1.2283	9	0 0 4	77.68
1.2086M	2	1 1 4	79.19
1.2086M		5 2 3	79.19
1.1979	1	6 5 1	80.04
1.1932	6	7 1 2	80.42
1.1751	11	6 4 2	81.92
1.1698	10	8 2 0	82.37
1.1631	2	7 4 1	82.95
1.1391M	3	3 1 4	85.10
1.1391M		6 1 3	85.10
1.1369	8	6 6 0	85.30
1.1259	4	7 3 2	86.34
1.1087	4	5 4 3	88.02
1.1004	11	8 3 1	88.86
1.0945	4	4 0 4	89.46

Nickel Arsenate Hydrate (Annabergite), $Ni_3(AsO_4)_2 \cdot 8H_2O$

Synonym
Nickel orthoarsenate octahydrate

CAS registry no.
54469-74-1

Sample
The sample was prepared at NBS. A solution of 2 gms $Ni(NO_3)_2 \cdot 6H_2O$ in 1 liter H_2O was added dropwise to a solution of 2 gms Na_2HAsO_4 in 1½ liters of warm H_2O. The combined solution was held at 70 to 80 °C for 3 weeks. The crystals were filtered off and washed with H_2O and C_2H_5OH.

Color
Light yellow green

Structure
Monoclinic, I2/m (12), Z = 2 (Barth, 1937). It is isostructural with vivianite, $Fe_3(PO_4)_2 \cdot 8H_2O$. The structure of vivianite was discussed by Mori and Ito (1950).

Lattice constants of this sample

a = 10.054(2) Å
b = 13.303(3)
c = 4.7159(10)
β = 102.10(2)°

a/b = 0.7558
c/b = 0.3545

Volume
616.73 Å^3

Density
(calculated) 3.221 g/cm^3

Figure of merit
F_{30} = 55.6(0.012,44)

Additional pattern
PDF card 11-625 (U.S. Bureau of Mines, Albany, Oregon)

References
Barth, T. F. W. (1937). Am. Mineral. 22, 325.

Mori, H. and Ito, T. (1950). Acta Crystallogr. 3, 1.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal std. Fluorophlogopite SRM 675

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
7.91	33	1 1 0	11.17
6.66	100	0 2 0	13.29
4.919	11	2 0 0	18.02
4.562	4	-1 0 1	19.44
4.363	20	0 1 1	20.34
4.044	6	1 3 0	21.96
3.954	8	2 2 0	22.47
3.879	16	1 0 1	22.91
3.765	3	-1 2 1	23.61
3.639	8	-2 1 1	24.44
3.347	5	1 2 1	26.61
3.326	4	0 4 0	26.78
3.198	43	0 3 1	27.88
2.982M	52	-3 0 1	29.94
2.982M		2 1 1	29.94
2.756	12	2 4 0	32.46
2.721	30	-3 2 1	32.89
2.687	21	-1 4 1	33.32
2.635	14	3 3 0	34.00
2.568	1	1 5 0	34.91
2.523	8	1 4 1	35.55
2.440	17	3 0 1	36.80
2.321	10	-1 1 2	38.76
2.304M	16	4 2 0	39.07
2.304M		0 5 1	39.07
2.217	3	0 6 0	40.66
2.178M	8	0 2 2	41.43
2.178M		-2 5 1	41.43
2.155	1	-2 2 2	41.89
2.102	1	-4 3 1	43.00
2.079	7	-3 1 2	43.49
2.066	8	3 5 0	43.79
2.021	1	2 6 0	44.80
1.9919	2	-1 6 1	45.50
1.9678	3	3 4 1	46.09
1.9463	6	5 1 0	46.63
1.9322	6	1 3 2	46.99
1.9006	9	-3 3 2	47.82
1.8240	3	4 3 1	49.96
1.7756	2	-4 5 1	51.42
1.7572	3	0 7 1	52.00
1.6915	1	-5 4 1	54.18
1.6713	8	1 5 2	54.89
1.6629	10	0 8 0	55.19
1.6505	11	-3 5 2	55.64

Nickel Arsenate Hydrate (Annabergite), $Ni_3(AsO_4)_2 \cdot 8H_2O$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
1.6405	11	3 6 1	56.01
1.6066	4	3 3 2	57.30
1.6002	5	4 5 1	57.55
1.5909	4	6 2 0	57.92
1.5807	2	5 5 0	58.33
1.5519M	2	-2 1 3	59.52
1.5519M		-6 3 1	59.52
1.5281M	3	1 8 1	60.54
1.5281M		-1 2 3	60.54
1.5191	2	-3 0 3	60.94
1.5028	3	5 4 1	61.67
1.4902	5	4 2 2	62.25
1.4791	4	-1 7 2	62.77

Nickel Molybdenum Oxide, $NiMoO_4$

Synonyms
Molybdenum nickel tetraoxide
Nickel molybdate

Sample
The sample was prepared at NBS. Stoichiometric amounts of NiO and MoO_3 were heated at 800 °C for 2 hours, then ground and reheated at 800 °C for 6 hours.

Color
Brilliant yellow green

Structure
Monoclinic, I2/m (12), Z = 8, isostructural with low temperature $CoMoO_4$ (Smith, 1962).

Lattice constants of this sample
a = 9.509(2)Å
b = 8.759(2)
c = 7.6678(15)
β = 113.13(2)°

a/b = 1.0856
c/b = 0.8754

Volume
587.3 Å^3

Density
(calculated) 4.946 g/cm^3

Polymorphism
Sleight and Chamberland (1968) report 3 polymorphs. The one described here occurs at low temperature when the heated reactants are cooled slowly. A second polymorph exists only at temperatures above 690 °C, and is isostructural with $MnMoO_4$. A third polymorph, isostructural with $NiWO_4$, can be prepared hydrothermally at 700 °C with pressures above 3 kbars.

Figure of merit
F_{30} = 27.7(0.017,63)

Additional patterns
PDF card 18-879 (Wetzlar, DEW-Technische Berichte, 1964)

PDF card 31-902 (Union Science and Technology Division, Union Oil Co. of California, Brea, CA 92621)

References
Sleight, A. W. and Chamberland, B. L. (1968). Inorg. Chem. 7, 1672.

Smith, G. W. (1962). Acta Crystallogr. 15, 1054.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.19	80	1 1 0	14.29
5.50	4	0 1 1	16.11
4.665	11	1 0 1	19.01
4.373M	1	0 2 0	20.29
4.373M		2 0 0	20.29
4.085	3	-2 1 1	21.74
3.711	15	-1 2 1	23.96
3.513	48	-1 1 2	25.33
3.166	5	-3 0 1	28.16
3.095	100	2 2 0	28.82
3.002	2	2 1 1	29.74
2.769M	15	1 3 0	32.31
2.769M		3 1 0	32.31
2.746	46	0 2 2	32.58
2.727	36	-3 1 2	32.82
2.465	1L	-2 3 1	36.42
2.331M	8	2 0 2	38.59
2.331M		-3 0 3	38.59
2.323	10	-1 3 2	38.74
2.307	4	-4 0 2	39.01
2.284	1	-4 1 1	39.42
2.188M	14	0 4 0	41.23
2.188M		4 0 0	41.23
2.154	1L	2 3 1	41.90
2.094	5	3 2 1	43.17
2.090	5	-1 4 1	43.26
2.062	45	3 3 0	43.87
1.998	1	-4 1 3	45.36
1.982	3	1 4 1	45.74
1.957M	4	2 4 0	46.37
1.957M		4 2 0	46.37
1.916	24	-2 0 4	47.40
1.847M	1	-5 1 2	49.30
1.847M		4 1 1	49.30
1.836	3	-1 1 4	49.60
1.828	2	-3 1 4	49.85
1.801	2	-3 4 1	50.63
1.759	1L	2 1 3	51.94
1.727	2	-5 2 1	52.98
1.716	10	5 1 0	53.34

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.7002	1	0 5 1	53.88
1.6789	1L	-4 3 3	54.62
1.6560	1L	-1 4 3	55.44
1.6456	1	-5 2 3	55.82
1.6357	9	0 2 4	56.19
1.6232	9	-4 2 4	56.66
1.5969+	11	3 3 2	57.68
1.5969+		2 4 2	57.68
1.5869M	9	-5 3 2	58.08
1.5869M		4 3 1	58.08
1.5602	1L	5 0 1	59.17
1.5472	1	4 4 0	59.72
1.5295M	1L	2 3 3	60.48
1.5295M		-6 1 1	60.48
1.4991	13	1 5 2	61.84
1.4954	10	-3 5 2	62.01
1.4900	8	-6 2 2	62.26
1.4583	5	-4 1 5	63.77
1.4418M	3	-2 4 4	64.59
1.4418M		-3 2 5	64.59
1.4394	2	-2 5 3	64.71
1.4293	1	-1 6 1	65.22
1.4094	8	1 3 4	66.26
1.3982M	6	-5 0 5	66.86
1.3982M		-5 3 4	66.86
1.3834	1	6 2 0	67.67
1.3711	1L	-6 3 1	68.36

Nickel Phosphate Hydrate, $Ni_3(PO_4)_2 \cdot 8H_2O$

Synonym
Nickel orthophosphate octahydrate

CAS registry no.
19033-89-7

Sample
The sample was made by adding a dilute solution of Na_2HPO_4 to dilute solution of $NiSO_4$ to which a small amount of NaOH had been added.

Color
Very light yellowish green.

Structure
Monoclinic, I2/m (12), $\dot{Z} = 2$. Vivianite structure, from the similarity of cell size, space group and chemistry. The structure of vivianite, $Fe_3(PO_4)_2 \cdot 8H_2O$, is discussed by Mori and Ito (1950).

Lattice constants of this sample

a = 9.846(4) Å
b = 13.203(4)
c = 4.6342(15)
β = 102.27(3)°

a/b = 0.7457
c/b = 0.3510

Volume
588.67 Å^3

Density
(calculated) 2.878 g/cm^3

Figure of merit
F_{30} = 31.9(0.016,58)

Additional pattern
PDF card 1-0126 (Hanawalt et al., 1938).

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

Mori, H. and Ito, T. (1950). Acta Crystallogr. 3, 1.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
7.77	36	1 1 0	11.38
6.62	100	0 2 0	13.36
4.808	61	2 0 0	18.44
4.480	32	-1 0 1	19.80
4.277	10	0 1 1	20.75
4.005	20	1 3 0	22.18
3.799	50	1 0 1	23.40
3.576	8	-2 1 1	24.88
3.297	2	0 4 0	27.02
3.159	33	0 3 1	28.23
2.924	72	-3 0 1	30.55
2.722	6	2 4 0	32.88
2.675	46	-3 2 1	33.47
2.657	35	-1 4 1	33.71
2.591	10	3 3 0	34.59
2.548	2	1 5 0	35.19
2.491	19	1 4 1	36.03
2.389	27	3 0 1	37.62
2.283M	17	-1 1 2	39.44
2.283M		0 5 1	39.44
2.241	2	-2 0 2	40.20
2.189	18	-3 4 1	41.20
2.153	14	-2 5 1	41.93
2.122	5	-2 2 2	42.56
2.079	3	1 1 2	43.49
2.039	11	3 5 0	44.39
1.975	1	-1 6 1	45.92
1.938	3	4 1 1	46.83
1.901	19	1 3 2	47.81
1.872	6	-3 3 2	48.61
1.857	5	-4 0 2	49.01
1.789	3	4 3 1	51.00
1.6503M	5	0 8 0	55.65
1.6503M		5 0 1	55.65

Nickel Sulfate Hydrate (Nickel-hexahydrite), β-$NiSO_4 \cdot 6H_2O$

Synonym
Nickel sulfate hexahydrate

CAS registry no.
10101-97-0

Sample
The sample was prepared by slow evaporation from a solution of nickel sulfate in an aqueous solution of H_3PO_4.

