



NBS MONOGRAPH 25—SECTION 20

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 20 — Data for 71 Substances

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## STANDARD X-RAY DIFFRACTION POWDER PATTERNS

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.

| NBS Publication | Order Number |
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### ERRATA

Monograph 25

Section 7, p. 160: The space group should be $P2_1/a$ (14).

Section 19, p. 24: The date for the Mitchell reference (3 locations) should be 1956.

# STANDARD X-RAY DIFFRACTION POWDER PATTERNS

## Section 20 --- Data for 71 Substances

by

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Standard x-ray powder diffraction patterns are presented for 71 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 70 experimental patterns, and is the thirtieth 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.

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

Interplanar spacings. All spacing determinations were made using one or more internal standards 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 calculated 2θ values used for them at 25 °C are given in Tables 1 and 2; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Standard Reference Material 640a [1982], Si powder (a=5.430825Å), was used for many patterns. 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 $10^5$ [Hubbard, 1982]. D-spacing results using SRM 640a will be in agreement with patterns recorded in this series of Monographs since 1966.

Another 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,

[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.

1983]. The calculated 2θ values of the 00ℓ lines are given in Table 2.

Table 1

| Calculated 2θ Angles, $CuK\alpha_1$ $\lambda$ = 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 |

Table 2

SRM 675, Fluorophlogopite (FP)

$d_{001}$ = 9.98104Å ± 0.00007

Calculated 2θ Angles, $CuK\alpha_1$ $\lambda$ = 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 room temperature 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: $\lambda(CuK\alpha_1, \text{peak})$ = 1.540598Å [Deslattes and Henins, 1973].

The majority of the patterns reported in this monograph 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 POWDER-PATTERN system of programs [Pyrros and Hubbard, 1983]. 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 read from strip chart recordings or 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. 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.

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.CALIBR was used to calculate a polynomial 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. 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. 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.

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 Visser's computer program, Ito 9 [Visser, 1969].

A least squares program, JCPDS-NBS*LSQ82, derived from the program of Evans, Appleman and Handwerker [1963], assigned hkℓ's and refined the lattice constants. The cell refinement was based only upon corrected 2θ values ($2\theta_{corr}$) which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{corr}-\theta_{calc})^2$. Generally, when two or more calculated 2θ's were within 0.03 degrees of the corrected 2θ, unique indices were not assigned. The possible multiple indices are reported. A plus sign (+) indicates more than 2 possible indices. Multiple hkℓ's were not utilized or reported in indexing cubic patterns. 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 $|2\theta_{corr} - 2\theta_{calc}|$ and the equation $\Delta d/d = -(\cot\theta)\overline{\Delta\theta}$. With these conditions, the rounded value of d agrees with its appropriate 2θ within the average error in 2θ. The value of $\overline{\Delta\theta}$ varies with the symmetry and crystallinity of each sample.

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

Figures 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. $M_{20}$ is defined by:

$$M_{20} = \frac{Q_{20}}{2\bar{\varepsilon}\ N_{20}}$$

where $Q_{20}$ is the value of $1/d^2$ for the 20th observed line (not counting unexplained lines), $N_{20}$ is the number of different calculated Q values up to $Q_{20}$, and $\bar{\varepsilon}$ is the average magnitude of the discrepancy in Q for these 20 lines. The number of unindexable lines occuring up to the 20th observed and indexed line is $X_{20}$. 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 the measured interplanar spacings is conveniently reported using the format:

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

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 the 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.

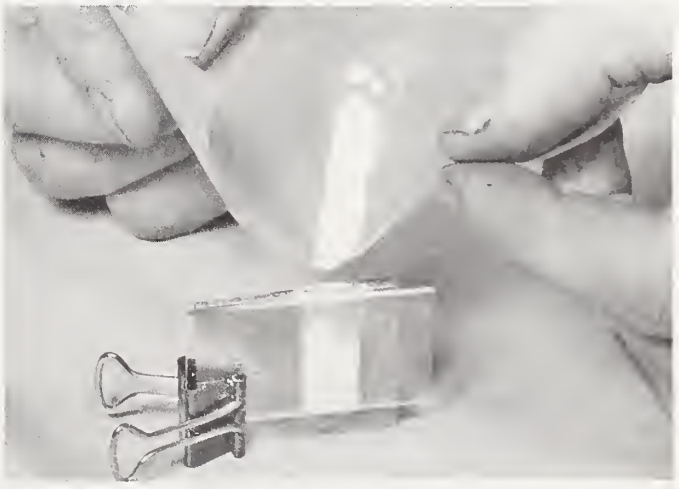

Figure 1.

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:

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

The estimated standard deviation, $\sigma$, 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 $\sigma_i$ was multiplied by the conversion factor

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

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 $gm/cm^3 = 10^3$ $kg/m^3$).


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We would like to thank Carolyn Wingo, Donna Gladhill, and Tracy Olert of the JCPDS Associateship for their assistance in keyboarding the data, proofreading of this manuscript, measuring intensities, and preparing compounds. Appreciation is also expressed to the Text Editing Facility of the National Measurement Laboratory of NBS for typing the manuscript.


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# Barium Cadmium Phosphate, $BaCd(PO_3)_4$

Synonym
Barium cadmium metaphosphate

Sample
The sample was made by heating $Ba(OH)_2 \cdot 8H_2O$, $CdCO_3$, and $(NH_4)_2HPO_4$ at 500 °C overnight. It was reground, heated at 700 °C for 2 days followed by heating at 800 °C overnight.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14). The structure of $BaCd(PO_3)_4$ was determined by Averbuch-Pouchot et al. (1975). This phase is isostructural with other phases with Mn, Ca, and Ag in place of Cd.

Crystallographic constants of this sample
a = 14.954(2) Å
b = 9.2066(11)
c = 7.2290(11)
β = 90.82(2)°

a/b = 1.6243
c/b = 0.7852

Z = 4
V = 995.15 Å$^3$
Density (calc) = 3.775 g/cm$^3$

Figure of merit
$F_{30}$ = 53.6(0.0087,64)

Additional patterns
PDF card 29-152 (Averbuch-Pouchot, 1975)
Majling et al. (1979) (calculated pattern)

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$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.8 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.84 | 8 | 1 1 0 | 11.280 |
| 7.48 | 3 | 2 0 0 | 11.821 |
| 5.801 | 38 | 2 1 0 | 15.262 |
| 5.686 | 8 | 0 1 1 | 15.573 |
| 5.333 | 3 | -1 1 1 | 16.609 |
| 4.604 | 14 | 0 2 0 | 19.262 |
| 4.497 | 4 | 2 1 1 | 19.727 |
| 4.397 | 32 | 1 2 0 | 20.179 |
| 4.135 | 1L | -3 0 1 | 21.471 |
| 3.919 | 8 | 2 2 0 | 22.674 |
| 3.754 | 69 | 1 2 1 | 23.681 |
| 3.737 | 68 | 4 0 0 | 23.789 |
| 3.615 | 5 | 0 0 2 | 24.608 |
| 3.462 | 100 | 4 1 0 | 25.709 |
| 3.456 | 98 | -2 2 1 | 25.761 |
| 3.432 | 20 | 2 2 1 | 25.943 |
| 3.291 | 16 | -1 1 2 | 27.070 |
| 3.270M | 15 | 1 1 2 | 27.249 |
| 3.270M | | -2 0 2 | 27.249 |
| 3.109 | 18 | 4 1 1 | 28.688 |
| 3.074 | 58 | -3 2 1 | 29.022 |
| 3.053M | 70 | 2 1 2 | 29.233 |
| 3.053M | | 3 2 1 | 29.233 |
| 3.006 | 11 | 1 3 0 | 29.694 |
| 2.845 | 22 | 5 1 0 | 31.414 |
| 2.825 | 20 | 0 3 1 | 31.647 |
| 2.805 | 22 | -3 1 2 | 31.874 |
| 2.778M | 54 | -1 3 1 | 32.192 |
| 2.778M | | -5 0 1 | 32.192 |
| 2.648M | 9 | -2 3 1 | 33.827 |
| 2.648M | | 2 2 2 | 33.827 |
| 2.616 | 10 | -4 0 2 | 34.253 |
| 2.580 | 13 | 4 0 2 | 34.742 |
| 2.517 | 11 | -4 1 2 | 35.637 |
| 2.509 | 6 | 5 2 0 | 35.763 |
| 2.491 | 5 | 6 0 0 | 36.020 |
| 2.464 | 9 | -3 3 1 | 36.427 |
| 2.458 | 10 | 3 2 2 | 36.528 |
| 2.452 | 6 | 3 3 1 | 36.621 |
| 2.405 | 10 | 6 1 0 | 37.359 |
| 2.372M | 6 | 1 0 3 | 37.893 |
| 2.372M | | 4 3 0 | 37.893 |
| 2.331 | 12 | 0 1 3 | 38.601 |
| 2.308M | 4 | -1 1 3 | 38.995 |
| 2.308M | | 1 3 2 | 38.995 |

Barium Cadmium Phosphate, $BaCd(PO_3)_4$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 2.2743+ | 16 | -4 2 2 | 39.596 |
| 2.2743+ | | 1 4 0 | 39.596 |
| 2.2597 | 10 | -4 3 1 | 39.862 |
| 2.2481 | 6 | 4 3 1 | 40.077 |
| 2.1679 | 12 | 1 4 1 | 41.626 |
| 2.1168 | 4 | -1 2 3 | 42.680 |
| 2.1046 | 14 | -6 2 1 | 42.939 |
| 2.0906M | 5 | 6 2 1 | 43.240 |
| 2.0906M | | 3 4 0 | 43.240 |
| 2.0723 | 12 | -5 2 2 | 43.643 |
| 2.0589M | 23 | -2 2 3 | 43.941 |
| 2.0589M | | -5 3 1 | 43.941 |
| 2.0484M | 28 | 5 2 2 | 44.178 |
| 2.0484M | | 5 3 1 | 44.178 |
| 2.0110 | 19 | -3 4 1 | 45.045 |
| 2.0046 | 15 | 3 4 1 | 45.196 |
| 1.9914M | 12 | 7 1 1 | 45.512 |
| 1.9914M | | -4 3 2 | 45.512 |
| 1.9712 | 6 | -3 2 3 | 46.005 |
| 1.9602 | 3 | 4 4 0 | 46.279 |
| 1.9268 | 4 | -1 4 2 | 47.130 |
| 1.8947M | 3 | -4 4 1 | 47.976 |
| 1.8947M | | 0 3 3 | 47.976 |
| 1.8833M | 8 | -1 3 3 | 48.285 |
| 1.8833M | | -2 4 2 | 48.285 |
| 1.8775M | 18 | -7 2 1 | 48.446 |
| 1.8775M | | 1 3 3 | 48.446 |
| 1.8652 | 10 | 7 2 1 | 48.785 |
| 1.8325M | 8 | 2 3 3 | 49.715 |
| 1.8325M | | 8 1 0 | 49.715 |
| 1.8276 | 6 | 1 5 0 | 49.856 |
| 1.8130M | 3 | -7 1 2 | 50.285 |
| 1.8130M | | -3 4 2 | 50.285 |
| 1.8074 | 4 | 0 0 4 | 50.452 |
| 1.7841 | 5 | 0 5 1 | 51.158 |
| 1.7724M | 10 | -1 5 1 | 51.522 |
| 1.7724M | | -5 4 1 | 51.522 |

# Barium Titanium Oxide, $BaTiO_3$

Synonym
Barium titanate

CAS registry no.
12047-27-7

Sample
The sample was prepared by heating $BaTiO_3$ at 1550 °C for one hour and quenching it in water.

Color
Light gray

Structure
Hexagonal, $P6_3/mmc$ (194). The structure was determined by Burbank and Evans (1948).

Crystallographic constants of this sample
a = 5.72481(11) Å
c = 13.9673(3)

c/a = 2.4398

Z = 6
V = 396.43 $Å^3$
Density (calc) = 5.862 $g/cm^3$

Figure of merit
$F_{30}$ = 105.1(0.0071,40)

Polymorphism
Blattner et al. (1947) reported the existence of two polymorphs, cubic and tetragonal. The rhombohedral form reported by Megaw (1946) is the same as the phase being reported here.

Additional patterns
PDF card 8-372 (Rase and Roy, 1955)
Dickson et al. (1961)
Arend and Kihlborg (1969)


References
Arend, H. and Kihlborg, L. (1969). J. Am. Ceram. Soc. 52, No. 2, 63.

Blattner, H., Matthias, B., and Merz, W. (1947). Helv. Phys. Acta 20, 225.

Burbank, R. D. and Evans, H. T., Jr. (1948). Acta Crystallogr. 1, 330.

Dickson, J. G., Katz, L., and Ward, R. (1961). J. Am. Chem. Soc. 83, 3026.

Megaw, H. D. (1946). Proc. Phys. Soc., London, 58, 133.

Rase, D. E. and Roy, R. (1955). J. Am. Ceram. Soc. 38, 108.