Color
Strong green

Structure
Monoclinic, A2/a (15), Z = 8. Isostructural with other divalent hexahydrate sulfates (Sutor, 1959). The structure of $MgSO_4 \cdot 6H_2O$ was discussed by Ide (1938).

Lattice constants of this sample
a = 24.188(5) Å
b = 7.2410(14)
c = 9.895(2)
β = 98.41(2)°

a/b = 3.3404
c/b = 1.3665

Volume
1714.4 Å^3

Density
(calculated) 2.037 g/cm^3

Polymorphism
$NiSO_4 \cdot 6H_2O$ also occurs in a tetragonal form as the mineral retgersite.

Figure of merit
F_{30} = 52.3(0.013,45)

Additional patterns
PDF card 18-891 (Oleinikov et al., 1965)

PDF card 26-1288 (Nawaz, 1973)

References

Ide, K. H. (1938). Naturwissenschaften, 26, 411.

Nawaz, R. (1973). Mineral. Mag. 39, 246.

Oleinikov, B. V., Shvartsev, S. L., Mandrikova, N. T., and Oleinikova, N. N. (1965). Zap. Vses. Mineral, O-Va. 94, 534.

Sutor, D. J. (1959). Acta Crystallogr. 12, 72.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
5.98	5	4 0 0	14.80
5.824	20	0 1 1	15.20
5.538	6	1 1 1	15.99
5.424	21	-2 1 1	16.33
5.061	21	2 1 1	17.51
4.900M	51	-3 1 1	18.09
4.900M		0 0 2	18.09
4.782	24	-2 0 2	18.54
4.519	6	3 1 1	19.63
4.367	100	-4 1 1	20.32
4.314	21	2 0 2	20.57
4.096	22	-4 0 2	21.68
4.003	60	4 1 1	22.19
3.865	4	-5 1 1	22.99
3.625	14	0 2 0	24.54
3.576	9	1 2 0	24.88
3.544M	20	5 1 1	25.11
3.544M		4 0 2	25.11
3.466	3	2 2 0	25.68
3.432	8	-6 1 1	25.94
3.340	8	-6 0 2	26.67
3.162	7	6 1 1	28.20
3.068	2	-7 1 1	29.08
3.001	6	-1 1 3	29.75
2.992	11	8 0 0	29.84
2.979	17	-2 1 3	29.97
2.916M	26	-1 2 2	30.63
2.916M		-3 1 3	30.63
2.890M	38	6 0 2	30.92
2.890M		5 2 0	30.92
2.860	1	1 2 2	31.25
2.818	8	-4 1 3	31.73
2.801	1	2 1 3	31.92
2.774	9	2 2 2	32.25
2.737	2	-8 0 2	32.69
2.711	1L	-4 2 2	33.02
2.690	5	-5 1 3	33.28
2.681	5	6 2 0	33.39
2.660	5	3 2 2	33.66
2.588	1L	-5 2 2	34.63
2.570	9	8 1 1	34.88
2.553	2	-6 1 3	35.12
2.471	12	-2 0 4	36.33
2.454	3	-6 2 2	36.59
2.408	2	-7 1 3	37.31

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ			2θ(°)
2.392M	3	10	0	0	37.57
2.392M		-4	0	4	37.57
2.342+	1	0	3	1	38.41
2.342+		9	1	1	38.41
2.331	1	2	0	4	38.59
2.306	5	8	2	0	39.03
2.285+	4	-10	0	2	39.41
2.285+		2	3	1	39.41
2.272	13	-3	3	1	39.64
2.246	5	6	1	3	40.12
2.229	2	3	3	1	40.44
2.209	5	-4	3	1	40.82
2.183	3	-8	2	2	41.32
2.157M	3	4	0	4	41.85
2.157M		4	3	1	41.85
2.135	1	-5	3	1	42.30
2.098	1L	-11	1	1	43.08
2.076	1	5	3	1	43.57
2.052M	4	-9	2	2	44.09
2.052M		-6	3	1	44.09
2.047	3	-8	0	4	44.22
2.041M	2	-1	2	4	44.35
2.041M		-2	2	4	44.35
2.028	3	0	2	4	44.64
1.995M	7	-4	2	4	45.43
1.995M		12	0	0	45.43
1.990	10	6	3	1	45.55
1.981M	12	11	1	1	45.76
1.981M		8	1	3	45.76
1.954	5	-5	2	4	46.43
1.9199	3	1	3	3	47.31
1.9092	5	-2	1	5	47.59
1.8901M	7	0	1	5	48.10
1.8901M		2	3	3	48.10
1.8791M	4	-4	1	5	48.40
1.8791M		-11	1	3	48.40
1.8769	4	-8	3	1	48.46
1.8536	14	4	2	4	49.11
1.8378	4	12	1	1	49.56

Niobium, Nb

Synonym
Columbium

CAS registry no.
7440-03-1

Sample
The sample was obtained from Fansteel Products Co., N. Chicago, IL.

Color
Dark gray

Structure
Cubic, Im3m, Z = 2. The structure was determined by McLennan and Monkman (1929), Hägg (1930), and others.

Lattice constant of this sample
$a = 3.30332(13)$ Å

Volume
36.046 Å^3

Density
(calculated) 8.560 g/cm^3

Figure of merit
$F_8 = 102.8(0.010,8)$

Additional patterns
PDF card 16-1 (Hanawalt et al., 1938)

Nadler and Kempter (1959)

References

Hägg, G. (1930). Z. Phys. Chem. B 11, 433.

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

McLennan, J. C. and Monkman, R. J. (1929). Trans. R. Soc. Can. Sec. 3 23, 255.

Nadler, M. R. and Kempter, C. P. (1959). Anal. Chem. 31 1922.

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

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
2.336	100	1 1 0	38.51
1.6519	18	2 0 0	55.59
1.3484	28	2 1 1	69.68
1.1678	8	2 2 0	82.54
1.0446	11	3 1 0	95.02
.9535	3	2 2 2	107.78
.8830	13	3 2 1	121.48
.8258	2	4 0 0	137.74

Potassium Barium Phosphate, $KBaPO_4$

Synonym
Potassium barium orthophosphate

CAS registry no.
25640-29-3

Sample
The sample was made by heating a 1:1 molar mixture of $Ba(OH)_2$ and KH_2PO_4 at 750 °C for 2 days, regrinding and heating to 900 °C for 1 hour.

Color
Colorless

Structure
Orthorhombic, Pnam (62), Z = 4. (Struck and White, 1962). Isostructural with β-K_2SO_4, arcanite.

Lattice constants of this sample
a = 7.7084(5) Å
b = 9.9783(8)
c = 5.6649(5)

a/b = 0.7725
c/b = 0.5677

Volume
435.73 $Å^3$

Density
(calculated) 4.137 g/cm^3

Polymorphism
$KBaPO_4$ is reported to have a high temperature form which is hexagonal (Klement and Uffelmann, 1941). This is questioned by Struck and White (1962).

Figure of merit
F_{30} = 111.6(0.008,35)

Additional patterns
PDF card 14-229 (Struck and White, 1962)

Wanmaker and Spier (1962)

Majling, et al. (1979) calculated pattern

References

Klement, R. and Uffelmann, R. (1941). Naturwissenschaften 29, 300.

Majling, J., Raninec, Š., and Ďurovič, S. (1979). Calculated Powder Diffraction Patterns for Anhydrous Phosphates (Veda, Bratislova, Czechoslovakia.)

Struck, C. W. and White, J. (1962). Acta Crystallogr. 15, 290.

Wanmaker, W. L. and Spier, H. L. (1962). J. Electrochem. Soc. 109, 109.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.100	8	1 1 0	14.51
4.990	18	0 2 0	17.76
4.927	33	0 1 1	17.99
4.189	4	1 2 0	21.19
4.153	3	1 1 1	21.38
3.854	6	2 0 0	23.06
3.594	4	2 1 0	24.75
3.368	40	1 2 1	26.44
3.186	3	2 0 1	27.98
3.052M	94	1 3 0	29.24
3.052M		2 2 0	29.24
3.036	100	2 1 1	29.40
2.868	41	0 3 1	31.16
2.832	39	0 0 2	31.57
2.685M	4	1 3 1	33.34
2.685M		2 2 1	33.34
2.569	6	1 1 2	34.90
2.518	4	2 3 0	35.63
2.488	19	3 1 0	36.07
2.463	2	0 2 2	36.45
2.3732	2	1 4 0	37.88
2.3464	3	1 2 2	38.33
2.3008	5	2 3 1	39.12
2.2823M	14	3 2 0	39.45
2.2823M		2 0 2	39.45
2.2768	13	3 1 1	39.55
2.2250	7	2 1 2	40.51
2.1888	33	1 4 1	41.21
2.1187	3	3 2 1	42.64
2.0939	4	2 4 0	43.17
2.0765M	54	1 3 2	43.55
2.0765M		2 2 2	43.55
2.0335	15	3 3 0	44.52
1.9646	1L	2 4 1	46.17
1.9318	14	1 5 0	47.00
1.9271	14	4 0 0	47.12
1.9134	1L	3 3 1	47.48
1.8817M	4	0 5 1	48.33
1.8817M		2 3 2	48.33
1.8693	7	3 1 2	48.67
1.8557	4	0 1 3	49.05
1.8237	1L	4 0 1	49.97
1.7942	16	4 1 1	50.85
1.7724	1L	2 5 0	51.52
1.7218	5	1 2 3	53.15

Potassium Barium Phosphate, $KBaPO_4$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.7067	19	3 4 1	53.66
1.6719	12	2 1 3	54.87
1.6516	6	3 3 2	55.60
1.6424	6	0 3 3	55.94
1.6000	7	4 3 1	57.56
1.5962	17	1 5 2	57.71
1.5929	11	4 0 2	57.84
1.5765	2	3 5 0	58.50
1.5626	7	1 6 1	59.07
1.5268	7	2 6 0	60.60
1.5182	1	4 2 2	60.98
1.4776	9	1 4 3	62.84
1.4738	9	2 6 1	63.02
1.4554	1	3 2 3	63.91
1.4368	1	4 3 2	64.84
1.4255	3	5 2 1	65.42
1.4164	5	0 0 4	65.89
1.4017	2	1 7 0	66.67
1.3984	3	5 3 0	66.85
1.3823	6	0 7 1	67.73
1.3789	5	1 1 4	67.92
1.3770	1	3 5 2	68.03
1.3555	4	3 6 1	69.26
1.3442	4	2 6 2	69.93
1.3368M	4	2 7 0	70.37
1.3368M		4 1 3	70.37
1.3069	2	5 2 2	72.23
1.3015M	5	4 2 3	72.58
1.3015M		2 7 1	72.58
1.2992	2	3 4 3	72.73
1.2850M	7	1 3 4	73.66
1.2850M		6 0 0	73.66
1.2777	4	5 4 1	74.15
1.2564	5	1 7 2	75.63
1.2544	2	5 3 2	75.77
1.2431	4	6 1 1	76.58
1.2321M	4	1 6 3	77.39
1.2321M		0 4 4	77.39
1.2202	1	5 5 0	78.29
1.2173	1	3 7 1	78.51
1.1929	2	5 5 1	80.44
1.1868M	1	2 8 0	80.94
1.1868M		4 4 3	80.94
1.1728M	1	2 4 4	82.11
1.1728M		6 3 1	82.11
1.1703	2	6 0 2	82.33
1.1624M	2	3 3 4	83.01
1.1624M		6 1 2	83.01

Potassium Calcium Phosphate, $KCaPO_4$

Synonym
Potassium calcium orthophosphate

CAS registry no.
18901-69-4

Sample
The sample was made at NBS by heating equimolar amounts of $CaCO_3$ and KH_2PO_4 at 800 °C over night, reground, heated to 900° over night and then at 1100 °C for 1 hour.

Color
Colorless

Structure
Hexagonal, $P\bar{3}ml$ (164), Z = 2. (Bredig, 1941)
Isostructural with aphthitalite, $(K,Na)_3Na(SO_4)_2$
The structure of aphthitalite was determined by Gossner (1928).

Lattice constants of this sample
a = 5.5085(4)Å
c = 7.5020(8)

c/a = 1.3619

Volume
197.14 $Å^3$

Density
(calculated) 2.934 g/cm^3

Polymorphism
There are several other forms of $KCaPO_4$ (Znamierowska, 1979). Bredig (1941) refers to the present form as α.

Figure of merit
F_{27} = 38.1(0.011,65)

Additional patterns
PDF card 3-619 (Bredig, 1942)

Wanmaker and Spier (1962)

References

Bredig, J. (1941). J. Am. Chem. Soc. 63, 2533.

Bredig, J. (1942). J. Phys. Chem. 46, 747.

Gossner (1928). Neues. Jahrb. Mineral. Geol. Palaeontol. Abh. Abt. A, 57, 89.

Wanmaker, W. L. and Spier, H. L. (1962). J. Electrochem. Soc. 109, 109.

Znamierowska, T. (1979). Pol. J. Chem. 53, 1415.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±1	hkℓ			2θ(°)
4.024	8	1	0	1	22.07
3.750	12	0	0	2	23.71
2.949	100	1	0	2	30.28
2.754	100	1	1	0	32.49
2.386	2	2	0	0	37.67
2.272	17	2	0	1	39.64
2.0125	39	2	0	2	45.01
1.8762	6	0	0	4	48.48
1.8038	2	2	1	0	50.56
1.7450	3	1	0	4	52.39
1.7255	2	2	0	3	53.03
1.6251	14	2	1	2	56.59
1.5906	12	3	0	0	57.93
1.5497	12	1	1	4	59.61
1.4643	1L	3	0	2	63.48
1.3770	9	2	2	0	68.03
1.2929	1	2	2	2	73.14
1.2478	4	3	1	2	76.24
1.2128	3	3	0	4	78.86
1.2097	2	1	0	6	79.10
1.1365	1	4	0	2	85.34
1.1101	1	2	2	4	87.88
1.1073	1	2	0	6	88.16
1.0507	1	3	2	2	94.30
1.0410	2	4	1	0	95.46
1.0275	1L	2	1	6	97.13
1.0030	1L	4	1	2	100.35

Potassium Strontium Phosphate, $KSrPO_4$

Synonym
Potassium strontium orthophosphate

CAS registry no.
53201-92-6

Sample
The sample was made at NBS by heating equimolar amounts of KH_2PO_4 and $SrCO_3$ at 900 °C for 1 hour; it was reground and heated to 1250 °C for 1 hour.

Color
Colorless

Structure
Orthorhombic, Pnam (62), Z = 4. Isostructural with arcanite, β-K_2SO_4. (Klement and Kresse, 1961) The structure of arcanite was determined by Robinson, (1958). This phase of $KSrPO_4$ can also be indexed on a hexagonal cell with a = 11.124 and c = 7.350, this being similar to the high form of K_2SO_4, but with a doubled a.

Lattice constants of this sample
a = 7.3507(7) Å
b = 9.6340(9)
c = 5.5621(6)

a/b = 0.7630
c/b = 0.5773

Volume
393.89 Å^3

Density
(calculated) 3.738 g/cm^3

Polymorphism
$KSrPO_4$ is reported to have several other forms (Klement and Uffelmann, 1941).

Figure of merit
F_{30} = 82.0(0.008,45)

Additional patterns
PDF card 14-40 (Klement and Kresse, 1961)

Wanmaker and Spier, 1962

References
Klement, R. and Kresse, P. (1961). Z. Anorg. Allg. Chem. 310, 62.

Klement, R. and Uffelmann, R. (1941). Naturwissenschaften 29, 300.

Robinson, M. T. (1958). J. Phys. Chem. 62, 925.

Wanmaker, W. L. and Spier, H. L. (1962). J. Electrochem. Soc. 109, 109.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
5.836	5	1 1 0	15.17
4.813M	19	0 2 0	18.42
4.813M		0 1 1	18.42
4.028M	8	1 2 0	22.05
4.028M		1 1 1	22.05
3.433	2	2 1 0	25.93
3.263	27	1 2 1	27.31
3.066	5	2 0 1	29.10
2.943	32	1 3 0	30.35
2.922M	100	2 2 0	30.57
2.922M		2 1 1	30.57
2.780M	93	0 3 1	32.17
2.780M		0 0 2	32.17
2.587	3	2 2 1	34.65
2.512	4	1 1 2	35.72
2.418	8	2 3 0	37.15
2.4107M	5	0 4 0	37.27
2.4107M		0 2 2	37.27
2.3744	19	3 1 0	37.86
2.2890M	10	1 4 0	39.33
2.2890M		1 2 2	39.33
2.2177M	10	2 3 1	40.65
2.2177M		2 0 2	40.65
2.1843M	6	3 2 0	41.30
2.1843M		3 1 1	41.30
2.1613	7	2 1 2	41.76
2.1168	24	1 4 1	42.68
2.0330	6	3 2 1	44.53
2.0214	22	1 3 2	44.80
2.0150M	36	2 4 0	44.95
2.0150M		2 2 2	44.95
1.9478	9	3 3 0	46.59
1.8942	1	2 4 1	47.99
1.8639	8	1 5 0	48.82
1.8378M	6	3 3 1	49.56
1.8378M		4 0 0	49.56
1.8251	6	2 3 2	49.93
1.8203+	6	0 4 2	50.07
1.8203+		0 1 3	50.07
1.8061M	7	3 1 2	50.49
1.8061M		4 1 0	50.49
1.7447	1	4 0 1	52.40
1.7167+	11	4 2 0	53.32
1.7167+		4 1 1	53.32
1.7064	1	2 5 0	53.67

Potassium Strontium Phosphate, $KSrPO_4$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
1.6840	3	1 2 3	54.44
1.6552	1	2 0 3	55.47
1.6413M	12	3 4 1	55.98
1.6413M		4 2 1	55.98
1.6314M	9	2 4 2	56.35
1.6314M		2 1 3	56.35
1.6056M	6	0 6 0	57.34
1.6056M		0 3 3	57.34
1.5951M	4	3 3 2	57.75
1.5951M		4 3 0	57.75
1.5655	1L	2 2 3	58.95
1.5481	8	1 5 2	59.68
1.5332M	6	4 3 1	60.32
1.5332M		4 0 2	60.32
1.5141M	3	3 5 0	61.16
1.5141M		4 1 2	61.16
1.5101	5	1 6 1	61.34
1.4713M	2	2 6 0	63.14
1.4713M		2 3 3	63.14
1.4610M	4	4 4 0	63.64
1.4610M		4 2 2	63.64
1.4408	4	1 4 3	64.64
1.4222	1	2 6 1	65.59
1.4132M	1	3 2 3	66.06
1.4132M		4 4 1	66.06
1.4058M	3	5 2 0	66.45
1.4058M		5 1 1	66.45
1.3907M	6	0 6 2	67.27
1.3907M		0 0 4	67.27
1.3836	1	4 3 2	67.66
1.3634	1	5 2 1	68.80
1.3526	1	1 1 4	69.43
1.3365M	3	5 3 0	70.39
1.3365M		0 7 1	70.39

Silver Telluride (Hessite), Ag_2Te

CAS registry no.
12002-98-1

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA.

Color
Unground: medium gray
Ground: dark gray

Structure
Monoclinic, P2/n (13), Z = 8. The space group was assumed from absences in the present powder data. The cell having "b" equal to half our value below would not allow an index for the very weak line at d = 8.91. This reflection appeared consistently in patterns from randomly oriented samples, but only appeared intermittently from non-randomly oriented mountings. Frueh (1959) gave the space group $P2_1/n$ with b'=b/2.

Lattice constants of this sample
a = 8.1698(15) Å
b = 8.940(2)
c = 8.0653(15)
β = 112.793(15)°

a/b = 0.9138
c/b = 0.9022

Volume
543.07 $Å^3$

Density
(calculated) 8.399 g/cm^3

Polymorphism
Frueh (1959) uses the following nomenclature. Form III (described here) is stable from room temperature up to a range from 105 °C to 145 °C. Form II is stable between the ranges 105 to 145 °C and 690 to 802 °C. Form I is stable between the range 690 to 802 °C and the melting point.

Figure of merit
F_{30} = 23.1(0.015,89)

Additional patterns
PDF card 12-695 (Thompson, 1949)

Frueh (1959)

Tokody (1932)

References

Frueh, A. J., Jr. (1959). Z. Kristallogr. Kristallgeom. Kristallphys. Kristallchem. 112, 44.

Thompson, R. M. (1949). Am. Mineral. 34, 342.