$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26±2 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.989 | 2 | 0 0 2 | 12.655 |
| 4.674 | 2 | 1 0 1 | 18.970 |
| 4.043 | 9 | 1 0 2 | 21.968 |
| 3.492 | 1L | 0 0 4 | 25.488 |
| 3.394 | 26 | 1 0 3 | 26.239 |
| 2.863 | 100 | 1 1 0 | 31.213 |
| 2.855 | 91 | 1 0 4 | 31.302 |
| 2.649 | 1L | 1 1 2 | 33.811 |
| 2.4408 | 6 | 2 0 1 | 36.793 |
| 2.4337 | 4 | 1 0 5 | 36.905 |
| 2.3365 | 16 | 2 0 2 | 38.498 |
| 2.3290 | 15 | 0 0 6 | 38.628 |
| 2.2136 | 3 | 1 1 4 | 40.728 |
| 2.1882 | 22 | 2 0 3 | 41.222 |
| 2.1073 | 1L | 1 0 6 | 42.882 |
| 2.0214 | 33 | 2 0 4 | 44.800 |
| 1.8539 | 13 | 2 0 5 | 49.102 |
| 1.8514 | 10 | 1 0 7 | 49.173 |
| 1.8102 | 5 | 2 1 2 | 50.370 |
| 1.8061 | 8 | 1 1 6 | 50.492 |
| 1.7466 | 2 | 0 0 8 | 52.338 |
| 1.7389 | 8 | 2 1 3 | 52.587 |
| 1.6513 | 32 | 2 1 4 | 55.612 |
| 1.6470 | 29 | 1 0 8 | 55.768 |
| 1.5544 | 9 | 2 0 7 | 59.414 |
| 1.4942 | 1 | 3 0 4 | 62.066 |
| 1.4908 | 6 | 1 1 8 | 62.224 |
| 1.4813 | 3 | 1 0 9 | 62.668 |
| 1.4595 | 1L | 2 1 6 | 63.709 |
| 1.4312 | 15 | 2 2 0 | 65.123 |
| 1.4277 | 12 | 2 0 8 | 65.305 |
| 1.3686 | 3 | 3 1 1 | 68.504 |
| 1.3658 | 8 | 2 1 7 | 68.664 |
| 1.3494 | 4 | 3 1 2 | 69.617 |
| 1.3475 | 4 | 3 0 6 | 69.729 |
| 1.3443 | 4 | 1 0 10 | 69.922 |
| 1.3243 | 1L | 2 2 4 | 71.136 |
| 1.3188 | 5 | 3 1 3 | 71.477 |
| 1.3154 | 6 | 2 0 9 | 71.688 |
| 1.2793 | 11 | 3 1 4 | 74.046 |
| 1.2772 | 5 | 2 1 8 | 74.185 |
| 1.2552 | 1L | 1 1 10 | 75.712 |
| 1.2340 | 1 | 3 1 5 | 77.255 |
| 1.2301 | 2 | 1 0 11 | 77.540 |
| 1.2190 | 6 | 2 2 6 | 78.380 |

| d(Å) | $I^{rel}$ $\sigma = \pm 1$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.2002 | 2 | 3 0 8 | 79.850 |
| 1.1977 | 4 | 4 0 3 | 80.052 |
| 1.1953 | 4 | 2 1 9 | 80.250 |
| 1.1681 | 4 | 4 0 4 | 82.519 |
| 1.1638 | 2 | 0 0 12 | 82.884 |
| 1.1323 | 3 | 3 1 7 | 85.737 |
| 1.1302 | 2 | 2 0 11 | 85.935 |
| 1.1225 | 1L | 3 2 2 | 86.666 |
| 1.1198 | 3 | 2 1 10 | 86.930 |
| 1.1067 | 1 | 2 2 8 | 88.214 |
| 1.1049 | 3 | 3 2 3 | 88.399 |
| 1.0816 | 12 | 3 2 4 | 90.829 |
| 1.0781 | 4 | 1 1 12 | 91.200 |
| 1.0691 | 1L | 4 1 2 | 92.193 |
| 1.0667 | 1L | 3 0 10 | 92.467 |
| 1.0528 | 3 | 4 0 7 | 94.049 |
| 1.0512 | 3 | 2 1 11 | 94.242 |
| 1.0501 | 3 | 1 0 13 | 94.372 |
| 1.0334 | 1L | 4 1 4 | 96.391 |
| 1.0292 | 2 | 3 1 9 | 96.909 |
| 1.0106 | 1 | 4 0 8 | 99.321 |
| .9996 | 1L | 2 2 10 | 100.813 |
| .9881 | 2 | 3 2 7 | 102.441 |
| .9857 | 3 | 2 0 13 | 102.787 |
| .9811 | 3 | 4 1 6 | 103.463 |
| .9799 | 1L | 3 1 10 | 103.652 |
| .9698 | 1 | 5 0 3 | 105.174 |
| .9684 | 1 | 4 0 9 | 105.386 |
| .9539 | 4 | 5 0 4 | 107.713 |
| .9530 | 1L | 3 2 8 | 107.859 |
| .9516 | 4 | 3 0 12 | 108.094 |
| .9421 | 1L | 1 1 14 | 109.707 |
| .9348 | 1L | 4 2 1 | 110.973 |
| .9329 | 3 | 3 1 11 | 111.321 |
| .9321 | 3 | 2 1 13 | 111.466 |
| .9286 | 1L | 4 2 2 | 112.100 |
| .9271 | 1L | 4 0 10 | 112.381 |
| .9196 | 3 | 4 1 8 | 113.776 |
| .9185 | 3 | 4 2 3 | 113.998 |
| .9174 | 3 | 3 2 9 | 114.212 |
| .9049 | 5 | 4 2 4 | 116.689 |
| .9031 | 5 | 2 2 12 | 117.076 |

# Barium Titanium Oxide, $BaTi_2O_5$

Synonyms
Barium titanate
Barium metadititanate

Sample
The sample was prepared by fusing an equimolar mixture of $BaTiO_3$ and $TiO_2$ at 1375 °C for one hour, then quenching in water.

Color
Light gray

Structure
Monoclinic, C2/m (12). The structure of $BaTi_2O_5$ was determined by Harrison (1956).

Crystallographic constants of this sample
a = 16.9140(12) Å
b = 3.9345(3)
c = 9.4122(7)
β = 103.114(6)°

a/b = 4.2989
c/b = 2.3922

Z = 6
V = 610.04 $Å^3$
Density (calc) = 5.112 $g/cm^3$

Figure of merit
$F_{30}$ = 90.6(0.0077,43)

Additional pattern
PDF card 8-368 (Rase and Roy, 1955)

References
Harrison, F. W. (1956). Acta Cryst. 9, 495.

Rase, D. E. and Roy, R. (1955). J. Am. Ceram. Soc. 38, No. 3, 102.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26±2 °C
Internal standards W, a = 4.0861 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.25 | 9 | 2 0 0 | 10.718 |
| 6.976 | 7 | -2 0 1 | 12.680 |
| 4.585 | 19 | 0 0 2 | 19.344 |
| 4.460 | 4 | -2 0 2 | 19.893 |
| 4.123 | 28 | -4 0 1 | 21.537 |
| 3.827 | 7 | 1 1 0 | 23.225 |
| 3.668 | 6 | 2 0 2 | 24.246 |
| 3.473 | 100 | 4 0 1 | 25.632 |
| 3.152 | 86 | -3 1 1 | 28.287 |
| 3.105 | 35 | -2 0 3 | 28.727 |
| 3.056 | 23 | 0 0 3 | 29.200 |
| 3.016 | 76 | -1 1 2 | 29.596 |
| 2.904 | 59 | 3 1 1 | 30.764 |
| 2.864 | 62 | 1 1 2 | 31.207 |
| 2.802 | 28 | -3 1 2 | 31.909 |
| 2.772 | 69 | -4 0 3 | 32.266 |
| 2.746 | 28 | 6 0 0 | 32.581 |
| 2.674 | 17 | 2 0 3 | 33.480 |
| 2.634 | 4 | -6 0 2 | 34.008 |
| 2.552 | 28 | -5 1 1 | 35.141 |
| 2.525 | 8 | 5 1 0 | 35.520 |
| 2.479 | 9 | 6 0 1 | 36.201 |
| 2.451 | 5 | -1 1 3 | 36.627 |
| 2.3957 | 5 | -5 1 2 | 37.511 |
| 2.3717 | 33 | -3 1 3 | 37.906 |
| 2.3333 | 27 | 5 1 1 | 38.554 |
| 2.3292 | 26 | 1 1 3 | 38.624 |
| 2.2910 | 16 | 0 0 4 | 39.294 |
| 2.2237 | 15 | 4 0 3 | 40.535 |
| 2.1504 | 6 | 6 0 2 | 41.981 |
| 2.1377 | 9 | -5 1 3 | 42.242 |
| 2.1138 | 3 | -8 0 1 | 42.743 |
| 2.0891 | 57 | 2 0 4 | 43.274 |
| 2.0758 | 17 | 3 1 3 | 43.566 |
| 2.0610 | 70 | -8 0 2 | 43.893 |
| 2.0200 | 35 | 7 1 0 | 44.833 |
| 2.0137 | 32 | -1 1 4 | 44.982 |
| 1.9960 | 25 | -6 0 4 | 45.401 |
| 1.9674 | 53 | 0 2 0 | 46.100 |
| 1.9221M | 7 | 1 1 4 | 47.252 |
| 1.9221M | | -8 0 3 | 47.252 |
| 1.9175 | 6 | 8 0 1 | 47.372 |
| 1.8823 | 5 | -2 0 5 | 48.313 |
| 1.8666 | 5 | -5 1 4 | 48.747 |
| 1.8600 | 5 | -7 1 3 | 48.929 |

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.8452 | 3L | 6 | 0 | 3 | 49.349 |
| 1.8329M | 7 | 4 | 0 | 4 | 49.701 |
| 1.8329M | | 0 | 0 | 5 | 49.701 |
| 1.8081 | 10 | 0 | 2 | 2 | 50.430 |
| 1.7992 | 30 | 5 | 1 | 3 | 50.700 |
| 1.7751M | 8 | -4 | 2 | 1 | 51.437 |
| 1.7751M | | 4 | 2 | 0 | 51.437 |
| 1.7559 | 6 | 3 | 1 | 4 | 52.040 |
| 1.7365 | 7 | 8 | 0 | 2 | 52.668 |
| 1.7281 | 12 | 7 | 1 | 2 | 52.943 |
| 1.7144 | 20 | -6 | 0 | 5 | 53.400 |
| 1.7116 | 3L | 4 | 2 | 1 | 53.494 |
| 1.6896M | 28 | -3 | 1 | 5 | 54.248 |
| 1.6896M | | -10 | 0 | 1 | 54.248 |
| 1.6867 | 28 | -7 | 1 | 4 | 54.348 |
| 1.6744 | 5 | -9 | 1 | 2 | 54.779 |
| 1.6613 | 20 | -2 | 2 | 3 | 55.248 |
| 1.6598 | 21 | 9 | 1 | 0 | 55.302 |
| 1.6246 | 5 | -5 | 1 | 5 | 56.606 |
| 1.6108 | 7 | -10 | 0 | 3 | 57.137 |
| 1.6041 | 20 | -4 | 2 | 3 | 57.396 |
| 1.5996 | 19 | 6 | 2 | 0 | 57.576 |
| 1.5909 | 3L | 6 | 0 | 4 | 57.918 |
| 1.5667 | 3 | 5 | 1 | 4 | 58.903 |
| 1.5610 | 10 | 10 | 0 | 1 | 59.138 |
| 1.5520M | 5 | 8 | 0 | 3 | 59.514 |
| 1.5520M | | -4 | 0 | 6 | 59.514 |
| 1.5491 | 5 | 4 | 0 | 5 | 59.638 |
| 1.5281 | 7 | 0 | 0 | 6 | 60.544 |
| 1.5117 | 3L | -7 | 1 | 5 | 61.270 |
| 1.5070 | 7 | 3 | 1 | 5 | 61.480 |
| 1.4984 | 7 | -9 | 1 | 4 | 61.871 |
| 1.4928 | 7 | 0 | 2 | 4 | 62.131 |
| 1.4856 | 12 | -6 | 0 | 6 | 62.463 |
| 1.4733 | 5 | 4 | 2 | 3 | 63.045 |
| 1.4667 | 8 | 9 | 1 | 2 | 63.362 |
| 1.4553 | 3 | -3 | 1 | 6 | 63.918 |
| 1.4492 | 10 | 10 | 0 | 2 | 64.219 |
| 1.4323 | 23 | 2 | 2 | 4 | 65.068 |
| 1.4293 | 25 | -11 | 1 | 1 | 65.224 |
| 1.4230 | 35 | -8 | 2 | 2 | 65.546 |
| 1.4049 | 5 | -12 | 0 | 1 | 66.500 |
| 1.4013 | 7 | -6 | 2 | 4 | 66.693 |
| 1.3938 | 19 | 1 | 1 | 6 | 67.098 |
| 1.3890 | 25 | -11 | 1 | 3 | 67.362 |
| 1.3861 | 20 | 6 | 0 | 5 | 67.523 |
| 1.3835 | 20 | 8 | 0 | 4 | 67.665 |
| 1.3746M | 12 | -8 | 2 | 3 | 68.164 |
| 1.3746M | | 5 | 1 | 5 | 68.164 |

# Barium Titanium Oxide, $BaTi_4O_9$

Synonym
Barium tetratitanate

CAS registry no.
12009-31-3

Sample
The sample was prepared using $BaTiO_3$ and $TiO_2$ (rutile). The reactants in a 1:3 molar ratio were blended by grinding under acetone. The following heating schedule, with periodic grinding, yielded a nearly single phase product, containing less than 1% of an extra phase: 800 °C for 20 hours; 1175 °C for 25 hours; 1250 °C for 20 hours; 1325 °C for 4 days.

Color
Colorless

Structure
Orthorhombic, Pnmm (59). The structure was determined by Lukaszewicz (1957). Temperature factors as well as atomic coordinates were given by Templeton and Dauben (1960).

Crystallographic constants of this sample

a = 6.2940(5) Å
b = 14.5324(11)
c = 3.7972(3)

a/b = 0.4331
c/b = 0.2613

Z = 2
V = 347.32 $Å^3$
Density (calc) = 4.522 $g/cm^3$

Figure of merit
$F_{30}$ = 124.6(0.0065,37)

Additional pattern
PDF card 8-367 (Rase and Roy, 1955)

References
Lukaszewicz, K. (1957). Rocz. Chem. 31, 1111.