Tokody, L. (1932). Z. Kristallogr. Kristallgeom. Kristallphys. Kristallchem. 82, 154.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
8.91	5	0 1 0	9.92
6.76	10	-1 0 1	13.08
4.492	8	1 0 1	19.75
3.764	5	2 0 0	23.62
3.726	7	-1 2 1	23.86
3.382	8	-2 0 2	26.33
3.169	24	1 2 1	28.14
3.003	52	-2 2 1	29.73
2.983M	59	-1 2 2	29.93
2.983M		0 3 0	29.93
2.880	100	2 2 0	31.03
2.857	24	0 2 2	31.28
2.695	10	-2 2 2	33.21
2.453	6	2 2 1	36.60
2.444	6	1 2 2	36.75
2.323M	41	0 3 2	38.73
2.323M		-3 2 1	38.73
2.301	96	-1 2 3	39.12
2.254	58	-3 0 3	39.97
2.246M	61	-3 2 2	40.11
2.246M		2 0 2	40.11
2.235+	30	0 4 0	40.33
2.235+		-2 2 3	40.33
2.189	30	3 2 0	41.21
2.167	12	0 2 3	41.65
2.141+	54	3 0 1	42.17
2.141+		0 4 1	42.17
2.122M	22	1 0 3	42.57
2.122M		-1 4 1	42.57
2.026	15	-4 0 2	44.70
2.012	6	-3 2 3	45.03
2.002M	4	-2 0 4	45.25
2.002M		1 4 1	45.25
1.958M	6	-3 3 2	46.33
1.958M		-2 4 1	46.33
1.953M	5	-2 1 4	46.45
1.953M		-1 4 2	46.45
1.930	10	3 2 1	47.04
1.884	1L	4 0 0	48.27
1.863	3	-2 4 2	48.84
1.858	5	0 0 4	48.98
1.845	2	-4 2 2	49.36
1.821M	4	-1 2 4	50.06
1.821M		0 1 4	50.06
1.7737	11	1 4 2	51.48
1.7355M	2	-3 2 4	52.70
1.7355M		4 2 0	52.70
1.6950	9	-3 4 2	54.06
1.6904	9	-4 0 4	54.22
1.6020	6	-5 0 1	57.48

Silver Telluride (Hessite), Ag_2Te - (continued)

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.5874M	5	-2 1 5	58.06
1.5874M		-3 4 3	58.06
1.5839	9	2 4 2	58.20
1.5797M	7	-2 5 2	58.37
1.5797M		-1 0 5	58.37
1.5752	4	-3 0 5	58.55
1.5578	2	1 2 4	59.27
1.5399	2	1 4 3	60.03
1.5077	2	-5 2 1	61.45
1.4974M	2	3 0 3	61.92
1.4974M		-5 2 3	61.92
1.4573M	2	2 0 4	63.82
1.4573M		3 5 0	63.82
1.4454	11	-4 4 3	64.41
1.4404M	8	-3 4 4	64.66
1.4404M		4 4 0	64.66
1.4107M	3	-5 3 1	66.19
1.4107M		0 2 5	66.19
1.4036	15	-4 2 5	66.57
1.3965M	18	-1 6 2	66.95
1.3965M		-1 3 5	66.95
1.3931	4	4 2 2	67.14
1.3761	2	5 0 1	68.08
1.3411+	6	-2 0 6	70.11
1.3411+		4 4 1	70.11
1.3283	3	2 6 1	70.89
1.3263M	2	1 6 2	71.01
1.3263M		-2 1 6	71.01
1.3077	10	-2 4 5	72.18
1.3029M	11	1 2 5	72.49
1.3029M		-1 6 3	72.49
1.2994	8	-6 0 4	72.71
1.2946	7	-5 2 5	73.03
1.2901+	8	-2 6 3	73.32
1.2901+		-1 4 5	73.32
1.2814	10	3 6 0	73.90
1.2773M	5	0 7 0	74.18
1.2773M		0 6 3	74.18
1.2555M	4	6 0 0	75.69
1.2555M		-1 7 1	75.69
1.2489	7	5 4 0	76.16
1.2390+	5	1 3 5	76.88
1.2390+		-4 2 6	76.88
1.2271+	2	5 1 2	77.77
1.2271+		3 2 4	77.77

Sodium Barium Phosphate, $NaBaPO_4$

Synonym
Sodium barium orthophosphate

CAS registry no.
53201-91-5

Sample
The sample was prepared at NBS. Na_2CO_3 and $2BaHPO_4$ were ground together, heated up gradually to 800 °C, re-ground, returned to oven at 800 °C, heated to 1000 °C, and held there for 1 hour.

Color
Colorless

Optical data
Low double refraction with an average value ~1.612.

Structure
Hexagonal, $P\bar{3}m1$ (164), Z = 2, isostructural with aphthitalite, $(K,Na)_3Na(SO_4)_2$. The structure was determined by Calvo and Faggiani (1975).

Lattice constants of this sample
a = 5.6181(3) Å
c = 7.2636(5)

c/a = 1.2929

Volume
198.55 $Å^3$

Density
(calculated) 4.270 g/cm^3

Polymorphism
Forms with other than hexagonal symmetry have been reported (Klement and Kresse, 1961; Kolsi et al., 1981; Paques-Ledent, 1974). Their cells may be related to the hexagonal cell above. An unrelated tetragonal form was reported by Klement and Uffelmann (1941).

Figure of merit
F_{30} = 82.1(0.010,38)

Additional patterns
PDF card 14-204 (Wanmaker and Spier, 1962), indexed as orthorhombic

Majling et al. (1979) (calculated pattern)

Comment
A pattern given by Kolsi et al., (1981) is called monoclinic but can be indexed with the hexagonal cell here which has ½ the volume of the monoclinic cell.

References
Calvo, C. and Faggiani, R. (1975). Can. J. Chem. 53, 1849.

Klement, R. and Kresse, P. (1961). Z. Anorg. Allg. Chem. 310, 62.

Klement, R. and Uffelmann, R. (1941). Naturwissenschaften 29, 300.

Kolsi, A. W., Quarton, M., and Freundlich, W. (1981). Ann. Chim. Paris 6, 411.

Majling, J., Raninec, Š., and Ďurovič, S. (1979). Calculated Powder Diffraction Patterns for Anhydrous Phosphates (VEDA, Bratislava, Czechoslovakia).

Paques-Ledent, M.-Th. (1974). Ind. Chim. Belge 39, 845.

Wanmaker, W. L. and Spier, H. L. (1962). J. Electrochem. Soc. 109, 109.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal std. Fluorophlogopite SRM 675

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
7.27	4	0 0 1	12.17
4.868	3	1 0 0	18.21
4.044	59	1 0 1	21.96
3.632	1	0 0 2	24.49
2.910	100	1 0 2	30.70
2.808	100	1 1 0	31.84
2.620	8	1 1 1	34.20
2.423	22	0 0 3	37.08
2.307	32	2 0 1	39.01
2.222	7	1 1 2	40.57
2.1672	6	1 0 3	41.64
2.0210	50	2 0 2	44.81
1.8337	25	1 1 3	49.68
1.8155	3	0 0 4	50.21
1.7824	11	2 1 1	51.21
1.7008	13	1 0 4	53.86
1.6405	24	2 1 2	56.01
1.6219	14	3 0 0	56.71
1.5826	1	3 0 1	58.25
1.5247	3	1 1 4	60.69
1.4802	1	3 0 2	62.72
1.4641	2	2 1 3	63.49
1.4548	10	2 0 4	63.94
1.4045	12	2 2 0	66.52
1.3920	5	1 0 5	67.20
1.3472	6	3 0 3	69.75
1.3265	3	3 1 1	71.00
1.2920	10	2 1 4	73.20
1.2651	8	3 1 2	75.02
1.2474	3	2 0 5	76.27
1.2148	5	2 2 3	78.71
1.2095	2	3 0 4	79.12
1.1996	2	4 0 1	79.90
1.1786	1	3 1 3	81.62
1.1748	1	1 0 6	81.94

Sodium Barium Phosphate, $NaBaPO_4$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.1537	2	4 0 2	83.78
1.1400	4	2 1 5	85.02
1.1116	5	1 1 6	87.73
1.1031	2	3 2 1	88.58
1.0868	1L	4 0 3	90.27
1.0831	4	3 1 4	90.66
1.0669	4	3 2 2	92.44
1.0620	3	4 1 0	92.99
1.0150	2	1 0 7	98.74
1.0110	2	2 1 6	99.27
.9887	2	3 1 5	102.36
.9724	3	4 1 3	104.77
.9702	4	3 0 6	105.12
.9546	2	2 0 7	107.60
.9511	3	3 2 4	108.18

Sodium Strontium Phosphate, $NaSrPO_4$

Synonym
Sodium strontium orthophosphate

CAS registry no.
19553-80-1

Sample
The sample was made at NBS by heating a 2:2:1 molar mixture of $(NH_4)_2HPO_4$, $SrCO_3$, and Na_2CO_3 at 1000 °C for 2 days.

Color
Colorless

Structure
Monoclinic, A*/*, Z = 16. The unit cell was determined by the Visser program (1969), and the Z assumed for a reasonable density.

Lattice constants of this sample

a = 20.414(4)Å
b = 5.429(11)
c = 17.246(3)
β = 101.76(2)°

a/b = 3.7602
c/b = 3.1766

Volume
1871.21 $Å^3$

Density
(calculated) 2.919 g/cm^3

Polymorphism
Several other cells have been reported (Klement and Uffelmann, 1941; Bredig, 1942). Both of these references and Klement and Steckenreiter (1940) assume there is a transformation. The phase in this study is assumed to be the low temperature form.

Figure of merit
F_{30} = 43.4(0.011,63)

M_{20} = 20.6

Additional pattern
PDF card 14-269 (Wanmaker and Spier, 1962)

References
Bredig, M. A. (1942). J. Phys. Chem. 46, 749.

Klement, R. and Steckenreiter, F. (1940). Z. Anorg. Allg. Chem. 245, 236.

Klement, R. and Uffelmann, R. (1941). Naturwissenschaften 29, 300.

Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

Wanmaker, W. L. and Spier, H. L. (1962). J. Electrochem. Soc. 109, 109.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±5	hkℓ	2θ(°)
9.98	2	2 0 0	8.85
8.43M	10	0 0 2	10.48
8.43M		-1 0 2	10.48
7.20	2	-2 0 2	12.28
6.66	4	3 0 0	13.28
5.886	1L	2 0 2	15.04
5.836	1	-3 0 2	15.17
5.166	9	0 1 1	17.15
5.078	1	-1 1 1	17.45
4.930	1	1 1 1	17.98
4.779	3	3 0 2	18.55
4.709	4	-2 1 1	18.83
4.478	6	2 1 1	19.81
4.209M	5	-3 1 1	21.09
4.209M		-2 0 4	21.09
3.996	3	5 0 0	22.23
3.961M	7	3 1 1	22.43
3.961M		4 0 2	22.43
3.931	8	-5 0 2	22.60
3.906	11	0 1 3	22.75
3.828	5	-2 1 3	23.22
3.632	7	2 0 4	24.49
3.602M	12	-4 0 4	24.70
3.602M		-3 1 3	24.70
3.484	10	4 1 1	25.55
3.356	6	5 0 2	26.54
3.330	9	6 0 0	26.75
3.180	4	3 1 3	28.04
2.922	30	-6 0 4	30.57
2.903	44	6 0 2	30.78
2.886M	55	4 1 3	30.96
2.886M		-6 1 1	30.96
2.866M	62	0 1 5	31.18
2.866M		-2 0 6	31.18
2.805	2	-3 0 6	31.88
2.772	11	1 1 5	32.27
2.732	100	-6 1 3	32.75
2.715	48	0 2 0	32.97
2.646	1L	5 0 4	33.85
2.615	7	5 1 3	34.26
2.585M	5	0 2 2	34.67
2.585M		-1 2 2	34.67
2.576	6	2 0 6	34.80
2.550	4	-5 1 5	35.17
2.514	1	3 2 0	35.68

d(Å)	I^{rel} $\sigma = \pm 5$	hkℓ	2θ(°)
2.464	2	2 2 2	36.43
2.387M	9	-6 1 5	37.66
2.387M		4 2 0	37.66
2.356	1	-4 2 2	38.16
2.320	1	4 1 5	38.78
2.306	2	-8 1 1	39.02
2.282M	2	0 2 4	39.45
2.282M		-2 2 4	39.45
2.262	29	4 0 6	39.82
2.246M	15	-7 0 6	40.11
2.246M		5 2 0	40.11
2.238M	12	-1 1 7	40.27
2.238M		-3 2 4	40.27
2.219M	2	9 0 0	40.62
2.219M		-3 1 7	40.62
2.205	3	0 1 7	40.90
2.196	4	8 1 1	41.06
2.175	7	2 2 4	41.49
2.169M	3	-4 2 4	41.60
2.169M		7 0 4	41.60
2.148	3	1 1 7	42.03
2.105M	9	6 2 0	42.94
2.105M		-4 0 8	42.94
2.092M	3	-8 0 6	43.22
2.092M		3 2 4	43.22
2.0550	4	1 0 8	44.03
2.0466M	7	9 0 2	44.22
2.0466M		-5 0 8	44.22
2.0409	7	-10 0 2	44.35

Sodium Titanium Phosphate, $NaTi_2(PO_4)_3$

Synonyms
Sodium titanium orthophosphate
NTP

CAS registry no.
22239-24-3

Sample
The sample was made at NBS by heating a 1:2:2 molar mixture of $NaH_2PO_4 \cdot H_2O$, $(NH_4)_2HPO_4$, and TiO_2 (anatase) at 1000 °C. It was then re-ground and heated at 1200° C for 18 hours.

Color
Colorless

Structure
Rhombohedral, $R\bar{3}c$ (167). Isostructural with $NaZr_2(PO_4)_3$ and other similar phosphates. The structure of $NaZr_2(PO_4)_3$ was determined by Hagman and Kierkegaard (1968).

Lattice constants of this sample
Hexagonal axes
a = 8.4912(3)Å
c = 21.7858(12)

c/a = 2.5657
Z = 6

Volume
1360.35 $Å^3$

Density
(calculated) 2.957 g/cm^3

Polymorphism
Götz and Niebergall (1969) report a cubic form of $NaTi_2(PO_4)_3$ in the ternary system $NaPO_3$-NaF-TiO_2.

Figure of merit
F_{30} = 112.7(0.007,36)

Additional patterns
PDF card 23-1410 (Hagman and Kierkegaard, 1968)

Chernorukov (1978)

References

Chernorukov, N. G. (1978). Russ. J. Inorg. Chem. Engl. Transl. 51, 425.

Götz, W. and Niebergall, R. (1969). Naturwissenschaften 56, 35.

Hagman, L.-O. and Kierkegaard, P. (1968). Acta Chem. Scand. 22, 1822.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.095	14	0 1 2	14.52
4.377	20	1 0 4	20.27
4.245	32	1 1 0	20.91
3.666	100	1 1 3	24.26
3.632	10	0 0 6	24.49
3.485	4	2 0 2	25.54
3.048	28	0 2 4	29.28
2.759M	64	1 1 6	32.42
2.759M		2 1 1	32.42
2.694	2	1 2 2	33.23
2.5532	1	0 1 8	35.12
2.4761	2	2 1 4	36.25
2.4520	16	3 0 0	36.62
2.1883	2	2 0 8	41.22
2.1032	7	1 1 9	42.97
2.0733	2	2 1 7	43.62
2.0378	5	2 2 3	44.42
2.0322M	6	3 0 6	44.55
2.0322M		1 3 1	44.55
2.0053	1	3 1 2	45.18
1.9455	15	1 2 8	46.65
1.9100	3	1 3 4	47.57
1.8740	2	0 2 10	48.54
1.8473	2	3 1 5	49.29
1.8330	16	2 2 6	49.70
1.8152	5	0 0 12	50.22
1.8128	6	0 4 2	50.29
1.7419	1L	4 0 4	52.49
1.7144	9	2 1 10	53.40
1.7058	7	1 3 7	53.69
1.6821	1L	3 2 1	54.51
1.6674	1	2 3 2	55.03
1.6328	6	3 1 8	56.30
1.6115	5	3 2 4	57.11
1.6048	11	4 1 0	57.37
1.5959	2	2 2 9	57.72
1.5733	2	2 3 5	58.63
1.5670	4	4 1 3	58.89
1.5236	5	0 4 8	60.74
1.4889	6	1 3 10	62.31
1.4678	6	4 1 6	63.31
1.4589	2	3 0 12	63.74
1.4331	5	2 0 14	65.03
1.4199	4	0 5 4	65.71
1.4153	3	3 3 0	65.95
1.4051	2	4 0 10	66.49
1.3890	1L	3 3 3	67.36
1.3798	1	2 2 12	67.87
1.3741	3	1 1 15	68.19
1.3583	3	1 2 14	69.10

Sodium Titanium Phosphate, $NaTi_2(PO_4)_3$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.3467	1	2 4 4	69.78
1.3373	1	4 1 9	70.34
1.3338	1	3 2 10	70.55
1.3239	1L	4 2 5	71.16
1.3183M	1	3 3 6	71.51
1.3183M		5 1 1	71.51
1.2942M	1	1 3 13	73.05
1.2942M		5 0 8	73.05
1.2837	9	5 1 4	73.75
1.2642	4	1 5 5	75.08
1.2371	2	3 1 14	77.02
1.2257	7	6 0 0	77.87
1.2157	3	5 1 7	78.64
1.2102	1	0 0 18	79.06
1.2014	1L	3 4 2	79.76
1.1886M	1	3 2 13	80.79
1.1886M		1 5 8	80.79
1.1772	1	5 2 0	81.74
1.1717	1L	2 4 10	82.21
1.1637M	1	1 1 18	82.90
1.1637M		1 2 17	82.90
1.1438	3	2 3 14	84.67
1.1267	1L	4 3 7	86.26
1.1200M	4	5 2 6	86.91
1.1200M		1 6 1	86.91
1.1049	2	3 4 8	88.40
1.0984	7	1 6 4	89.06

Sodium Zirconium Phosphate, $NaZr_2(PO_4)_3$

Synonyms
Sodium zirconium orthophosphate
NZP

CAS registry no.
19527-81-2

Sample
The sample was made at NBS by heating a 1:2:2 molar mixture of $NaH_2PO_4 \cdot H_2O$, $(NH_4)_2HPO_4$, and ZrO_2, slowly up to 1000 °C. It was then re-ground and heated to 1200 °C overnight.

Color
Colorless

Structure
Rhombohedral, $R\bar{3}c(167)$. Isostructural with $NaTi_2(PO_4)_3$ and many other similar phosphates. The structure has been determined by Hagman and Kierkegaard, (1968) and confirmed by Hong (1976).

Lattice constants of this sample
Hexagonal axes

a = 8.8048(4) Å
c = 22.7572(14)

c/a = 2.5846
Z = 6

Volume
1527.88 $Å^3$

Density
(calculated) 3.198 g/cm^3

Figure of merit
F_{30} = 103.6(0.007,43)

Additional patterns
PDF card 23-1411 (Hagman and Kierkegaard, 1968)

PDF card 24-1180 (Clearfield et al., 1969)

Majling, et al. (1979) calculated pattern

References

Clearfield, A., Duax, W. L., Medina, A. S., Smith, G. D., and Thomas, J. R. (1969). J. Phys. Chem. 73, 3424.

Hagman, L-O. and Kierkegaard, P. (1968). Acta Chem. Scand. 22, 1822.

Hong, H. Y-P. (1976). Mater. Res. Bull. 11, 173.

Majling, J., Raninec, Š., and Ďurovič, S. (1979). Calculated Powder Diffraction Patterns for Anhydrous Phosphates. (VEDA, Bratislava, Czechoslovakia)

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.430825 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
6.325	22	0 1 2	13.99
4.556	75	1 0 4	19.47
4.399	97	1 1 0	20.17
3.807	100	1 1 3	23.35
3.614	1	2 0 2	24.61
3.166	54	0 2 4	28.16
2.873	94	1 1 6	31.10
2.666	3	0 1 8	33.59
2.571	24	2 1 4	34.87
2.5419	42	3 0 0	35.28
2.2801	7	2 0 8	39.49
2.2016	6	2 2 0	40.96
2.1929	3	1 1 9	41.13
2.1802	3	1 0 10	41.38
2.1568	2	2 1 7	41.85
2.1116	10	3 0 6	42.79
2.0797	3	3 1 2	43.48
2.0248	21	1 2 8	44.72
1.9824	12	1 3 4	45.73
1.9542	6	0 2 10	46.43
1.9039	29	2 2 6	47.73
1.8802	5	0 4 2	48.37
1.8078	1	4 0 4	50.44
1.7860	22	2 1 10	51.10
1.7727	4	1 3 7	51.51
1.6967	9	3 1 8	54.00
1.6719	14	3 2 4	54.87
1.6638	25	4 1 0	55.16
1.6328	1	2 3 5	56.30
1.6251	2	4 1 3	56.59
1.5894	5	0 1 14	57.98
1.5834	4	0 4 8	58.22
1.5490	12	1 3 10	59.64
1.5401	1	3 2 7	60.02
1.5236	14	4 1 6	60.74
1.5197	1	3 0 12	60.91
1.4950	7	2 0 14	62.03
1.4787	4	3 1 11	62.79
1.4730	6	0 5 4	63.06
1.4676	7	3 3 0	63.32
1.4610	4	4 0 10	63.64
1.4406	1	3 3 3	64.65
1.4340	3	1 1 15	64.98
1.4157	9	1 2 14	65.93
1.3969	5	2 4 4	66.93

Sodium Zirconium Phosphate, $NaZr_2(PO_4)_3$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
1.3900	3	4 1 9	67.31
1.3869	5	3 2 10	67.48
1.3738	1	4 2 5	68.21
1.3688	3	3 3 6	68.49
1.3487	1	1 3 13	69.66
1.3314	8	5 1 4	70.70
1.3113	1	1 5 5	71.95
1.2886	1	3 1 14	73.42
1.2855	5	4 2 8	73.63
1.2751	1	2 1 16	74.33
1.2709	7	6 0 0	74.62
1.2643	3	0 0 18	75.07
1.2619	2	5 1 7	75.24
1.2373M	1	3 2 13	77.01
1.2373M		0 4 14	77.01
1.2243	1	4 3 4	77.98
1.2210	4	5 2 0	78.23
1.2176	4	2 4 10	78.49
1.2053M	2	5 2 3	79.45
1.2053M		6 0 6	79.45
1.1907	5	2 3 14	80.62
1.1738	1L	5 1 10	82.03
1.1624	5	5 2 6	83.01
1.1473	3	3 4 8	84.35
1.1421	1	1 5 11	84.82
1.1395	2	1 6 4	85.06
1.1319	2	3 0 18	85.77
1.1255	2	0 1 20	86.38
1.1122	3	5 0 14	87.67
1.1039	1	3 2 16	88.50
1.1008	2	4 4 0	88.82
1.0982	6	4 3 10	89.08
1.0903	1L	2 0 20	89.90
1.0879	1L	3 5 1	90.16
1.0845	1	0 7 2	90.52

Yttrium Chromium Oxide, $YCrO_3$

Synonym
Yttrium orthochromite

Sample
The sample was prepared at NBS by T. Negas.