Rase, D. E. and Roy, R. (1955). J. Am. Ceram. Soc. 38, 102.

Templeton, D. H. and Dauben, C. H. (1960). J. Chem. Phys. 32, 1515.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C
Internal standards Ag, a = 4.08651 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.267 | 1L | 0 2 0 | 12.170 |
| 6.295 | 1L | 1 0 0 | 14.057 |
| 5.777 | 15 | 1 1 0 | 15.324 |
| 4.758 | 16 | 1 2 0 | 18.634 |
| 3.840 | 36 | 1 3 0 | 23.141 |
| 3.675 | 5 | 0 1 1 | 24.198 |
| 3.631 | 5 | 0 4 0 | 24.494 |
| 3.250 | 21 | 1 0 1 | 27.417 |
| 3.173 | 18 | 1 1 1 | 28.098 |
| 3.147M | 67 | 1 4 0 | 28.341 |
| 3.147M | | 2 0 0 | 28.341 |
| 3.077 | 2 | 2 1 0 | 28.999 |
| 2.988 | 93 | 0 3 1 | 29.874 |
| 2.968 | 100 | 1 2 1 | 30.089 |
| 2.888 | 1L | 2 2 0 | 30.936 |
| 2.700 | 1 | 1 3 1 | 33.155 |
| 2.639M | 68 | 2 3 0 | 33.942 |
| 2.639M | | 1 5 0 | 33.942 |
| 2.4225+ | 17 | 2 0 1 | 37.081 |
| 2.4225+ | | 1 4 1 | 37.081 |
| 2.3899 | 10 | 2 1 1 | 37.606 |
| 2.3779 | 8 | 2 4 0 | 37.803 |
| 2.3080 | 11 | 0 5 1 | 38.994 |
| 2.2975 | 8 | 2 2 1 | 39.179 |
| 2.2604 | 8 | 1 6 0 | 39.848 |
| 2.1666M | 22 | 1 5 1 | 41.653 |
| 2.1666M | | 2 3 1 | 41.653 |
| 2.1337 | 1L | 2 5 0 | 42.325 |
| 2.0989 | 1L | 3 0 0 | 43.061 |
| 2.0159M | 26 | 2 4 1 | 44.929 |
| 2.0159M | | 3 2 0 | 44.929 |
| 1.9716 | 1 | 1 7 0 | 45.996 |
| 1.9422 | 5 | 1 6 1 | 46.732 |
| 1.9250 | 15 | 3 3 0 | 47.177 |
| 1.9200 | 10 | 2 6 0 | 47.305 |
| 1.8985 | 30 | 0 0 2 | 47.876 |
| 1.8611 | 5 | 2 5 1 | 48.900 |
| 1.8368M | 7 | 0 2 2 | 49.590 |
| 1.8368M | | 3 0 1 | 49.590 |
| 1.8220M | 13 | 3 1 1 | 50.021 |
| 1.8220M | | 0 7 1 | 50.021 |
| 1.8167+ | 15 | 3 4 0 | 50.175 |
| 1.8167+ | | 0 8 0 | 50.175 |
| 1.8042 | 3 | 1 1 2 | 50.548 |
| 1.7805 | 10 | 3 2 1 | 51.268 |

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.7634 | 2 | 1 2 2 | 51.804 |
| 1.7328 | 5 | 2 7 0 | 52.787 |
| 1.7128 | 3 | 2 6 1 | 53.452 |
| 1.7015M | 16 | 1 3 2 | 53.835 |
| 1.7015M | | 3 5 0 | 53.835 |
| 1.6821 | 1 | 0 4 2 | 54.508 |
| 1.6390 | 1 | 3 4 1 | 56.065 |
| 1.6259M | 13 | 2 0 2 | 56.557 |
| 1.6259M | | 1 4 2 | 56.557 |
| 1.5858+ | 23 | 1 8 1 | 58.122 |
| 1.5858+ | | 3 6 0 | 58.122 |
| 1.5766 | 12 | 2 7 1 | 58.496 |
| 1.5733M | 14 | 2 8 0 | 58.630 |
| 1.5733M | | 4 0 0 | 58.630 |
| 1.5640M | 5 | 1 9 0 | 59.014 |
| 1.5640M | | 4 1 0 | 59.014 |
| 1.5525 | 9 | 3 5 1 | 59.495 |
| 1.5414M | 21 | 2 3 2 | 59.966 |
| 1.5414M | | 1 5 2 | 59.966 |
| 1.5377 | 12 | 4 2 0 | 60.124 |
| 1.4965 | 6 | 4 3 0 | 61.958 |
| 1.4838 | 2 | 2 4 2 | 62.549 |
| 1.4632 | 2 | 3 6 1 | 63.532 |
| 1.4537+ | 8 | 1 6 2 | 63.998 |
| 1.4537+ | | 4 0 1 | 63.998 |
| 1.4460M | 3 | 1 9 1 | 64.380 |
| 1.4460M | | 4 1 1 | 64.380 |
| 1.4257 | 1L | 4 2 1 | 65.410 |
| 1.3923 | 3 | 4 3 1 | 67.183 |
| 1.3819 | 6 | 3 2 2 | 67.757 |
| 1.3732 | 1L | 3 8 0 | 68.246 |
| 1.3519 | 8 | 3 3 2 | 69.473 |
| 1.3497M | 7 | 4 4 1 | 69.603 |
| 1.3497M | | 2 6 2 | 69.603 |
| 1.3267 | 1 | 1 10 1 | 70.985 |
| 1.3195M | 1L | 4 6 0 | 71.437 |
| 1.3195M | | 2 10 0 | 71.437 |
| 1.3126M | 4 | 3 4 2 | 71.870 |
| 1.3126M | | 0 8 2 | 71.870 |
| 1.3001 | 2 | 4 5 1 | 72.668 |
| 1.2932 | 4 | 1 11 0 | 73.120 |
| 1.2915 | 5 | 3 8 1 | 73.231 |
| 1.2798M | 2 | 2 7 2 | 74.010 |
| 1.2798M | | 3 9 0 | 74.010 |
| 1.2670 | 5 | 3 5 2 | 74.886 |

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.2541M | 1L | 5 1 0 | 75.789 |
| 1.2541M | | 4 7 0 | 75.789 |
| 1.2478 | 6 | 0 11 1 | 76.241 |
| 1.2464M | 3 | 4 6 1 | 76.346 |
| 1.2464M | | 2 10 1 | 76.346 |
| 1.2406M | 2 | 1 0 3 | 76.768 |
| 1.2406M | | 5 2 0 | 76.768 |
| 1.2247 | 5 | 0 3 3 | 77.950 |
| 1.2232 | 5 | 1 2 3 | 78.059 |
| 1.2185M | 1L | 5 3 0 | 78.420 |
| 1.2185M | | 2 11 0 | 78.420 |
| 1.2115M | 6 | 4 0 2 | 78.959 |
| 1.2115M | | 2 8 2 | 78.959 |
| 1.2072M | 4 | 4 1 2 | 79.302 |
| 1.2072M | | 1 9 2 | 79.302 |
| 1.1948+ | 1L | 5 0 1 | 80.291 |
| 1.1948+ | | 3 10 0 | 80.291 |
| 1.1909M | 3 | 5 1 1 | 80.608 |
| 1.1909M | | 4 7 1 | 80.608 |

# Barium Titanium Phosphate, $BaTi_4(PO_4)_6$

Sample
The sample was prepared by heating stoichiometric proportions of $BaCO_3$, $TiO_2$ (anatase), and $(NH_4)_2HPO_4$ at 500 °C. The phase was then reground and heated at 1200 °C for 3 days.

Color
Bluish white

Structure
Rhombohedral, $R\bar{3}c$ (167). Similar to $BaZr_4(PO_4)_6$, $NaZr_2(PO_4)_3$, and other phosphates of this type. The structure of $NaZr_2(PO_4)_3$ was determined by Hagman and Kierkegaard (1968).

Crystallographic constants of this sample (Hexagonal axes)
$a = 8.3483(2)$ Å
$c = 23.0193(9)$

$c/a = 2.7574$

$Z = 3$
$V = 1389.37$ Å$^3$
Density (calc) = 3.222 g/cm$^3$

Figure of merit
$F_{30} = 188.2(0.0048,33)$

Additional pattern
PDF card 12-685 (Harrison, 1960)

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

Harrison, D. E. (1960). J. Electrochem. Soc. 107, 217.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 26.0 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.124 | 5 | 0 1 2 | 14.453 |
| 4.502 | 4 | 1 0 4 | 19.702 |
| 4.176 | 59 | 1 1 0 | 21.261 |
| 3.667 | 100 | 1 1 3 | 24.253 |
| 3.449 | 12 | 2 0 2 | 25.812 |
| 3.061 | 16 | 0 2 4 | 29.146 |
| 2.8245 | 93 | 1 1 6 | 31.652 |
| 2.7132 | 12 | 2 1 1 | 32.987 |
| 2.6731 | 12 | 0 1 8 | 33.496 |
| 2.6584 | 14 | 1 2 2 | 33.687 |
| 2.4682 | 2 | 2 1 4 | 36.370 |
| 2.4098 | 22 | 3 0 0 | 37.284 |
| 2.3502 | 3 | 1 2 5 | 38.266 |
| 2.2511 | 5 | 2 0 8 | 40.020 |
| 2.1934 | 5 | 1 0 10 | 41.121 |
| 2.1809 | 8 | 1 1 9 | 41.367 |
| 2.1014 | 2 | 2 1 7 | 43.007 |
| 2.0872 | 2 | 2 2 0 | 43.314 |
| 2.0409 | 13 | 3 0 6 | 44.349 |
| 2.0137 | 3 | 2 2 3 | 44.980 |
| 1.9976 | 2 | 1 3 1 | 45.363 |
| 1.9815 | 12 | 1 2 8 | 45.753 |
| 1.9411 | 2 | 0 2 10 | 46.762 |
| 1.9176 | 4 | 0 0 12 | 47.370 |
| 1.8938 | 1L | 1 3 4 | 48.002 |
| 1.8331 | 30 | 2 2 6 | 49.697 |
| 1.7854 | 1 | 0 4 2 | 51.118 |
| 1.7602 | 6 | 2 1 10 | 51.906 |
| 1.7430 | 3 | 1 1 12 | 52.455 |
| 1.7240 | 3 | 4 0 4 | 53.078 |
| 1.7119 | 6 | 1 3 7 | 53.484 |
| 1.6613 | 1L | 1 2 11 | 55.247 |
| 1.6451 | 10 | 3 1 8 | 55.841 |
| 1.6412 | 4 | 2 3 2 | 55.985 |
| 1.6169 | 1 | 2 2 9 | 56.900 |
| 1.6032 | 2 | 0 1 14 | 57.434 |
| 1.5935 | 1 | 3 2 4 | 57.815 |
| 1.5776 | 13 | 4 1 0 | 58.454 |
| 1.5605 | 1 | 2 3 5 | 59.158 |
| 1.5452 | 3 | 4 1 3 | 59.802 |
| 1.5306 | 6 | 0 4 8 | 60.435 |
| 1.5121 | 5 | 1 3 10 | 61.253 |
| 1.5008 | 11 | 3 0 12 | 61.762 |
| 1.4969 | 11 | 2 0 14 | 61.941 |
| 1.4808 | 2 | 3 2 7 | 62.689 |

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4590 | 11 | 4 1 6 | 63.734 |
| 1.4481 | 1L | 3 1 11 | 64.271 |
| 1.4402 | 2 | 1 1 15 | 64.666 |
| 1.4368 | 2 | 2 3 8 | 64.840 |
| 1.4216 | 2 | 4 0 10 | 65.621 |
| 1.4126 | 1L | 2 2 12 | 66.091 |
| 1.4091 | 6 | 1 2 14 | 66.275 |
| 1.4023 | 1L | 0 5 4 | 66.641 |
| 1.3915 | 5 | 3 3 0 | 67.223 |
| 1.3693 | 1L | 3 3 3 | 68.466 |
| 1.3429 | 1 | 4 1 9 | 70.005 |
| 1.3269 | 1 | 1 3 13 | 70.975 |
| 1.3100 | 2 | 4 2 5 | 72.034 |
| 1.3080 | 2 | 3 3 6 | 72.162 |
| 1.2963 | 2 | 5 1 1 | 72.915 |
| 1.2902 | 1L | 1 5 2 | 73.314 |
| 1.2789 | 1L | 0 0 18 | 74.071 |
| 1.2714 | 4 | 3 1 14 | 74.582 |
| 1.2666 | 3 | 5 1 4 | 74.912 |
| 1.2497 | 2 | 1 5 5 | 76.104 |
| 1.2344 | 1L | 4 2 8 | 77.218 |
| 1.2227 | 1 | 1 1 18 | 78.097 |
| 1.2185 | 2 | 4 1 12 | 78.420 |
| 1.2133 | 2 | 1 2 17 | 78.820 |
| 1.2105 | 3 | 3 2 13 | 79.036 |
| 1.2077 | 4 | 5 1 7 | 79.256 |
| 1.2049 | 5 | 6 0 0 | 79.477 |
| 1.1824 | 1L | 3 4 2 | 81.306 |
| 1.1677 | 4 | 2 3 14 | 82.551 |
| 1.1578 | 2 | 5 2 0 | 83.413 |
| 1.1497 | 1L | 6 0 6 | 84.137 |
| 1.1447 | 1L | 5 2 3 | 84.584 |
| 1.1367 | 4 | 0 1 20 | 85.322 |
| 1.1311 | 1 | 5 1 10 | 85.850 |
| 1.1264 | 1 | 3 3 12 | 86.292 |
| 1.1177 | 1L | 4 3 7 | 87.128 |
| 1.1034 | 2 | 1 5 11 | 88.552 |
| 1.0986 | 4 | 3 4 8 | 89.042 |
| 1.0967 | 2 | 2 0 20 | 89.234 |

# Barium Zirconium Phosphate, $BaZr_4(PO_4)_6$

Synonym
Barium zirconium orthophosphate

CAS registry no.
6792-89-8

Sample
The sample was made by heating a 1:4:6 molar mixture of $BaCO_3$, $ZrO_2$, and $(NH_4)_2HPO_4$ at 500 °C. This was followed by grinding and heating to 1600 °C for 1 day.