Color
Medium yellowish green

Structure
Orthorhombic, Pnma (62), Z = 4, isostructural with $GdFeO_3$ (Geller and Wood, 1956). The structure of $GdFeO_3$ was determined by Geller (1956).

Lattice constants of this sample
a = 5.5237(3)Å
b = 7.5343(5)
c = 5.2427(3)

a/b = 0.7331
c/b = 0.6958

Volume
218.19 Å^3

Density
(calculated) 5.751 g/cm^3

Figure of merit
F_{30} = 116.2(0.008,31)

Additional patterns
PDF card 25-1078 (Gallagher and McCarthy, Penn State University, University Park, PA)

Geller and Wood (1956)

Keith and Roy (1954)

Looby and Katz (1954) (indexed with a monoclinic supercell)

References

Geller, S. (1956). J. Chem. Phys. 24, 1236.

Geller, S. and Wood, E. A. (1956). Acta Crystallogr. 9, 563.

Keith, M. L. and Roy, R. (1954). Am. Mineral. 39, 1.

Looby, J. T. and Katz, L. (1954). J. Am. Chem. Soc. 76, 6029.

Ruggiero, A. and Ferro, R. (1955). Gazz. Chim. Ital. 85, 892.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
4.306	2	0 1 1	20.61
3.805	5	1 0 1	23.36
3.770	5	0 2 0	23.58
3.396	22	1 1 1	26.22
2.762	22	2 0 0	32.39
2.676	100	1 2 1	33.46
2.621	27	0 0 2	34.18
2.593	11	2 1 0	34.56
2.443	1L	2 0 1	36.76
2.3678	2	1 0 2	37.97
2.3248	1	2 1 1	38.70
2.2647	5	0 3 1	39.77
2.2592	9	1 1 2	39.87
2.2276	6	2 2 0	40.46
2.1509	9	0 2 2	41.97
2.0967	11	1 3 1	43.11
2.0497	3	2 2 1	44.15
2.0049	2	1 2 2	45.19
1.9013	24	2 0 2	47.80
1.8831	18	0 4 0	48.29
1.8582	8	2 3 0	48.98
1.8434	13	2 1 2	49.40
1.7516	1L	2 3 1	52.18
1.7376	2	3 0 1	52.63
1.7230	2	1 3 2	53.11
1.7020	1	0 1 3	53.82
1.6933	20	3 1 1	54.12
1.6878	1	1 4 1	54.31
1.6665	1L	1 0 3	55.06
1.6264	3	1 1 3	56.54
1.5772	9	3 2 1	58.47
1.5564	11	2 4 0	59.33
1.5291	17	0 4 2	60.50
1.5238	27	1 2 3	60.73
1.5157	6	2 3 2	61.09
1.5066	1L	3 0 2	61.50
1.4764	1	2 0 3	62.90
1.4482	1L	0 5 1	64.27
1.4344	1L	0 3 3	64.96
1.4286	8	3 3 1	65.26
1.4008	1	1 5 1	66.72
1.3883	1L	1 3 3	67.40
1.3809	1L	4 0 0	67.81
1.3752	1L	2 2 3	68.13
1.3583	3	4 1 0	69.10

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.3380	10	2 4 2	70.30
1.3229	1	2 5 0	71.22
1.3107	4	0 0 4	71.99
1.2965	1	4 2 0	72.90
1.2920	1	3 3 2	73.20
1.2825	1L	2 5 1	73.83
1.2769	1L	3 4 1	74.21
1.2751	1	1 0 4	74.33
1.2713	1	1 5 2	74.59
1.2574	2	1 1 4	75.56
1.2558	1	0 6 0	75.67
1.2499	4	3 1 3	76.09
1.2481	2	1 4 3	76.22
1.2382	1L	0 2 4	76.94
1.2219	1	4 0 2	78.16
1.2101	1	4 3 0	79.07
1.2062	4	4 1 2	79.38
1.2015	3	3 2 3	79.75
1.1923	7	1 6 1	80.49
1.1841	3	2 0 4	81.16
1.1810	5	2 5 2	81.42
1.1699	3	2 1 4	82.36
1.1623M	3	4 2 2	83.02
1.1623M		2 4 3	83.02
1.1384	5	3 5 1	85.16
1.1315	3	3 3 3	85.81
1.1176	1	1 5 3	87.14
1.1137	1L	4 4 0	87.52
1.0987	4	4 3 2	89.03
1.0894	1L	4 4 1	90.00
1.0833	1L	4 0 3	90.64
1.0809	2	5 0 1	90.90
1.0758	2	0 4 4	91.45
1.0708	3	2 3 4	92.00
1.0699	3	5 1 1	92.10

Zinc Arsenate Hydrate (Koettigite), $Zn_3(AsO_4)_2 \cdot 8H_2O$

Synonyms
Zinc arsenate octahydrate
Zinc orthoarsenate octahydrate

Sample
The sample was made at NBS by adding a dilute solution of Na_2HAsO_4 dropwise to a slightly alkaline dilute solution of $ZnSO_4$.

Spectrographic analysis
Major impurities
0.05 to 0.25% P
0.002 to 0.01% B,Cu,Fe,Ni,Pb,Si
<0.005% Al, Mg

Color
Colorless

Structure
Monoclinic, I2/m (12), Z = 2. Vivianite structure (Wolfe, 1940). The structure of vivianite ($Fe_3(PO_4)_2 \cdot 8H_2O$) was discussed by Mori and Ito (1950).

Lattice constants of this sample
a = 10.118(2)Å
b = 13.431(2)
c = 4.7615(12)
β = 101.81(2)°

a/b = 0.7533
c/b = 0.3545

Volume
633.37 Å^3

Density
(calculated) 3.241 g/cm^3

Comment
Note the similarity between the data above and the data for the phase $Co_3(AsO_4)_2 \cdot 8H_2O$ also appearing in this Monograph.

Figure of merit
F_{30} = 67.1(0.010,44)

Additional pattern
PDF card 1-0744 (New Jersey Zinc Co.)

References

Mori, H. and Ito, T. (1950). Acta Crystallogr. 3, 1.

Wolfe, C. W. (1940). Am. Mineral. 25, 787.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
7.97	24	1 1 0	11.09
6.72	100	0 2 0	13.17
4.951	10	2 0 0	17.90
4.595	5	-1 0 1	19.30
4.403	14	0 1 1	20.15
4.083	9	1 3 0	21.75
3.987	6	2 2 0	22.28
3.923	15	1 0 1	22.65
3.660	7	-2 1 1	24.30
3.385	3	1 2 1	26.31
3.357	4	0 4 0	26.53
3.229	47	0 3 1	27.60
3.013	34	2 1 1	29.63
3.002	36	-3 0 1	29.74
2.900	1	-2 3 1	30.81
2.779	8	2 4 0	32.19
2.736	28	-3 2 1	32.70
2.711	25	-1 4 1	33.01
2.657	16	3 3 0	33.70
2.593	2	1 5 0	34.57
2.549	9	1 4 1	35.18
2.468	16	3 0 1	36.38
2.343	10	-1 1 2	38.39
2.328	22	0 5 1	38.64
2.238M	5	0 6 0	40.27
2.238M		-3 4 1	40.27
2.200	4	0 2 2	40.99
2.195	9	-2 5 1	41.08
2.1154	1	-4 3 1	42.71
2.0838	11	3 5 0	43.39
2.0396	1	2 6 0	44.38
2.0120	2	-1 6 1	45.02
1.9915	2	4 4 0	45.51
1.9874	2	3 4 1	45.61
1.9594M	8	2 0 2	46.30
1.9594M		5 1 0	46.30
1.9542	8	1 3 2	46.43
1.9443	3	1 6 1	46.68
1.9153M	3	-3 3 2	47.43
1.9153M		0 4 2	47.43
1.8434	7	4 3 1	49.40
1.7925	2	-3 6 1	50.90
1.7893	3	-4 5 1	51.00
1.7744	2	0 7 1	51.46
1.6884	9	1 5 2	54.29
1.6789	11	0 8 0	54.62
1.6643	11	-3 5 2	55.14
1.6604	10	4 6 0	55.28
1.6154	3	4 5 1	56.96
1.6023	2	6 2 0	57.47
1.5941	1	5 5 0	57.79
1.5621	3	-6 3 1	59.09
1.5441	2	1 8 1	59.85

Zinc Sulfate Hydrate (Gunningite), $ZnSO_4 \cdot H_2O$

Synonym
Zinc sulfate monohydrate

CAS registry no.
7446-19-7

Sample
The sample was made by allowing $ZnSO_4 \cdot 6H_2O$ to stay in dry air for several days.

Color
Colorless

Structure
Monoclinic, A2/a (15), Z = 4. Isostructural with kieserite ($MgSO_4 \cdot H_2O$), (Pistorius, 1961). The structure of kieserite was determined by Leonhardt and Weiss (1957).

Lattice constants of this sample
a = 7.5079(6)Å
b = 7.5871(6)
c = 6.9355(6)
β = 116.248(7)°

Volume
354.3 $Å^3$

Density
(calculated) 3.364 g/cm^3

Figure of merit
F_{30} = 122.5(0.006,38)

Additional pattern
PDF card 12-781 (Pistorius)

References
Leonhardt, H. J. and Weiss, R. (1957). Naturwissenschaften 44, 338.

Pistorius, C. W. F. T. (1961). Acta Crystallogr. 14, 534.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
4.810	39	0 1 1	18.43
4.759	39	-1 1 1	18.63
3.794	11	0 2 0	23.43
3.404	100	1 1 1	26.16
3.348	23	-2 1 1	26.60
3.307	28	1 2 0	26.94
3.056	47	-2 0 2	29.20
2.5595	16	-1 2 2	35.03
2.5185	46	2 2 0	35.62
2.4051	3	0 2 2	37.36
2.3989	3	2 1 1	37.46
2.3805	5	-2 2 2	37.76
2.3678	6	-3 1 1	37.97
2.3370	13	-1 3 1	38.49
2.1888	18	-1 1 3	41.21
2.1064	9	1 3 1	42.90
2.0934	4	-2 3 1	43.18
2.0536	10	1 2 2	44.06
2.0223	2	-3 2 2	44.78
1.9674	14	-3 1 3	46.10
1.9318	2	3 2 0	47.00
1.9036	7	2 0 2	47.74
1.8979	5	0 4 0	47.89
1.8105	9	3 1 1	50.36
1.7912	1	-4 1 1	50.94
1.7886	1	2 3 1	51.02
1.7753	1	-3 3 1	51.43
1.7330	3	-2 0 4	52.78
1.7011	7	2 2 2	53.85
1.6964	5	-1 3 3	54.01
1.6909	1L	-4 1 3	54.20
1.6835	4	4 0 0	54.46
1.6738	15	-4 2 2	54.80
1.6522	8	2 4 0	55.58
1.6193	10	0 4 2	56.81
1.6035	1	0 3 3	57.42
1.5861	9	-3 3 3	58.11
1.5765	4	-2 2 4	58.50
1.5557	6	0 0 4	59.36
1.5420	3	-1 2 4	59.94
1.5383	1	4 2 0	60.10
1.5279M	3	-3 2 4	60.55
1.5279M		-4 0 4	60.55
1.5006	7	3 3 1	61.77
1.4857	1L	-3 4 2	62.46
1.4726	1	-1 5 1	63.08
1.4518	3	1 3 3	64.09
1.4486	2	3 4 0	64.25
1.4390	3	0 2 4	64.73
1.4364	4	-5 1 3	64.86
1.4301	1	-5 1 1	65.18
1.4172M	3	-4 2 4	65.85
1.4172M		3 2 2	65.85
1.4094	3	1 5 1	66.26
1.3962	1	-5 2 2	66.97
1.3541	1	-3 1 5	69.34
1.3302	2	-4 4 2	70.77
1.3024	1	1 2 4	72.52
1.2795	5	-2 4 4	74.03
1.2693	2	5 2 0	74.73

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
1.2646M	5	4 0 2	75.05
1.2646M		0 6 0	75.05
1.2618M	5	-5 3 1	75.25
1.2618M		-2 5 3	75.25
1.2535	2	-3 4 4	75.83
1.2269	1L	-6 1 3	77.78
1.2168	1L	-3 5 3	78.55
1.1998	1L	4 2 2	79.89
1.1949M	1	5 1 1	80.28
1.1949M		-6 0 4	80.28

Phenobarbital Hydrate, $C_{12}H_{12}N_2O_3 \cdot H_2O$

This pattern is calculated from published crystal structure data. The calculation procedure follows the method described in previous sections 15 and 16 of NBS Monograph 25.

Synonyms
5-Ethyl-5-phenyl-2,4,6(1H,3H,5H)-pyrimidinetrione hydrate
Phenobarbitone monohydrate
5-Ethyl-5-phenylbarbituric acid hydrate

CAS registry no.
24486-13-3

Structure
Orthorhombic, Pbca (61), Z = 8. The structure was refined from single crystal data (Williams, 1973).

Atom positions
All atoms were in general positions 8(c).

Lattice constants
a = 7.157 Å
b = 30.881
c = 10.871

(published values: 7.157 Å, 30.879, 10.870 for CuKα = 1.54178; Williams, 1973)

CD cell: 10.871 Å, 30.881, 7.157, sp. gp. Pcab; a/b = 0.3520, c/b = 0.2318

Volume
2402.7 Å^3

Density
(calculated) 1.384 g/cm^3

Thermal parameters
Isotropic for hydrogen atoms (ibid.).
Isotropic B_i for other atoms, estimated from U_{ij} for each atom.

Scattering factors
Zero ionization (International Tables, 1962)

Scale factors
$\gamma = 0.2009 \times 10^{-2}$
$I/I_{corundum}$ (calculated) = 0.812 for reflection with hkℓ = 020.

Comment
This phase was earlier thought to be number V of the numerous polymorphs of anhydrous phenobarbitone. It was later referred to as form XIII, but now has been shown to be a monohydrate (Williams, op. cit.).

Additional patterns
PDF card 22-1883 (Nogami et al., 1969)

PDF cards 27-1592 (Cleverly and Williams, 1959) and 27-1848 (Mesley et al., 1968) may be essentially the phase described here, though each card appears to have minor amounts of a 2nd phase.

References

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

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England), p. 202.

Mesley, R. J., Clements, R. L., Flaherty, B., and Goodhead, K. (1968). J. Pharm. Pharmacol. 20, 329.

Nogami, H., Nagai, T., and Yotsuyanagi, T. (1969). Chem. Pharm. Bull. Tokyo 17, 499.

Williams, P. P. (1973). Acta Crystallogr. B29, 1572.

Calculated Pattern (Peak heights)
λ=1.540598Å

d(Å)	I^{rel}	hkℓ	2θ(°)
15.44	100	0 2 0	5.72
8.87	1	0 2 1	9.96
7.72	30	0 4 0	11.46
5.863	90	1 1 1	15.10
5.569	7	1 2 1	15.90
5.434	45	0 0 2	16.30
5.163	12	1 3 1	17.16
4.726	9	1 4 1	18.76
4.653	2	0 6 1	19.06
4.283	2	1 1 2	20.72
3.897	80	1 6 1	22.80
3.773	2	1 4 2	23.56
3.736	3	0 6 2	23.80
3.548	15	1 7 1	25.08
3.485	8	2 2 0	25.54
3.378	6	2 3 0	26.36
3.312	1	1 6 2	26.90
3.243+	1	1 8 1	27.48
3.164	1	1 2 3	28.18
3.085+	13	1 3 3	28.92
2.976+	22	1 9 1	30.00
2.938	2	2 6 0	30.40
2.864+	12	1 5 3	31.20
2.779+	27	2 7 0	32.18
2.743+	2	1 10 1	32.62
2.685	5	0 10 2	33.34
2.624	4	2 8 0	34.14
2.608	7	1 7 3	34.36
2.585	6	2 6 2	34.68
2.477+	2	2 9 0	36.24
2.3624	1	2 8 2	38.06
2.3376	2	2 10 0	38.48
2.3248+	2	0 12 2	38.70
2.2224	5	0 8 4	40.56
2.2088	2	2 11 0	40.82

+ More than one hkℓ possible

d(Å)	I^{rel}	hkℓ	2θ(°)
2.1642	2	2 0 4	41.70
2.1436	1	2 2 4	42.12
2.0888	1	2 12 0	43.28
2.0751	2	1 1 5	43.58
2.0616	2	1 2 5	43.88
2.0129	2	1 12 3	45.00
1.9953+	1	3 8 1	45.42
1.9788	1	2 13 0	45.82
1.9279+	6	3 9 1	47.10
1.8597	1	3 10 1	48.94
1.8309+	1	1 8 5	49.76
1.8220	1	1 14 3	50.02
1.7932	1	3 11 1	50.88
1.7750	1	2 14 2	51.44
1.7156	1	0 18 0	53.36
1.6985	1	2 16 0	53.94
1.6402	1	0 8 6	56.02
1.6046	1	3 1 5	57.38

Calculated Pattern (Integrated)
λ=1.540598Å

d(Å)	I^{rel}	hkℓ	2θ(°)
15.44	100	0 2 0	5.72
8.891	1	0 2 1	9.94
7.722	31	0 4 0	11.45
5.870	97	1 1 1	15.08
5.573	5	1 2 1	15.89
5.437	48	0 0 2	16.29
5.169	11	1 3 1	17.14
5.148	3	0 6 0	17.21
5.128	2	0 2 2	17.28
4.7263	10	1 4 1	18.76
4.6526	1	0 6 1	19.06
4.2875	2	1 1 2	20.70
3.9904	1	1 3 2	22.26
3.9005	93	1 6 1	22.78
3.7763	1	1 4 2	23.54
3.7372	3	0 6 2	23.79
3.5787	2	2 0 0	24.86
3.5492	17	1 7 1	25.07
3.4863	9	2 2 0	25.53
3.3796	8	2 3 0	26.35
3.3129	1	1 6 2	26.89
3.2431	1	1 8 1	27.48
3.1641	1	1 2 3	28.18
3.1112	1	2 4 1	28.67
3.0880	6	0 10 0	28.89
3.0849	10	1 3 3	28.92
2.9820	8	1 4 3	29.94
2.9762	19	1 9 1	30.00
2.9752	2	2 1 2	30.01
2.9379	2	2 6 0	30.40
2.8707	4	2 3 2	31.13
2.8644	12	1 5 3	31.20
2.7870	23	2 4 2	32.09
2.7794	19	2 7 0	32.18
2.7437	2	1 10 1	32.61
2.7380	1	1 6 3	32.68
2.6853	6	0 10 2	33.34
2.6242	4	2 8 0	34.14
2.6079	8	1 7 3	34.36
2.5845	7	2 6 2	34.68
2.4788	1	1 8 3	36.21
2.4768	2	2 9 0	36.24
2.3630	2	2 8 2	38.05
2.3382	2	2 10 0	38.47
2.3260	1	0 12 2	38.68
2.3237	1	3 1 1	38.72
2.2224	7	0 8 4	40.56
2.2088	1	2 11 0	40.82
2.1642	3	2 0 4	41.70
2.1431	2	2 2 4	42.13
2.0893	2	2 12 0	43.27
2.0756	2	1 1 5	43.57
2.0616	2	1 2 5	43.88
2.0133	2	1 12 3	44.99
1.9948	1	3 8 1	45.43
1.9792	2	2 13 0	45.81
1.9287	1	1 6 5	47.08
1.9275	7	3 9 1	47.11
1.8600	1	3 10 1	48.93
1.8220	2	1 14 3	50.02
1.7929	1	3 11 1	50.89
1.7747	1	2 14 2	51.45
1.7629	1	4 3 0	51.82
1.7156	1	0 18 0	53.36
1.6988	1	2 16 0	53.93
1.6402	1	0 8 6	56.02
1.6048	2	3 1 5	57.37

INORGANIC NAMES

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.