Color
Colorless

Structure
Rhombohedral, R** (166). The structure was similar to that of $NaZr_2(PO_4)_3$ (Chernorukov et al., 1978).

Crystallographic constants of this sample (Hexagonal axes)
a = 8.6468(5) Å
c = 23.984(2)

c/a = 2.7737

Z = 3
V = 1552.97 $Å^3$
Density (calc) = 3.439 $g/cm^3$

Figure of merit
$F_{30}$ = 91.7(0.0091,36)

Reference
Chernorukov, N. G., Korshunov, I. A., and Prokof'eva, T. V. (1978). Sov. Phys. Crystallogr. (Engl. Transl.) 23, 475.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.0 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±4 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.01 | 1L | 0 0 3 | 11.039 |
| 7.16 | 1 | 1 0 1 | 12.353 |
| 6.359 | 1 | 0 1 2 | 13.915 |
| 4.681 | 7 | 1 0 4 | 18.942 |
| 4.324 | 36 | 1 1 0 | 20.522 |
| 4.040 | 2 | 0 1 5 | 21.986 |
| 3.999 | 1 | 0 0 6 | 22.213 |
| 3.804 | 40 | 1 1 3 | 23.368 |
| 3.695 | 3 | 0 2 1 | 24.063 |
| 3.576 | 2 | 2 0 2 | 24.876 |
| 3.176 | 20 | 0 2 4 | 28.071 |
| 3.114 | 2 | 1 0 7 | 28.647 |
| 2.936 | 100 | 1 1 6 | 30.422 |
| 2.811 | 8 | 2 1 1 | 31.810 |
| 2.784 | 7 | 0 1 8 | 32.126 |
| 2.755 | 2 | 1 2 2 | 32.473 |
| 2.559 | 2 | 2 1 4 | 35.032 |
| 2.496 | 30 | 3 0 0 | 35.952 |
| 2.437 | 2 | 1 2 5 | 36.850 |
| 2.384 | 1 | 3 0 3 | 37.709 |
| 2.340 | 6 | 2 0 8 | 38.435 |
| 2.2684 | 4 | 1 1 9 | 39.703 |
| 2.1829 | 4 | 2 1 7 | 41.328 |
| 2.1613 | 6 | 2 2 0 | 41.760 |
| 2.1173 | 14 | 3 0 6 | 42.669 |
| 2.0865 | 2 | 2 2 3 | 43.330 |
| 2.0683 | 4 | 1 3 1 | 43.731 |
| 2.0581 | 11 | 1 2 8 | 43.960 |
| 2.0193 | 4 | 0 2 10 | 44.849 |
| 1.9977 | 2 | 0 0 12 | 45.360 |
| 1.9625 | 2 | 1 3 4 | 46.221 |
| 1.9014 | 28 | 2 2 6 | 47.798 |
| 1.8501 | 1L | 0 4 2 | 49.209 |
| 1.8295 | 12 | 2 1 10 | 49.801 |
| 1.8140 | 2 | 1 1 12 | 50.255 |
| 1.7760 | 2 | 1 3 7 | 51.409 |
| 1.7072 | 6 | 3 1 8 | 53.642 |
| 1.6788 | 2 | 2 2 9 | 54.623 |
| 1.6702 | 4 | 0 1 14 | 54.929 |
| 1.6513 | 4 | 3 2 4 | 55.613 |
| 1.6339 | 14 | 4 1 0 | 56.257 |
| 1.6167 | 1L | 2 3 5 | 56.909 |
| 1.6008 | 1L | 4 1 3 | 57.526 |
| 1.5877 | 2 | 0 4 8 | 58.048 |
| 1.5700 | 6 | 1 3 10 | 58.766 |
| 1.5602 | 9 | 3 0 12 | 59.172 |
| 1.5573 | 9 | 2 0 14 | 59.292 |
| 1.5356 | 2 | 3 2 7 | 60.214 |
| 1.5126 | 15 | 4 1 6 | 61.230 |
| 1.4995 | 1 | 1 1 15 | 61.823 |
| 1.4905 | 1L | 2 3 8 | 62.235 |
| 1.4863 | 1 | 5 0 2 | 62.432 |
| 1.4756 | 2 | 4 0 10 | 62.934 |
| 1.4657 | 10 | 1 2 14 | 63.413 |
| 1.4531 | 2 | 0 5 4 | 64.026 |
| 1.4411 | 5 | 3 3 0 | 64.625 |

# Bismuth Germanium Oxide, $Bi_4(GeO_4)_3$

Synonyms
Bismuth germanate, BGO
Bismuth orthogermanate
Germanium bismuthate

CAS registry no.
12233-56-6

Sample
The sample was donated by Harshaw Chemical Co.

Color
Colorless

Structure
Cubic, $I\bar{4}3d$ (220), isostructural with $Bi_4(SiO_4)_3$. The structure of $Bi_4(SiO_4)_3$ was determined by Durif (1957).

Crystallographic constants of this sample
$a = 10.5187(2)$ Å

$Z = 4$
$V = 1163.8$ Å$^3$
Density (calc) = 7.109 g/cm$^3$

Figure of merit
$F_{30} = 106.9(0.0091,31)$

Additional patterns
PDF card 11-320 (Durif, 1958)
PDF card 17-809 (Gattow and Fricke, 1963)

References
Durif, A. (1958). Anal. Chem. 30, 1161.

Durif, A. (1957). C. R. Hebd. Séances Acad. Sci. 244, 2815, and ibid. 245, 1095.

Gattow, G. and Fricke, H. (1963). Z. Anorg. Allg. Chem. 324, 287.

| $CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 24.9 °C<br>Internal standard Si, SRM 640a | | | | | |
|---|---|---|---|---|---|
| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | h | k | ℓ | 2θ(°) |
| 4.293 | 62 | 2 | 1 | 1 | 20.673 |
| 3.719 | 1 | 2 | 2 | 0 | 23.911 |
| 3.326 | 94 | 3 | 1 | 0 | 26.786 |
| 2.811 | 100 | 3 | 2 | 1 | 31.803 |
| 2.631 | 14 | 4 | 0 | 0 | 34.052 |
| 2.352 | 2 | 4 | 2 | 0 | 38.242 |
| 2.2423 | 2 | 3 | 3 | 2 | 40.185 |
| 2.1470 | 44 | 4 | 2 | 2 | 42.051 |
| 2.0622 | 34 | 5 | 1 | 0 | 43.867 |
| 1.9200 | 6 | 5 | 2 | 1 | 47.306 |
| 1.8594 | 2 | 4 | 4 | 0 | 48.946 |
| 1.8038 | 18 | 5 | 3 | 0 | 50.560 |
| 1.7059 | 38 | 6 | 1 | 1 | 53.685 |
| 1.6626 | 14 | 6 | 2 | 0 | 55.203 |
| 1.6226 | 22 | 5 | 4 | 1 | 56.685 |
| 1.5505 | 15 | 6 | 3 | 1 | 59.577 |
| 1.5183 | 6 | 4 | 4 | 4 | 60.975 |
| 1.4874 | 21 | 7 | 1 | 0 | 62.382 |
| 1.4585 | 2 | 6 | 4 | 0 | 63.759 |
| 1.4313 | 8 | 7 | 2 | 1 | 65.120 |
| 1.4053 | 7 | 6 | 4 | 2 | 66.478 |
| 1.3809 | 1 | 7 | 3 | 0 | 67.813 |
| 1.3360 | 3 | 6 | 5 | 1 | 70.422 |
| 1.2947 | 8 | 7 | 4 | 1 | 73.022 |
| 1.2758 | 1L | 8 | 2 | 0 | 74.280 |
| 1.2571 | 3 | 6 | 5 | 3 | 75.579 |
| 1.2397 | 14 | 6 | 6 | 0 | 76.831 |
| 1.2227 | 10 | 7 | 5 | 0 | 78.100 |
| 1.1908 | 6 | 7 | 5 | 2 | 80.610 |
| 1.1760 | 1 | 8 | 4 | 0 | 81.842 |
| 1.1617 | 2 | 9 | 1 | 0 | 83.071 |
| 1.1477 | 1L | 8 | 4 | 2 | 84.319 |
| 1.1343 | 9 | 7 | 6 | 1 | 85.551 |
| 1.1213 | 2 | 6 | 6 | 4 | 86.779 |
| 1.1088 | 9 | 9 | 3 | 0 | 88.007 |
| 1.0850 | 3 | 7 | 6 | 3 | 90.461 |
| 1.0736 | 4 | 8 | 4 | 4 | 91.698 |
| 1.0626 | 10 | 9 | 4 | 1 | 92.923 |
| 1.0415 | 6 | 10 | 1 | 1 | 95.393 |
| 1.0314 | 1 | 10 | 2 | 0 | 96.632 |
| 1.0216 | 2 | 9 | 5 | 0 | 97.873 |
| 1.0029 | 9 | 10 | 3 | 1 | 100.355 |
| .9852 | 2 | 8 | 7 | 1 | 102.869 |
| .9766 | 1 | 10 | 4 | 0 | 104.136 |
| .9683 | 1 | 9 | 6 | 1 | 105.402 |
| .9602 | 4 | 10 | 4 | 2 | 106.681 |
| .9523 | 6 | 11 | 1 | 0 | 107.966 |
| .9371 | 1 | 10 | 5 | 1 | 110.568 |
| .9298 | 1L | 8 | 8 | 0 | 111.882 |
| .9226 | 2 | 9 | 7 | 0 | 113.216 |
| .9087 | 11 | 9 | 7 | 2 | 115.925 |
| .9020 | 5 | 10 | 6 | 0 | 117.298 |
| .8954 | 1 | 11 | 4 | 1 | 118.687 |

# Bismuth Germanium Oxide, $Bi_{12}GeO_{20}$

CAS registry no.
12233-73-7

Sample
$Bi_2O_3$ and $GeO_2$ were melted together in a 6 to 1 molar ratio and a single crystal was pulled from the melt by the Czochralski technique (Levin and Roth, 1964).

Color
Single crystal: dark yellow
Ground: yellowish white

Structure
Cubic, I23 (197). The structure was determined by Abrahams et al. (1967).

Crystallographic constants of this sample
$a = 10.14558(14)$ Å

$Z = 2$
$V = 144.31$ Å$^3$
Density (calc) = 9.223 g/cm$^3$

Figure of merit
$F_{30} = 117.3(0.0085,30)$

Additional patterns
PDF card 17-812 (Gattow and Fricke, 1963)
PDF card 23-71 (Bernstein, 1967)


References
Abrahams, S. C., Jamieson, P. B., and Bernstein, J. L. (1967). J. Chem. Phys. 47, 4034.

Bernstein, J. L. (1967). J. Cryst. Growth 1, 45.

Gattow, G. and Fricke, H. (1963). Z. Anorg. Allg. Chem. 324, 287.

Levin, E. M. and Roth, R. S. (1964). J. Res. Natl. Bur. Stand., Sect. A, 68, 197.


$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 25.8 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.18 | 1 | 1 1 0 | 12.323 |
| 5.072 | 2 | 2 0 0 | 17.470 |
| 4.146 | 4 | 2 1 1 | 21.415 |
| 3.587 | 22 | 2 2 0 | 24.800 |
| 3.208 | 100 | 3 1 0 | 27.785 |
| 2.930 | 26 | 2 2 2 | 30.484 |
| 2.712 | 76 | 3 2 1 | 33.002 |
| 2.537 | 4 | 4 0 0 | 35.344 |
| 2.391 | 12 | 3 3 0 | 37.585 |
| 2.2681 | 12 | 4 2 0 | 39.707 |
| 2.1628 | 19 | 3 3 2 | 41.729 |
| 2.0712 | 15 | 4 2 2 | 43.667 |
| 1.9899 | 23 | 5 1 0 | 45.549 |
| 1.8519 | 12 | 5 2 1 | 49.158 |
| 1.7927 | 1 | 4 4 0 | 50.894 |
| 1.7396 | 46 | 5 3 0 | 52.567 |
| 1.6910 | 25 | 6 0 0 | 54.198 |
| 1.6460 | 36 | 5 3 2 | 55.808 |
| 1.6036 | 1 | 6 2 0 | 57.418 |
| 1.5656 | 6 | 5 4 1 | 58.945 |
| 1.5294 | 6 | 6 2 2 | 60.485 |
| 1.4960 | 28 | 6 3 1 | 61.981 |
| 1.4640 | 4 | 4 4 4 | 63.493 |
| 1.4347 | 12 | 5 5 0 | 64.945 |
| 1.4070 | 3 | 6 4 0 | 66.387 |
| 1.3807 | 8 | 7 2 1 | 67.824 |
| 1.3559 | 5 | 6 4 2 | 69.234 |
| 1.3320 | 2 | 7 3 0 | 70.663 |
| 1.2887 | 7 | 6 5 1 | 73.414 |
| 1.2683 | 1 | 8 0 0 | 74.799 |
| 1.2487 | 6 | 7 4 1 | 76.177 |
| 1.2303 | 3 | 6 4 4 | 77.524 |
| 1.2128 | 17 | 6 5 3 | 78.861 |
| 1.1956 | 16 | 6 6 0 | 80.219 |
| 1.1795 | 17 | 7 5 0 | 81.549 |
| 1.1640 | 1 | 6 6 2 | 82.869 |
| 1.1489 | 6 | 7 5 2 | 84.204 |
| 1.1343 | 2 | 8 4 0 | 85.543 |
| 1.1205 | 4 | 9 1 0 | 86.860 |
| 1.1071 | 6 | 8 4 2 | 88.182 |
| 1.0942 | 9 | 7 6 1 | 89.500 |
| 1.0814 | 1 | 6 6 4 | 90.845 |
| 1.0695 | 8 | 9 3 0 | 92.148 |
| 1.0464 | 5 | 9 3 2 | 94.804 |
| 1.0355 | 1L | 8 4 4 | 96.133 |

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.0248 | 16 | 7 | 7 | 0 | 97.468 |
| 1.0145 | 3 | 8 | 6 | 0 | 98.802 |
| 1.0047 | 1 | 10 | 1 | 1 | 100.122 |
| .9948 | 3 | 10 | 2 | 0 | 101.482 |
| .9854 | 9 | 9 | 5 | 0 | 102.835 |
| .9763 | 3 | 10 | 2 | 2 | 104.187 |
| .9673 | 9 | 10 | 3 | 1 | 105.571 |
| .9501 | 4 | 8 | 7 | 1 | 108.333 |
| .9419 | 3 | 10 | 4 | 0 | 109.729 |
| .9340 | 6 | 10 | 3 | 3 | 111.130 |
| .9261 | 2 | 10 | 4 | 2 | 112.569 |
| .9185 | 7 | 11 | 1 | 0 | 113.999 |
| .9038 | 7 | 10 | 5 | 1 | 116.923 |
| .8897 | 8 | 9 | 7 | 0 | 119.940 |
| .8831 | 10 | 10 | 4 | 4 | 121.448 |
| .8764 | 12 | 9 | 7 | 2 | 123.021 |
| .8699 | 3 | 10 | 6 | 0 | 124.630 |
| .8637 | 5 | 11 | 4 | 1 | 126.225 |
| .8514 | 6 | 9 | 6 | 5 | 129.591 |
| .8454 | 4 | 12 | 0 | 0 | 131.320 |
| .8397 | 17 | 11 | 5 | 0 | 133.089 |
| .8284 | 6 | 10 | 7 | 1 | 136.826 |
| .8230 | 2 | 10 | 6 | 4 | 138.783 |
| .8176 | 4 | 12 | 3 | 1 | 140.829 |
| .8072 | 5 | 11 | 6 | 1 | 145.237 |

# Bismuth Titanium Oxide, $Bi_{12}TiO_{20}$

CAS registry no.
12441-73-5

Sample
$Bi_2O_3$ and $TiO_2$ were melted together in the ratio of 6 to 1 moles and a single crystal was pulled by the Czochralski technique (Levin and Roth, 1964).

Color
Single crystal: dark red brown
Ground: grayish yellow

Structure
Cubic, I23 (197). Assumed to be isomorphous with $Bi_{12}GeO_{20}$ (Abrahams et al., 1967).

Crystallographic constants of this sample
$a = 10.17391(13)$ Å

$Z = 2$
$V = 1053.08$ Å$^3$
Density (calc) = 9.069 g/cm$^3$

Figure of merit
$F_{30} = 111.0(0.0090,30)$

References
Abrahams, S. C., Jamieson, P. B., and Bernstein, J. L. (1967). J. Chem. Phys. 47, 4034.

Levin, E. M. and Roth, R. S. (1964). J. Res. Natl. Bur. Stand., Sect. A, 68, 197.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 25.9 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.19 | 1 | 1 1 0 | 12.296 |
| 5.080 | 3 | 2 0 0 | 17.444 |
| 4.152 | 4 | 2 1 1 | 21.381 |
| 3.595 | 23 | 2 2 0 | 24.747 |
| 3.218 | 100 | 3 1 0 | 27.701 |
| 2.936 | 25 | 2 2 2 | 30.424 |
| 2.720 | 77 | 3 2 1 | 32.901 |
| 2.543 | 3 | 4 0 0 | 35.263 |
| 2.398 | 11 | 3 3 0 | 37.482 |
| 2.2750 | 12 | 4 2 0 | 39.583 |
| 2.1691 | 20 | 3 3 2 | 41.603 |
| 2.0763 | 13 | 4 2 2 | 43.554 |
| 1.9959 | 20 | 5 1 0 | 45.403 |
| 1.8578 | 11 | 5 2 1 | 48.993 |
| 1.7982 | 1 | 4 4 0 | 50.729 |
| 1.7447 | 46 | 5 3 0 | 52.401 |
| 1.6959 | 22 | 6 0 0 | 54.028 |
| 1.6506 | 35 | 6 1 1 | 55.637 |
| 1.6090 | 1 | 6 2 0 | 57.207 |
| 1.5700 | 4 | 5 4 1 | 58.766 |
| 1.5335 | 6 | 6 2 2 | 60.307 |
| 1.4996 | 26 | 6 3 1 | 61.816 |
| 1.4687 | 3 | 4 4 4 | 63.268 |
| 1.4389 | 10 | 5 5 0 | 64.736 |
| 1.4107 | 2 | 6 4 0 | 66.192 |
| 1.3844 | 9 | 7 2 1 | 67.617 |
| 1.3599 | 4 | 6 4 2 | 69.002 |
| 1.3359 | 2 | 7 3 0 | 70.426 |
| 1.2920 | 6 | 6 5 1 | 73.196 |
| 1.2716 | 1 | 8 0 0 | 74.569 |
| 1.2522 | 5 | 7 4 1 | 75.929 |
| 1.2336 | 2 | 6 4 4 | 77.277 |
| 1.2158 | 16 | 6 5 3 | 78.626 |
| 1.1991 | 14 | 6 6 0 | 79.939 |
| 1.1827 | 13 | 7 5 0 | 81.277 |
| 1.1670 | 1 | 6 6 2 | 82.612 |
| 1.1519 | 4 | 7 5 2 | 83.941 |
| 1.1374 | 2 | 8 4 0 | 85.256 |
| 1.1235 | 4 | 9 1 0 | 86.569 |
| 1.1100 | 5 | 8 4 2 | 87.886 |
| 1.0972 | 8 | 7 6 1 | 89.189 |
| 1.0847 | 1 | 6 6 4 | 90.498 |
| 1.0724 | 5 | 9 3 0 | 91.824 |
| 1.0493 | 3 | 9 3 2 | 94.463 |
| 1.0384 | 1 | 8 4 4 | 95.770 |
| 1.0278 | 12 | 7 7 0 | 97.094 |
| 1.0174 | 3 | 10 0 0 | 98.423 |
| 1.0075 | 3 | 10 1 1 | 99.738 |
| .9976 | 3 | 10 2 0 | 101.089 |
| .9882 | 5 | 9 5 0 | 102.433 |
| .9792 | 2 | 10 2 2 | 103.752 |
| .9701 | 6 | 10 3 1 | 105.132 |
| .9529 | 3 | 8 7 1 | 107.877 |
| .9446 | 3 | 10 4 0 | 109.269 |
| .9365 | 5 | 9 6 1 | 110.673 |
| .9287 | 2 | 10 4 2 | 112.081 |
| .9211 | 4 | 11 1 0 | 113.501 |
| .9064 | 5 | 10 5 1 | 116.398 |
| .8923 | 3 | 9 7 0 | 119.364 |
| .8855 | 6 | 10 4 4 | 120.891 |
| .8789 | 9 | 9 7 2 | 122.442 |
| .8725 | 2 | 10 6 0 | 123.984 |
| .8661 | 4 | 11 4 1 | 125.586 |
| .8538 | 4 | 9 6 5 | 128.910 |
| .8478 | 3 | 12 0 0 | 130.612 |
| .8419 | 10 | 11 5 0 | 132.384 |
| .8307 | 4 | 10 7 1 | 136.025 |
| .8253 | 2 | 12 2 2 | 137.941 |
| .8198 | 3 | 12 3 1 | 139.973 |
| .8093 | 3 | 11 6 1 | 144.260 |
| .7993 | 2 | 9 9 0 | 149.017 |

# Boron Nitride, BN

CAS registry no.
10294-33-4

Sample
The sample was obtained from the Carborundum Co., Niagara Falls, N.Y.

Color
Colorless

Structure
Hexagonal, $P6_3/mmc$ (194). The structure was determined by Pease (1952).

Crystallographic constants of this sample
$a = 2.50441(7)$ Å
$c = 6.6562(4)$

$c/a = 2.6578$

$Z = 2$
$V = 36.158$ Å$^3$
Density (calc) = 2.280 g/cm$^3$

Figure of merit
$F_{20} = 71.5(0.011,25)$

Polymorphism
A high pressure wurtzite-type form (borazon) was described by Soma et al. (1974) and another high pressure zinc blende type structure was described by Coleburn and Forbes (1968).

Additional pattern
PDF card 9-12 (Hatfield Ltd., Sheffield and A.E.R.E. Harwell, Didcot, Berks, England).

References

Coleburn, N. L. and Forbes, J. W. (1968). J. Chem. Phys. 48, 555.

Pease, R. S. (1952). Acta Crystallogr. 5, 356.

Soma, T., Sawaoka, A., and Saito, S. (1974). Mater. Res. Bull. 9, 755.


$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 26±2 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 3.328 | 100 | 0 0 2 | 26.765 |
| 2.169 | 15 | 1 0 0 | 41.598 |
| 2.0619 | 6 | 1 0 1 | 43.874 |
| 1.8176 | 9 | 1 0 2 | 50.150 |
| 1.6636 | 6 | 0 0 4 | 55.165 |
| 1.5509 | 1L | 1 0 3 | 59.561 |
| 1.3198 | 2 | 1 0 4 | 71.412 |
| 1.2521 | 5 | 1 1 0 | 75.934 |
| 1.1720 | 5 | 1 1 2 | 82.177 |
| 1.1346 | 1L | 1 0 5 | 85.521 |
| 1.1095 | 1L | 0 0 6 | 87.943 |
| 1.0843 | 1L | 2 0 0 | 90.535 |
| 1.0311 | 1 | 2 0 2 | 96.667 |
| 1.0005 | 3 | 1 1 4 | 100.690 |
| .9877 | 1L | 1 0 6 | 102.501 |
| .9086 | 1L | 2 0 4 | 115.941 |
| .8319 | 1L | 0 0 8 | 135.641 |
| .8304 | 1 | 1 1 6 | 136.150 |
| .8197 | 1L | 2 1 0 | 140.003 |
| .7960 | 1L | 2 1 2 | 150.810 |

# Boron Phosphate, $BPO_4$

Synonym
Boron orthophosphate

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

Color
Colorless

Structure
Tetragonal, $I\bar{4}$ (82). The structure was determined by Schulze (1934).

Crystallographic constants of this sample
$a = 4.34253(15)$ Å
$c = 6.6415(4)$

$c/a = 1.5294$

$Z = 2$
$V = 125.24$ Å$^3$
Density (calc) = 2.805 g/cm$^3$

Figure of merit
$F_{28} = 112.1(0.0063,36)$

Polymorphism
Three other forms of $BPO_4$ are reported. A quartz-like hexagonal (Shafer et al., 1956) and two high pressure hexagonal forms (Mackenzie et al., 1959, and Dachille and Dent-Glasser, 1959).

Additional pattern
PDF card 14-696 (deWolff, priv. comm.)

References

Dachille, F. and Dent-Glasser, L. S. (1959). Acta Crystallogr. 12, 280.

Mackenzie, J. D., Roth, W. L., and Wentorf, R. H. (1959). Acta Crystallogr. 12, 79.

Schulze, G. E. R. (1934). Z. Phys. Chem. B. 24, 215.

Shafer, E. C., Shafer, M. W., and Roy, R. (1956). Z. Kristallogr. 108, 263.


$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 26±1 °C
Internal standard Ag, a = 4.08651 Å

| d(Å) | $I^{rel}$ $\sigma = \pm 1$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 3.635 | 100 | 1 0 1 | 24.468 |
| 3.321 | 3 | 0 0 2 | 26.826 |
| 3.070 | 4 | 1 1 0 | 29.064 |
| 2.2546 | 34 | 1 1 2 | 39.956 |
| 1.9719 | 2 | 1 0 3 | 45.988 |
| 1.8641 | 10 | 2 1 1 | 48.815 |
| 1.8175 | 5 | 2 0 2 | 50.152 |
| 1.6604 | 1L | 0 0 4 | 55.282 |
| 1.5354 | 1 | 2 2 0 | 60.222 |
| 1.4597 | 10 | 2 1 3 | 63.700 |
| 1.4146 | 1L | 3 0 1 | 65.987 |
| 1.3936 | 1L | 2 2 2 | 67.109 |
| 1.3732 | 2 | 3 1 0 | 68.244 |
| 1.3192 | 5 | 2 0 4 | 71.454 |
| 1.2689 | 4 | 3 1 2 | 74.753 |
| 1.2114 | 2 | 3 0 3 | 78.970 |
| 1.1851 | 4 | 3 2 1 | 81.084 |
| 1.1272 | 1 | 2 2 4 | 86.218 |
| 1.1069 | 1L | 0 0 6 | 88.198 |
| 1.0964 | 2 | 2 1 5 | 89.265 |
| 1.0859 | 1L | 4 0 0 | 90.370 |
| 1.0580M | 1 | 3 1 4 | 93.450 |
| 1.0580M | | 3 2 3 | 93.450 |
| 1.0402 | 3 | 4 1 1 | 95.558 |
| 1.0319 | 1L | 4 0 2 | 96.569 |
| .9861 | 1L | 2 0 6 | 102.726 |
| .9781 | 1 | 3 3 2 | 103.915 |
| .9511 | 1L | 4 1 3 | 108.181 |
| .9319 | 1L | 4 2 2 | 111.497 |

# Cadmium Aluminum Oxide, $CdAl_2O_4$

Synonyms
Cadmium aluminate
Cadmium metaaluminate

CAS registry no.
12252-16-3

Sample
The sample was prepared by heating CdO and $\gamma$-$Al_2O_3$ in a sealed platinum tube for 18 hours at 975 °C, followed by 20 hours at 1200 °C.