		Vol. or Sec.	Page
$C_6H_{12}O_6$	α-D-Glucose	11m	28
$C_6H_{15}HoO_{12}S_3 \cdot 9H_2O$	Holmium ethylsulfate hydrate	1m	18
$C_6H_{15}NdO_{12}S_3 \cdot 9H_2O$	Neodymium ethylsulfate hydrate	9	41
$C_7H_5BrO_2$	o-Bromobenzoic acid	16m	22
$C_7H_5ClO_2$	m-Chlorobenzoic acid	16m	30
$C_7H_5FO_2$	p-Fluorobenzoic acid	16m	36
$C_7H_5IO_2$	p-Iodobenzoic Acid	19m	47
$C_7H_9NO_2S$	Methyl sulfonanilide	9m	78
$C_7H_{12}O_4$	Pimelic acid	7m	153
$C_8H_4Hg_2O_4$	Mercury o-phthalate	10m	113
$C_8H_5KO_4$	Potassium hydrogen o-phthalate	4m	30
$C_8H_5O_4Tl$	Thallium hydrogen phthalate	16m	75
$C_8H_7N_3O_7$	2,4,6-Trinitrophenetole	8m	152
$C_8H_8O_3$	p-Anisic acid	16m	11
C_8H_9NO	Acetanilide (calc. pattern)	14m	38
C_8H_9NO	Acetanilide	16m	7
$C_8H_{11}N_2NaO_3$	Sodium barbital	16m	157
$C_8H_{12}N_2O_3$	Barbital, form I	15m	126
$C_8H_{12}N_2O_3$	Barbital, form II	15m	128
$C_8H_{12}N_2O_3$	Barbital, form IV	15m	130
$C_9H_{14}N_2O_3$	Metharbital	15m	177
$C_{10}H_{12}N_2O_3$	Allobarbital	14m	41
$C_{10}H_{12}N_2O_8$	Ethylenediaminetetraacetic Acid	19m	45
$C_{10}H_{15}NO \cdot HCl$	(-)-Ephedrine hydrochloride	16m	124
$C_{11}H_{16}N_2O_3$	Vinbarbital, form I	16m	162
$C_{11}H_{18}N_2O_3$	Amobarbital, form I	15m	114
$C_{11}H_{18}N_2O_3$	Amobarbital, form II	15m	117
$C_{12}H_{10}N_2$	Azobenzene	7m	86
$C_{12}H_{12}N_2 \cdot 2HCl$	Benzidine hydrochloride	18m	14
$C_{12}H_{12}N_2O_3$	Phenobarbital, form III	16m	144
$C_{12}H_{12}N_2O_3 \cdot 8H_2O$	Phenobarbital Hydrate	19m	88
$C_{12}H_{16}Cl_2CuN_8$	Copper tetrapyrazole chloride	8m	31
$C_{12}H_{16}Cl_2N_8Ni$	Nickel tetrapyrazole chloride	8m	44
$C_{12}H_{16}CuN_{10}O_6$	Copper tetraimidazole nitrate	13m	24
$C_{12}H_{16}N_2$	(N,N)-Dimethyltryptamine	14m	109
$C_{12}H_{16}N_2O$	Bufotenine	15m	133
$C_{12}H_{16}N_2O$	Psilocin	16m	152
$C_{12}H_{22}O_{11}$	Sucrose	11m	66
$C_{12}H_{26}N_2O_4$	Hexamethylenediammonium adipate	7m	121
$C_{13}H_{20}N_2O_2 \cdot HCl$	Procaine hydrochloride	16m	149
$C_{13}H_{21}N_2O_4P$	Psilocybin methanolate	16m	154
$C_{14}H_{11}FO$	4-Acetyl-2'-fluorodiphenyl	8m	91
$C_{14}H_{19}N_3S \cdot HCl$	Methapyrilene hydrochloride	14m	112
$C_{15}H_{12}N_2O$	β-Carbamazepine	18m	24
$C_{15}H_{12}O_2$	Dibenzoylmethane	7m	115
$C_{16}H_{13}ClN_2O$	Diazepam	14m	106
$C_{16}H_{13}N$	N-Phenyl-2-naphthylamine	6m	29
$C_{17}H_{19}ClN_2S$	Chlorpromazine	14m	60
$C_{17}H_{19}NO_3 \cdot HCl \cdot 3H_2O$	Morphine hydrochloride hydrate	16m	133
$C_{17}H_{21}NO_4 \cdot HCl$	L-Cocaine hydrochloride	16m	114
$C_{17}H_{25}N \cdot HCl$	Phencyclidine hydrochloride	16m	141
$C_{18}H_{21}NO_3 \cdot HBr \cdot 2H_2O$	Codeine hydrobromide hydrate	16m	117
$C_{18}H_{24}CdN_{14}O_6$	Cadmium hexaimidazole nitrate	8m	23
$C_{18}H_{24}N_{14}NiO_6$	Nickel hexaimidazole nitrate	7m	27
$C_{18}H_{28}N_2O_4S$	(+)-Amphetamine sulfate	15m	119
$C_{19}H_{21}NO_4 \cdot HCl \cdot 2H_2O$	Naloxone hydrochloride hydrate	16m	136
$C_{19}H_{22}N_2O$	Cinchonine	17m	26
$C_{19}H_{24}N_2 \cdot HCl$	Imipramine hydrochloride	16m	129
$C_{20}H_{25}NO_3 \cdot HCl$	Benactyzine hydrochloride	16m	92
$C_{20}H_{34}$	α-Dihydrophyllocladene, hartite (or bombiccite)	16m	122
$C_{21}H_{23}ClFNO_2$	Haloperidol	16m	127
$C_{21}H_{30}O_2$	Cannabidiol	16m	111
$C_{22}H_{25}ClN_2OS \cdot 2H_2O$	Clopenthixol hydrate	17m	28
$C_{22}H_{30}O_4$	Δ^9-Tetrahydrocannabinolic acid B	16m	160

		Vol. or Sec.	Page
$C_{24}H_{32}N_2O_2Pd$	Palladium bis-(N-isopropyl-3-ethylsalicylaldiminate)	7m	144
$C_{25}H_{15}N_6$	N-Methylphenazinium-7,7,8,8-tetracyanoquinodimethanide	7m	146
$C_{33}H_{40}N_2O_9$	Reserpine	8m	123

		Vol. or Sec.	Page
Imipramine hydrochloride	$C_{19}H_{24}N_2 \cdot HCl$	16m	129
p-Iodobenzoic acid	$C_7H_5IO_2$	19m	47
Iodoform	CHI_3	18m	34
Iron oxalate hydrate (humboldtine)	$FeC_2O_4 \cdot 2H_2O$	10m	24
Lead formate	$Pb(HCO_2)_2$	8	30
Lithium oxalate	$Li_2C_2O_4$	10m	34
Manganese tartrate	$C_4H_4MnO_6$	19m	57
Mercury acetate	$C_4H_6Hg_2O_4$	17m	51
Mercury o-phthalate	$C_6H_4(CO_2Hg)_2$	10m	113
Methapyrilene hydrochloride	$C_{14}H_{19}N_3S \cdot HCl$	14m	112
Metharbital	$C_9H_{14}N_2O_3$	15m	177
Methyl sulfonanilide	$C_6H_5NHSO_2CH_3$	9m	78
N-Methylphenazinium-7,7,8,8-tetra-cyanoquinodimethanide	$C_{25}H_{15}N_6$	7m	146
Morphine hydrochloride hydrate	$C_{17}H_{19}NO_3 \cdot HCl \cdot 3H_2O$	16m	133
Naloxone hydrochloride hydrate	$C_{19}H_{21}NO_4 \cdot HCl \cdot 2H_2O$	16m	136
2-Naphthylamine, N-phenyl-	$C_{10}H_7NHC_6H_5$	6m	29
Neodymium ethylsulfate hydrate	$Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$	9	41
Nickel acetate hydrate	$Ni(C_2H_3O_2)_2 \cdot 4H_2O$	13m	31
Nickel hexaimidazole nitrate	$Ni(C_3H_4N_2)_6(NO_3)_2$	7m	27
Nickel tetrapyrazole chloride	$Ni(C_3H_4N_2)_4Cl_2$	8m	44
Nicotinic acid	$C_6H_5NO_2$	16m	54
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (α-HMX)	$C_4H_8N_8O_8$	11m	100
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (β-HMX)	$C_4H_8N_8O_8$	11m	102
Oxalic acid hydrate	$C_2H_2O_4 \cdot 2H_2O$	16m	55
Palladium bis-(N-isopropyl-3-ethylsalicylaldiminate)	$Pd(C_{12}H_{16}NO)_2$	7m	144
Pentaerythritol	$C_5H_{12}O_4$	17m	55
Phencyclidine hydrochloride	$C_{17}H_{25}N \cdot HCl$	16m	141
Phenobarbital, form III	$C_{12}H_{12}N_2O_3$	16m	144
Phenobarbital hydrate	$C_{12}H_{12}N_2O_3 \cdot H_2O$	19m	88
Phenylhydrazine hydrochloride	$C_6H_8N_2 \cdot HCl$	17m	56
Picric acid	$C_6H_3N_3O_7$	16m	56
Pimelic acid	$(CH_2)_5(CO_2H)_2$	7m	153
Potassium formate-formic acid complex	$KO_2CH \cdot HO_2CH$	9m	93
Potassium hydrogen o-phthalate	$C_6H_4(COOH)(COOK)$	4m	30
Potassium hydrogen oxalate hydrate	$C_4H_3KO_8 \cdot 2H_2O$	17m	60
Potassium oxalate hydrate	$K_2C_2O_4 \cdot H_2O$	9m	39
Potassium oxalate perhydrate	$K_2C_2O_4 \cdot H_2O_2$	9m	96
Potassium sodium tartrate hydrate	$C_4H_4KNaO_6 \cdot 4H_2O$	15m	55
Procaine hydrochloride	$C_{13}H_{20}N_2O_2 \cdot HCl$	16m	149
Psilocin	$C_{12}H_{16}N_2O$	16m	152
Psilocybin methanolate	$C_{13}H_{21}N_2O_4P$	16m	154
Reserpine	$C_{33}H_{40}N_2O_9$	8m	123
Rubidium oxalate perhydrate	$Rb_2C_2O_4 \cdot H_2O_2$	9m	102
Silver oxalate	$Ag_2C_2O_4$	9m	47
Sodium acetate hydrate	$C_2H_3NaO_2 \cdot 3H_2O$	15m	66
Sodium barbital	$C_8H_{11}N_2NaO_3$	16m	157
Sodium glutamate hydrate	$C_5H_8NNaO_4 \cdot H_2O$	17m	70
Sodium hydrogen oxalate hydrate	$C_2HNaO_4 \cdot H_2O$	17m	72
Sodium oxalate	$Na_2C_2O_4$	6m	70
Sodium D-tartrate hydrate	$(CHOH\text{-}CO_2Na)_2 \cdot 2H_2O$	11m	110
Strontium formate	$Sr(CHO_2)_2$	8	55
Strontium formate hydrate	$Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic)	8	56
Sucrose	$C_{12}H_{22}O_{11}$	11m	66
Tartaric acid, D-	$(CHOHCO_2H)_2$	7m	168
Δ^9-Tetrahydrocannabinolic acid B	$C_{22}H_{30}O_4$	16m	160
Thallium hydrogen phthalate	$C_8H_5O_4Tl$	16m	75
Thiosemicarbazide	CH_5N_3S	17m	81
Thiourea	CH_4N_2S	17m	83
Trimethylammonium chloride	$C_3H_9N \cdot HCl$	9m	113
2,4,6-Trinitrophenetole	$C_8H_7N_3O_7$	8m	152
Uranyl acetate hydrate	$C_4H_6O_6U \cdot 2H_2O$	18m	76
Urea	$CO(NH_2)_2$	7	61
Uric acid, phase 1, (calc. pattern)	$C_5H_4N_4O_3$	8m	154
Uric acid (phase 1)	$C_5H_4N_4O_3$	16m	78
Vinbarbital, form I	$C_{11}H_{16}N_2O_3$	16m	162

*Natural mineral

NBS-114A (REV. 2-8C)

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET (See instructions)	1. PUBLICATION OR REPORT NO. Monogr. 25--Sec. 19	2. Performing Organ. Report No.	3. Publication Date December 1982

4. TITLE AND SUBTITLE

Standard X-ray Diffraction Powder Patterns

Section 19--Data for 51 Substances

5. AUTHOR(S) M. C. Morris, H. F. McMurdie, E. H. Evans, B. Paretzkin, H. S. Parker, N. P. Pyrros, and C. R. Hubbard

6. PERFORMING ORGANIZATION (*If joint or other than NBS, see instructions*)

NATIONAL BUREAU OF STANDARDS
DEPARTMENT OF COMMERCE
WASHINGTON, D.C. 20234

JCPDS--International Centre for Diffraction Data
Swarthmore, PA 19081

7. Contract/Grant No.

8. Type of Report & Period Covered

Final

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (*Street, City, State, ZIP*)

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10. SUPPLEMENTARY NOTES

Library of Congress Catalog Card Number: 53-61386

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (*A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here*)

Standard x-ray powder diffraction patterns are presented for 51 substances. These patterns, useful for identification, were obtained by manual or automated diffractometer methods, or were calculated from published crystal structure data. The lattice constants from the experimental work were refined by least-squares methods, and reflections were assigned Miller indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

12. KEY WORDS (*Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons*)

Crystal structure; densities; lattice constants; powder patterns; reference intensities; standard; x-ray diffraction.

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