Structure
Rhombohedral, $R\bar{3}$ (148). Phenakite type (Colin and Théry, 1966).

Crystallographic constants of this sample (Hexagonal axes)
a = 14.2146(3) Å
c = 9.5698(3)

c/a = 0.6732

Z = 18
V = 1674.57 $Å^3$
Density (calc) = 4.112 $g/cm^3$

Figure of merit
$F_{30}$ = 228.6(0.0031,43)

Polmorphism
At higher temperatures a cubic (spinel) form has been reported (Hahn et al., 1955).

Additional pattern
PDF card 22-119 (Colin and Théry, 1966)

References
Colin, F. and Théry, J. (1966). C. R. Séances Acad. Sci. Ser. C, 263, 1220.

Hahn, H., Günter, F., Klingler, W., Störger, D., and Störger, G. (1955). Z. Anorg. Allg. Chem. 279, 241.

$CuK\alpha_1$ $\lambda$ = 1.540598 Å; mean T = 26.1 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ $\sigma$ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.107 | 9 | 1 1 0 | 12.444 |
| 5.177 | 7 | 0 2 1 | 17.115 |
| 4.460 | 31 | 0 1 2 | 19.889 |
| 4.185 | 78 | 2 1 1 | 21.211 |
| 4.104 | 39 | 3 0 0 | 21.639 |
| 3.5527 | 86 | 2 2 0 | 25.045 |
| 3.3355 | 19 | 1 2 2 | 26.705 |
| 3.2157 | 28 | 1 3 1 | 27.719 |
| 2.9105 | 91 | 1 1 3 | 30.694 |
| 2.7794 | 6 | 3 1 2 | 32.180 |
| 2.6868 | 100 | 4 1 0 | 33.321 |
| 2.5889 | 5 | 0 4 2 | 34.620 |
| 2.4318 | 8 | 2 3 2 | 36.934 |
| 2.3737 | 58 | 2 2 3 | 37.873 |
| 2.3483 | 19 | 1 0 4 | 38.297 |
| 2.2605 | 11 | 2 4 1 | 39.847 |
| 2.1892 | 23 | 5 0 2 | 41.202 |
| 2.1541 | 3 | 5 1 1 | 41.905 |
| 2.1276 | 13 | 2 1 4 | 42.452 |
| 2.0923 | 8 | 4 2 2 | 43.205 |
| 2.0516 | 17 | 6 0 0 | 44.107 |
| 2.0071 | 18 | 1 5 2 | 45.136 |
| 1.9799 | 12 | 4 3 1 | 45.791 |
| 1.9711 | 13 | 5 2 0 | 46.008 |
| 1.9594 | 3 | 1 3 4 | 46.299 |
| 1.9021 | 37 | 3 3 3 | 47.780 |
| 1.8641 | 8 | 3 4 2 | 48.817 |
| 1.8425 | 2 | 1 6 1 | 49.425 |
| 1.8251 | 9 | 3 2 4 | 49.930 |
| 1.7768 | 2 | 4 4 0 | 51.384 |
| 1.7700 | 9 | 1 2 5 | 51.597 |
| 1.7474 | 2 | 6 1 2 | 52.313 |
| 1.7296 | 5 | 3 5 1 | 52.892 |
| 1.7254 | 7 | 6 0 3 | 53.032 |
| 1.7157 | 6 | 0 5 4 | 53.354 |
| 1.6805 | 13 | 6 2 1 | 54.565 |
| 1.6767 | 7 | 5 2 3 | 54.697 |
| 1.6684M | 8 | 3 1 5 | 54.992 |
| 1.6684M | | 2 4 4 | 54.992 |
| 1.6504 | 1 | 0 7 2 | 55.645 |
| 1.6303 | 13 | 7 1 0 | 56.391 |
| 1.6237 | 10 | 5 1 4 | 56.641 |
| 1.6079 | 1 | 2 6 2 | 57.248 |
| 1.5949 | 13 | 0 0 6 | 57.759 |
| 1.5510 | 10 | 6 3 0 | 59.558 |

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.5194 | 2 | 0 8 1 | 60.923 |
| 1.4971 | 1 | 4 5 2 | 61.933 |
| 1.4860M | 5 | 3 0 6 | 62.448 |
| 1.4860M | | 2 7 1 | 62.448 |
| 1.4778 | 3 | 4 2 5 | 62.830 |
| 1.4649 | 1 | 8 0 2 | 63.448 |
| 1.4554 | 12 | 2 2 6 | 63.914 |
| 1.4520 | 35 | 7 1 3 | 64.078 |
| 1.4249 | 2 | 8 1 1 | 65.450 |
| 1.4213 | 5 | 5 5 0 | 65.635 |
| 1.3947 | 19 | 6 3 3 | 67.049 |
| 1.3908 | 12 | 3 4 5 | 67.266 |
| 1.3796 | 2 | 1 8 2 | 67.883 |
| 1.3715 | 6 | 4 1 6 | 68.338 |
| 1.3679 | 10 | 9 0 0 | 68.543 |
| 1.3544 | 4 | 6 4 2 | 69.324 |
| 1.3430 | 1 | 8 2 0 | 70.000 |
| 1.3303 | 2 | 3 7 2 | 70.766 |
| 1.3117 | 2 | 2 1 7 | 71.925 |
| 1.2949 | 1 | 5 3 5 | 73.007 |
| 1.2766 | 4 | 7 4 0 | 74.230 |
| 1.2732 | 2 | 2 7 4 | 74.457 |
| 1.2693 | 1 | 1 3 7 | 74.728 |
| 1.2593 | 4 | 6 0 6 | 75.425 |
| 1.2459 | 2 | 5 6 2 | 76.377 |
| 1.2400 | 3 | 5 2 6 | 76.809 |
| 1.2161 | 2 | 4 6 4 | 78.605 |
| 1.2033 | 1 | 9 2 1 | 79.605 |
| 1.1990M | 2 | 8 0 5 | 79.948 |
| 1.1990M | | 7 3 4 | 79.948 |
| 1.1853 | 4 | 7 4 3 | 81.062 |
| 1.1825 | 4 | 7 2 5 | 81.298 |
| 1.1757 | 3 | 2 9 2 | 81.867 |
| 1.1703 | 4 | 5 7 1 | 82.323 |
| 1.1685 | 5 | 10 1 0 | 82.480 |
| 1.1584 | 1L | 1 2 8 | 83.356 |
| 1.1547 | 1 | 8 4 1 | 83.685 |
| 1.1402 | 6 | 7 1 6 | 84.999 |
| 1.1357 | 3 | 1 9 4 | 85.412 |
| 1.1329 | 3 | 4 3 7 | 85.678 |
| 1.1302 | 1L | 4 8 2 | 85.930 |
| 1.1120 | 4 | 6 3 6 | 87.691 |
| 1.0982 | 1 | 2 10 1 | 89.082 |
| 1.0970 | 1L | 10 1 3 | 89.201 |

# Cadmium Zinc Phosphate, $Cd_{0.9}Zn_{2.1}(PO_4)_2$

Sample
The sample was made by heating a mixture of $CdCO_3$, ZnO, and $(NH_4)_2HPO_4$ for 19 hours at 800 °C, followed by regrinding and heating for 2 days at 800 °C.

Color
Colorless

Structure
Monoclinic, $P2_1/c$ (14). The structure was determined by Calvo and Stephens (1968). The structure of this phase is related to graftonite $(Fe,Mn,Ca)_3(PO_4)_2$ and $Cd_2Zn(PO_4)_2$. This phase called "Bss" has a range of composition from 20% to 35% $Cd_3(PO_4)_2$ in the system $Cd_3(PO_4)_2$ - $Zn_3(PO_4)_2$ (Brown and Hummel, 1963).

Crystallographic constants of this sample

a = 9.0594(14) Å
b = 11.5369(14)
c = 5.9197(8)
β = 98.556(14)°

a/b = 0.7853
c/b = 0.5131

Z = 4
V = 611.83 $Å^3$
Density (calc) = 4.651 $g/cm^3$

Figure of merit
$F_{30}$ = 61.5(0.012,41)

Additional patterns
Brown and Hummel (1963)
Majling et al. (1979) Calculated pattern

References
Brown, J. J. and Hummel, F. A. (1963). J. Electrochem. Soc. 110, 1218.

Calvo, C. and Stephens, J. S. (1968). Can. J. Chem. 46, 903.

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; mean T = 25.1 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±4 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.96 | 10 | 1 0 0 | 9.868 |
| 7.06 | 1L | 1 1 0 | 12.523 |
| 5.760 | 1L | 0 2 0 | 15.370 |
| 5.212 | 1L | 0 1 1 | 16.997 |
| 4.800 | 2 | -1 1 1 | 18.471 |
| 4.480 | 8 | 2 0 0 | 19.803 |
| 4.274 | 4 | 1 1 1 | 20.765 |
| 4.177 | 13 | 2 1 0 | 21.253 |
| 4.112 | 6 | 0 2 1 | 21.594 |
| 3.889 | 13 | -1 2 1 | 22.850 |
| 3.648 | 33 | -2 1 1 | 24.383 |
| 3.592 | 22 | 1 2 1 | 24.768 |
| 3.532 | 53 | 1 3 0 | 25.196 |
| 3.213 | 10 | 0 3 1 | 27.744 |
| 3.107 | 9 | -1 3 1 | 28.713 |
| 2.988 | 35 | 3 0 0 | 29.880 |
| 2.950 | 47 | 1 3 1 | 30.277 |
| 2.926 | 47 | 0 0 2 | 30.522 |
| 2.916 | 49 | 2 3 0 | 30.633 |
| 2.883M | 100 | 0 4 0 | 30.989 |
| 2.883M | | 2 2 1 | 30.989 |
| 2.838 | 32 | 0 1 2 | 31.496 |
| 2.824 | 31 | -1 1 2 | 31.655 |
| 2.756 | 67 | -3 1 1 | 32.462 |
| 2.745 | 66 | 1 4 0 | 32.590 |
| 2.668 | 8 | 1 0 2 | 33.558 |
| 2.635 | 8 | -2 0 2 | 33.989 |
| 2.611 | 13 | 0 2 2 | 34.320 |
| 2.600M | 17 | -1 2 2 | 34.473 |
| 2.600M | | 1 1 2 | 34.473 |
| 2.569 | 8 | -2 1 2 | 34.892 |
| 2.546 | 2 | -3 2 1 | 35.228 |
| 2.455 | 19 | 3 1 1 | 36.574 |
| 2.424 | 9 | 2 4 0 | 37.054 |
| 2.398 | 2 | -2 2 2 | 37.467 |
| 2.329 | 15 | 0 3 2 | 38.623 |
| 2.308 | 5 | -2 4 1 | 39.002 |
| 2.284 | 12 | -3 3 1 | 39.424 |
| 2.266 | 4 | -3 0 2 | 39.744 |
| 2.240 | 1 | 4 0 0 | 40.222 |
| 2.198 | 12 | 4 1 0 | 41.039 |
| 2.135 | 2 | 2 2 2 | 42.302 |
| 2.114 | 5 | -1 5 1 | 42.732 |
| 2.109 | 8 | -3 2 2 | 42.851 |
| 2.103 | 2 | 3 3 1 | 42.971 |
| 2.063 | 3 | 1 5 1 | 43.860 |
| 2.051 | 10 | 2 5 0 | 44.109 |
| 1.9786 | 8 | -2 5 1 | 45.825 |
| 1.9734 | 1 | 2 3 2 | 45.951 |
| 1.9517 | 25 | -3 3 2 | 46.492 |

Cadmium Zinc Phosphate, $Cd_{0.9}Zn_{2.1}(PO_4)_2$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.9346 | 10 | 4 | 3 | 0 | 46.927 |
| 1.9234+ | 10 | 3 | 1 | 2 | 47.216 |
| 1.9234+ | | 0 | 6 | 0 | 47.216 |
| 1.9123 | 6 | -4 | 3 | 1 | 47.509 |
| 1.8968M | 12 | 2 | 5 | 1 | 47.920 |
| 1.8968M | | -4 | 1 | 2 | 47.920 |
| 1.8699 | 13 | -2 | 1 | 3 | 48.654 |
| 1.8494 | 2 | 0 | 2 | 3 | 49.230 |
| 1.8274M | 22 | 1 | 1 | 3 | 49.862 |
| 1.8274M | | 0 | 6 | 1 | 49.862 |
| 1.8100 | 6 | -1 | 5 | 2 | 50.374 |
| 1.8061 | 7 | -1 | 6 | 1 | 50.492 |
| 1.7976 | 7 | 2 | 4 | 2 | 50.746 |
| 1.7903 | 4 | -3 | 5 | 1 | 50.968 |
| 1.7719 | 22 | 4 | 3 | 1 | 51.535 |
| 1.7671 | 12 | 2 | 6 | 0 | 51.686 |
| 1.7519M | 4 | -1 | 3 | 3 | 52.169 |
| 1.7519M | | -4 | 4 | 1 | 52.169 |
| 1.7452 | 10 | 1 | 5 | 2 | 52.385 |
| 1.7404 | 15 | 0 | 3 | 3 | 52.539 |
| 1.7361 | 15 | -2 | 5 | 2 | 52.679 |
| 1.7111 | 2 | 5 | 2 | 0 | 53.510 |
| 1.7002M | 3 | -2 | 3 | 3 | 53.882 |
| 1.7002M | | 3 | 5 | 1 | 53.882 |
| 1.6813M | 9 | -3 | 2 | 3 | 54.536 |
| 1.6813M | | 2 | 1 | 3 | 54.536 |
| 1.6644 | 3 | 2 | 6 | 1 | 55.137 |
| 1.6410M | 2 | 4 | 4 | 1 | 55.990 |
| 1.6410M | | -5 | 0 | 2 | 55.990 |
| 1.6288M | 8 | 2 | 2 | 3 | 56.447 |
| 1.6288M | | 2 | 5 | 2 | 56.447 |
| 1.6248M | 6 | -5 | 1 | 2 | 56.601 |
| 1.6248M | | 5 | 3 | 0 | 56.601 |
| 1.6211 | 6 | 1 | 7 | 0 | 56.742 |
| 1.6162M | 7 | -3 | 5 | 2 | 56.930 |
| 1.6162M | | 0 | 4 | 3 | 56.930 |
| 1.5938 | 5 | -4 | 5 | 1 | 57.802 |
| 1.5837 | 3 | -2 | 4 | 3 | 58.206 |
| 1.5786M | 4 | -4 | 1 | 3 | 58.413 |
| 1.5786M | | -5 | 2 | 2 | 58.413 |
| 1.5739 | 1 | -1 | 7 | 1 | 58.603 |
| 1.5352 | 1 | -4 | 2 | 3 | 60.231 |
| 1.5271M | 14 | 3 | 6 | 1 | 60.586 |
| 1.5271M | | 4 | 3 | 2 | 60.586 |
| 1.5209 | 10 | -5 | 4 | 1 | 60.860 |
| 1.5147 | 1 | -2 | 7 | 1 | 61.133 |
| 1.4980 | 1 | -1 | 5 | 3 | 61.892 |
| 1.4896M | 1 | 0 | 5 | 3 | 62.278 |
| 1.4896M | | 3 | 5 | 2 | 62.278 |
| 1.4805 | 2 | 6 | 1 | 0 | 62.705 |
| 1.4768M | 1 | 2 | 7 | 1 | 62.881 |
| 1.4768M | | -4 | 5 | 2 | 62.881 |

# Calcium Iron Silicate (Kirschsteinite), $CaFeSiO_4$

Sample
The sample was prepared from $CaCO_3$, $Fe_2O_3$, and $SiO_2$. The components, in stoichiometric proportions, were blended with a mortar and pestle in acetone. After drying, the sample was heated in an iron crucible in three eight hour stages; 1075 °C, 1110 °C, and 1140 °C in a controlled atmosphere with the partial pressure of oxygen less than or equal to $10^{-18}$ atm.

Color
Yellowish gray

Structure
Orthorhombic, Pmnb (62). The structure was studied by Sahama and Hytönen (1958). Their results were derived by analogy of the fosterite-fayalite series as reported by Yoder and Sahama (1957).

Crystallographic constants of this sample
a = 6.4413(7) Å
b = 11.1586(12)
c = 4.8753(3)

a/b = 0.5772
c/b = 0.4369

Z = 4
V = 350.42 $Å^3$
Density (calc) = 3.564 $g/cm^3$

Figure of merit
$F_{30}$ = 92.1(0.0072,45)

Additional pattern
PDF card 11-477 (Sahama and Hytönen, 1958)

References
Sahama, Th. G. and Hytönen, K. (1958). Am. Mineral. 43, 862.

Yoder, H. S., Jr. and Sahama, Th. G. (1957). Am. Mineral. 42, 475.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26.0 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±5 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.579 | 31 | 0 2 0 | 15.872 |
| 4.466 | 13 | 0 1 1 | 19.865 |
| 4.217 | 16 | 1 2 0 | 21.049 |
| 3.886 | 11 | 1 0 1 | 22.864 |
| 3.672M | 39 | 0 2 1 | 24.221 |
| 3.672M | | 1 1 1 | 24.221 |
| 3.222 | 9 | 2 0 0 | 27.662 |
| 3.190 | 8 | 1 2 1 | 27.946 |
| 2.955 | 74 | 0 3 1 | 30.217 |
| 2.789M | 34 | 0 4 0 | 32.062 |
| 2.789M | | 2 2 0 | 32.062 |
| 2.687 | 67 | 1 3 1 | 33.315 |
| 2.612 | 100 | 2 1 1 | 34.298 |
| 2.5604 | 16 | 1 4 0 | 35.018 |
| 2.4375 | 12 | 0 0 2 | 36.845 |
| 2.4208M | 27 | 0 4 1 | 37.108 |
| 2.4208M | | 2 2 1 | 37.108 |
| 2.3809 | 7 | 0 1 2 | 37.753 |
| 2.2328M | 8 | 0 2 2 | 40.362 |
| 2.2328M | | 1 1 2 | 40.362 |
| 2.1779 | 15 | 2 3 1 | 41.426 |
| 2.1097M | 3 | 1 2 2 | 42.831 |
| 2.1097M | | 2 4 0 | 42.831 |
| 2.0381 | 5 | 0 3 2 | 44.414 |
| 2.0294 | 9 | 0 5 1 | 44.613 |
| 1.9644 | 1L | 3 0 1 | 46.174 |
| 1.9351+ | 10 | 2 4 1 | 46.914 |
| 1.9351+ | | 3 1 1 | 46.914 |
| 1.9150 | 2 | 2 1 2 | 47.437 |
| 1.8534 | 5 | 3 2 1 | 49.116 |
| 1.8353M | 85 | 0 4 2 | 49.634 |
| 1.8353M | | 2 2 2 | 49.634 |
| 1.7870 | 8 | 1 6 0 | 51.071 |
| 1.7649 | 9 | 1 4 2 | 51.757 |
| 1.7375M | 17 | 0 6 1 | 52.635 |
| 1.7375M | | 3 3 1 | 52.635 |
| 1.7167 | 18 | 2 5 1 | 53.322 |
| 1.7015 | 10 | 3 4 0 | 53.835 |
| 1.6105M | 51 | 2 6 0 | 57.150 |
| 1.6105M | | 4 0 0 | 57.150 |
| 1.5949M | 12 | 1 5 2 | 57.760 |
| 1.5949M | | 2 4 2 | 57.760 |
| 1.5603M | 7 | 0 2 3 | 59.167 |
| 1.5603M | | 1 1 3 | 59.167 |
| 1.5475M | 4 | 3 2 2 | 59.703 |

Calcium Iron Silicate (Kirschsteinite), $CaFeSiO_4$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 5$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.5475M | | 4 | 2 | 0 | 59.703 |
| 1.5154M | 17 | 0 | 7 | 1 | 61.103 |
| 1.5154M | | 4 | 1 | 1 | 61.103 |
| 1.4893 | 6 | 0 | 3 | 3 | 62.294 |
| 1.4743+ | 1 | 3 | 5 | 1 | 62.997 |
| 1.4743+ | | 4 | 2 | 1 | 62.997 |
| 1.4659 | 1L | 2 | 5 | 2 | 63.403 |
| 1.4508 | 4 | 1 | 3 | 3 | 64.139 |
| 1.4387 | 9 | 2 | 1 | 3 | 64.745 |
| 1.4143 | 8 | 4 | 3 | 1 | 66.004 |
| 1.4040M | 9 | 0 | 4 | 3 | 66.546 |
| 1.4040M | | 2 | 2 | 3 | 66.546 |
| 1.3949+ | 5 | 0 | 8 | 0 | 67.042 |
| 1.3949+ | | 4 | 4 | 0 | 67.042 |
| 1.3723 | 2 | 1 | 4 | 3 | 68.295 |
| 1.3518 | 2 | 2 | 3 | 3 | 69.478 |
| 1.3439M | 9 | 2 | 6 | 2 | 69.948 |
| 1.3439M | | 4 | 0 | 2 | 69.948 |
| 1.3344M | 1 | 0 | 7 | 2 | 70.514 |
| 1.3344M | | 4 | 1 | 2 | 70.514 |
| 1.3137 | 1 | 0 | 5 | 3 | 71.796 |
| 1.3061+ | 1 | 3 | 5 | 2 | 72.281 |
| 1.3061+ | | 4 | 2 | 2 | 72.281 |
| 1.2960 | 1 | 3 | 0 | 3 | 72.937 |
| 1.2871+ | 2 | 2 | 4 | 3 | 73.520 |
| 1.2871+ | | 3 | 1 | 3 | 73.520 |
| 1.2800 | 3 | 2 | 8 | 0 | 73.999 |
| 1.2614 | 2 | 4 | 5 | 1 | 75.279 |
| 1.2380+ | 1L | 2 | 8 | 1 | 76.955 |
| 1.2380+ | | 3 | 7 | 1 | 76.955 |
| 1.2235M | 1 | 0 | 6 | 3 | 78.040 |
| 1.2235M | | 3 | 3 | 3 | 78.040 |
| 1.2189 | 6 | 0 | 0 | 4 | 78.391 |
| 1.2164 | 7 | 2 | 5 | 3 | 78.585 |
| 1.2106M | 6 | 0 | 8 | 2 | 79.029 |
| 1.2106M | | 4 | 4 | 2 | 79.029 |

## Calcium Magnesium Silicate (Monticellite), $CaMgSiO_4$

Synonym
Calcium magnesium orthosilicate

CAS registry no.
14567-83-0

Sample
The sample was made by heating a mixture of $CaCO_3$, basic magnesium carbonate and $SiO_2$ at 900 °C, followed by heating at 1350-1380 °C for 420 hours with periodic grindings.

Color
Colorless

Optical data
$N_\alpha$ = 1.641, $N_\beta$ = 1.649, $N_\gamma$ = 1.655 (-) 2V = 80° (Sahama and Hytönen, 1958).

Structure
Orthorhombic, Pmnb (62). Olivine type (Brown and West, 1927). The structure was determined by Brown and West (1927) and refined by Onken (1964).

Crystallographic constants of this sample
a = 6.3666(6) Å
b = 11.0741(11)
c = 4.8224(6)

a/b = 0.5749
c/b = 0.4355

Z = 4
V = 340.00 Å$^3$
Density (calc) = 3.057 g/cm$^3$

Figure of merit
$F_{30}$ = 76.4(0.010,39)

Additional patterns
PDF card 19-240 (United Steel Co. Ltd., Rotherham, U.K.)

Sahama and Hytönen (1958)

References
Brown, G. B. and West, J. (1927). Z. Kristallogr., 66, 154.

Onken, H. (1964). Naturwissenschaften 51, 334.

Sahama, Th. G. and Hytönen, K. (1958). Am. Mineral. 43, 862.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26±2 °C
Internal standards Ag, a = 4.08651 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±4 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.538 | 8 | 0 2 0 | 15.990 |
| 4.425 | 3 | 0 1 1 | 20.052 |
| 4.183 | 25 | 1 2 0 | 21.225 |
| 3.845 | 13 | 1 0 1 | 23.113 |
| 3.634M | 51 | 0 2 1 | 24.474 |
| 3.634M | | 1 1 1 | 24.474 |
| 3.185 | 26 | 2 0 0 | 27.995 |
| 3.159 | 10 | 1 2 1 | 28.229 |
| 2.932 | 44 | 0 3 1 | 30.465 |
| 2.768 | 6 | 0 4 0 | 32.312 |
| 2.761 | 6 | 2 2 0 | 32.402 |
| 2.664 | 100 | 1 3 1 | 33.620 |
| 2.584 | 59 | 2 1 1 | 34.684 |
| 2.540 | 21 | 1 4 0 | 35.301 |
| 2.396 | 29 | 2 2 1 | 37.499 |
| 2.357 | 9 | 0 1 2 | 38.150 |
| 2.247 | 1 | 1 4 1 | 40.095 |
| 2.210M | 10 | 0 2 2 | 40.798 |
| 2.210M | | 1 1 2 | 40.798 |
| 2.1557 | 1 | 2 3 1 | 41.872 |
| 2.0893 | 4 | 2 4 0 | 43.269 |
| 2.0188 | 2 | 0 3 2 | 44.861 |
| 2.0127 | 2 | 0 5 1 | 45.004 |
| 1.9815 | 1L | 3 2 0 | 45.754 |
| 1.9424 | 1L | 3 0 1 | 46.729 |
| 1.9222 | 5 | 2 0 2 | 47.248 |
| 1.9131 | 9 | 3 1 1 | 47.486 |
| 1.8941 | 2 | 2 1 2 | 47.994 |
| 1.8462 | 1 | 0 6 0 | 49.320 |
| 1.8327 | 4 | 3 2 1 | 49.709 |
| 1.8160 | 60 | 2 2 2 | 50.198 |
| 1.7730 | 8 | 1 6 0 | 51.503 |
| 1.7485 | 10 | 1 4 2 | 52.276 |
| 1.7194 | 21 | 3 3 1 | 53.232 |
| 1.7013 | 6 | 2 5 1 | 53.842 |
| 1.6844 | 9 | 3 4 0 | 54.427 |
| 1.6637 | 1L | 1 6 1 | 55.161 |
| 1.5965 | 25 | 2 6 0 | 57.697 |
| 1.5919 | 27 | 4 0 0 | 57.877 |
| 1.5796M | 8 | 1 5 2 | 58.372 |

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.5796M | | 2 4 2 | 58.372 |
| 1.5433 | 9 | 1 1 3 | 59.883 |
| 1.5311 | 3 | 3 2 2 | 60.409 |
| 1.5032 | 12 | 0 7 1 | 61.653 |
| 1.4736 | 1L | 0 3 3 | 63.029 |
| 1.4578 | 1 | 4 2 1 | 63.796 |
| 1.4514 | 1 | 2 5 2 | 64.110 |
| 1.4357 | 1 | 1 3 3 | 64.897 |
| 1.4229 | 2 | 2 1 3 | 65.552 |
| 1.3987 | 6 | 4 3 1 | 66.833 |
| 1.3891 | 12 | 2 2 3 | 67.355 |
| 1.3804 | 3 | 3 4 2 | 67.837 |
| 1.3592 | 4 | 2 7 1 | 69.047 |
| 1.3312 | 1 | 2 6 2 | 70.708 |
| 1.3280 | 2 | 4 0 2 | 70.907 |
| 1.3188 | 1L | 4 1 2 | 71.477 |
| 1.2932 | 1 | 3 5 2 | 73.118 |
| 1.2731 | 4 | 3 1 3 | 74.466 |
| 1.2692 | 4 | 2 8 0 | 74.733 |

# Calcium Magnesium Silicate (Akermanite), $Ca_2MgSi_2O_7$

Sample
The sample was prepared from basic magnesium carbonate, $CaCO_3$ and $SiO_2$. The product was calcined at 850 °C then heated for 6 days between 1300-1380 °C with periodic grinding. To adjust the composition, 2% $SiO_2$ was added before the final heating at 1380 °C for 48 hours.

Color
Colorless

Structure
Tetragonal, $P\bar{4}2_1m$ (113), isostructural with $Ca_2ZnSi_2O_7$ (Andrews, 1948). The structure of $Ca_2ZnSi_2O_7$ was determined by Warren and Trautz (1930).

Crystallographic constants of this sample
$a = 7.8332(2)$ Å
$c = 5.0069(2)$

$c/a = 0.6392$

$Z = 2$
$V = 307.22$ Å$^3$
Density (calc) = 2.947 g/cm$^3$

Figure of merit
$F_{30} = 93.3(0.011,30)$

Additional patterns
PDF card 10-391 (Ervin and Osborn, 1949)
Andrews (1948)
O'Daniel and Tscheischwili (1945-48)

References

Andrews, K. W. (1948). Mineral. Mag. 28, 374.

Ervin, G., Jr. and Osborn, E. F. (1949). Am. Mineral. 34, 717.

O'Daniel, H. and Tscheischwili, L. (1945-48). Neues Jahrb. Mineral., Monatsh. A65, 60.

Warren, B. E. and Trautz, O. R. (1930). Z. Kristallogr. 75, 525.


$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 25±1 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 5.538 | 9 | 1 | 1 | 0 | 15.991 |
| 5.010 | 2 | 0 | 0 | 1 | 17.689 |
| 4.222 | 7 | 1 | 0 | 1 | 21.027 |
| 3.917 | 4 | 2 | 0 | 0 | 22.685 |
| 3.716 | 12 | 1 | 1 | 1 | 23.928 |
| 3.504 | 5 | 2 | 1 | 0 | 25.399 |
| 3.087 | 23 | 2 | 0 | 1 | 28.903 |
| 2.872 | 100 | 2 | 1 | 1 | 31.117 |
| 2.771 | 4 | 2 | 2 | 0 | 32.277 |
| 2.505 | 4 | 0 | 0 | 2 | 35.821 |
| 2.478 | 15 | 3 | 1 | 0 | 36.224 |
| 2.425 | 7 | 2 | 2 | 1 | 37.046 |
| 2.386 | 8 | 1 | 0 | 2 | 37.673 |
| 2.316 | 9 | 3 | 0 | 1 | 38.849 |
| 2.282 | 3 | 1 | 1 | 2 | 39.452 |
| 2.221 | 1 | 3 | 1 | 1 | 40.589 |
| 2.172 | 1L | 3 | 2 | 0 | 41.536 |
| 2.110 | 1 | 2 | 0 | 2 | 42.828 |
| 2.0372 | 13 | 2 | 1 | 2 | 44.434 |
| 1.9928 | 2 | 3 | 2 | 1 | 45.480 |
| 1.9581 | 6 | 4 | 0 | 0 | 46.331 |
| 1.9005 | 6 | 4 | 1 | 0 | 47.822 |
| 1.8572 | 5 | 2 | 2 | 2 | 49.009 |
| 1.8462 | 9 | 3 | 3 | 0 | 49.321 |
| 1.8237 | 1L | 4 | 0 | 1 | 49.969 |
| 1.8075 | 1 | 3 | 0 | 2 | 50.448 |
| 1.7764 | 10 | 4 | 1 | 1 | 51.396 |
| 1.7609 | 20 | 3 | 1 | 2 | 51.883 |
| 1.7519 | 8 | 4 | 2 | 0 | 52.169 |
| 1.7327 | 3 | 3 | 3 | 1 | 52.791 |
| 1.6690 | 2 | 0 | 0 | 3 | 54.974 |
| 1.6531 | 1 | 4 | 2 | 1 | 55.546 |
| 1.6411 | 2 | 3 | 2 | 2 | 55.989 |
| 1.6325 | 1 | 1 | 0 | 3 | 56.309 |
| 1.5980 | 2 | 1 | 1 | 3 | 57.637 |
| 1.5421 | 1L | 4 | 0 | 2 | 59.935 |
| 1.5355 | 2 | 2 | 0 | 3 | 60.221 |
| 1.5133 | 1L | 4 | 1 | 2 | 61.195 |
| 1.5066 | 5 | 2 | 1 | 3 | 61.499 |
| 1.4951 | 1L | 5 | 0 | 1 | 62.025 |
| 1.4861 | 2 | 3 | 3 | 2 | 62.442 |
| 1.4683 | 3 | 5 | 1 | 1 | 63.286 |
| 1.4544 | 1L | 5 | 2 | 0 | 63.959 |
| 1.4352 | 1 | 4 | 2 | 2 | 64.919 |
| 1.4296 | 4 | 2 | 2 | 3 | 65.208 |

Calcium Magnesium Silicate (Akermanite), $Ca_2MgSi_2O_7$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.4063 | 3 | 3 | 0 | 3 | 66.428 |
| 1.3966 | 7 | 5 | 2 | 1 | 66.949 |
| 1.3846 | 3 | 4 | 4 | 0 | 67.608 |
| 1.3435 | 3 | 5 | 3 | 0 | 69.968 |
| 1.3344 | 2 | 4 | 4 | 1 | 70.514 |
| 1.3282 | 1L | 4 | 3 | 2 | 70.893 |
| 1.3096 | 2 | 5 | 1 | 2 | 72.058 |
| 1.3054 | 2 | 6 | 0 | 0 | 72.324 |
| 1.2974 | 1 | 5 | 3 | 1 | 72.843 |
| 1.2879 | 1 | 6 | 1 | 0 | 73.469 |
| 1.2702 | 1 | 4 | 0 | 3 | 74.668 |
| 1.2576 | 4 | 5 | 2 | 2 | 75.546 |
| 1.2538 | 6 | 4 | 1 | 3 | 75.811 |
| 1.2516 | 2 | 0 | 0 | 4 | 75.971 |
| 1.2471 | 1 | 6 | 1 | 1 | 76.291 |
| 1.2380 | 2 | 3 | 3 | 3 | 76.956 |
| 1.2119 | 1 | 4 | 4 | 2 | 78.933 |
| 1.2083 | 1 | 4 | 2 | 3 | 79.213 |
| 1.2022 | 2 | 6 | 2 | 1 | 79.695 |
| 1.1922 | 1L | 2 | 0 | 4 | 80.495 |
| 1.1884 | 3 | 5 | 4 | 1 | 80.809 |
| 1.1838 | 1 | 5 | 3 | 2 | 81.193 |
| 1.1787 | 1 | 2 | 1 | 4 | 81.615 |
| 1.1677 | 1 | 6 | 3 | 0 | 82.551 |
| 1.1577 | 1 | 6 | 0 | 2 | 83.422 |
| 1.1450 | 1L | 6 | 1 | 2 | 84.557 |
| 1.1421 | 1 | 4 | 3 | 3 | 84.824 |
| 1.1405 | 1 | 2 | 2 | 4 | 84.976 |
| 1.1302 | 3 | 5 | 1 | 3 | 85.931 |
| 1.1287 | 2 | 3 | 0 | 4 | 86.072 |
| 1.1173 | 1 | 3 | 1 | 4 | 87.170 |
| 1.1101 | 2 | 6 | 2 | 2 | 87.882 |
| 1.1076 | 1L | 5 | 5 | 0 | 88.125 |
| 1.0990 | 1 | 5 | 4 | 2 | 88.997 |
| 1.0966 | 1 | 5 | 2 | 3 | 89.247 |
| 1.0864 | 1L | 6 | 4 | 0 | 90.314 |
| 1.0760 | 1L | 7 | 2 | 0 | 91.427 |
| 1.0584 | 1L | 6 | 3 | 2 | 93.408 |
| 1.0519 | 1L | 7 | 2 | 1 | 94.159 |
| 1.0452 | 1 | 4 | 1 | 4 | 94.948 |

# Calcium Magnesium Silicate (Merwinite), $Ca_3Mg(SiO_4)_2$

Synonym
Tricalcium magnesium orthosilicate

CAS registry no.
13596-18-4

Sample
The sample was made by heating $CaCO_3$, basic magnesium carbonate and $SiO_2$ overnight at 900 °C, followed by heating at 1380 °C for 39 hours, and 1350 °C for 240 hours with intermediate grindings.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14) (Yamaguchi and Suzuki, 1967). The structure was determined by Moore and Araki (1972).

Crystallographic constants of this sample
$a = 13.298(3)$ Å
$b = 5.3046(12)$
$c = 9.352(3)$
$\beta = 92.09(2)°$

$a/b = 2.5069$
$c/b = 1.7630$

$Z = 4$
$V = 659.26$ Å$^3$
Density (calc) 3.312 g/cm$^3$

Figure of merit
$F_{30} = 33.6(0.012,73)$

Additional patterns
PDF card 4-728 (Phemister et al., 1942)
PDF card 25-161 (Moore and Araki, 1972)
Yamaguchi and Suzuki (1967)

References
Moore, P. B. and Araki, T. (1972). Am. Mineral. 57, 1355.

Phemister, J., Nurse, R. W., and Bannister, F. A. (1942). Mineral. Mag. 26, 225.

Yamaguchi, G. and Suzuki, K. (1967). Yogyo Kyokaishi (J. Ceram. Assoc. Jpn.) 75, 220.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 26±2 °C
Internal standards Ag, a = 4.08651 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 9.33 | 1 | 0 0 1 | 9.473 |
| 6.64 | 3 | 2 0 0 | 13.317 |
| 4.609 | 3 | 0 1 1 | 19.242 |
| 4.379 | 2 | -1 1 1 | 20.264 |
| 4.335 | 3 | 1 1 1 | 20.471 |
| 3.890 | 6 | -2 0 2 | 22.843 |
| 3.759M | 2 | 2 0 2 | 23.647 |
| 3.759M | | 2 1 1 | 23.647 |
| 3.508 | 1 | 0 1 2 | 25.371 |
| 3.325 | 9 | 4 0 0 | 26.792 |
| 3.169M | 7 | -4 0 1 | 28.137 |
| 3.169M | | 3 1 1 | 28.137 |
| 3.067 | 2 | 2 1 2 | 29.096 |
| 2.816 | 2 | 4 1 0 | 31.746 |
| 2.756 | 26 | -4 0 2 | 32.458 |
| 2.719 | 12 | -4 1 1 | 32.920 |
| 2.687 | 100 | 0 1 3 | 33.324 |
| 2.671 | 65 | 4 1 1 | 33.521 |
| 2.653 | 47 | 0 2 0 | 33.758 |
| 2.509 | 1 | -1 2 1 | 35.765 |
| 2.465M | 3 | 2 1 3 | 36.423 |
| 2.465M | | 2 2 0 | 36.423 |
| 2.330 | 5 | -3 1 3 | 38.614 |
| 2.321 | 12 | -5 1 1 | 38.773 |
| 2.307 | 10 | 0 2 2 | 39.015 |
| 2.285 | 7 | 5 1 1 | 39.401 |
| 2.267M | 5 | 1 2 2 | 39.735 |
| 2.267M | | 3 1 3 | 39.735 |
| 2.230 | 9 | -2 0 4 | 40.413 |
| 2.214 | 19 | 6 0 0 | 40.724 |
| 2.192 | 2 | -2 2 2 | 41.155 |
| 2.179 | 10 | 2 0 4 | 41.411 |
| 2.168 | 11 | 2 2 2 | 41.626 |
| 2.137M | 1 | 0 1 4 | 42.256 |
| 2.137M | | 6 0 1 | 42.256 |
| 2.121M | 2 | -1 1 4 | 42.592 |
| 2.121M | | -4 1 3 | 42.592 |
| 2.100 | 1 | 1 1 4 | 43.037 |
| 2.061 | 10 | -3 2 2 | 43.895 |
| 2.031M | 14 | 3 2 2 | 44.574 |
| 2.031M | | -6 0 2 | 44.574 |
| 2.014 | 1 | 4 2 1 | 44.974 |
| 1.9834 | 1 | 6 1 1 | 45.706 |
| 1.9111 | 35 | -4 2 2 | 47.539 |
| 1.8787M | 24 | 4 0 4 | 48.412 |
| 1.8787M | | 4 2 2 | 48.412 |
| 1.8258 | 1 | -4 1 4 | 49.909 |

# Calcium Manganese Phosphate Fluoride, $Ca_8Mn_2(PO_4)_6F_2$

Synonym
Calcium manganese orthophosphate fluoride

Sample
The sample was obtained from the General Electric Co., Chemical Products Plant, Cleveland, OH.

Color
Pink white

Structure
Hexagonal, $P6_3/m$ (176) (Schroeder, 1982).

Crystallographic constants of this sample
$a = 9.3286(4)$ Å
$c = 6.7678(9)$

$c/a = 0.7255$

$Z = 1$
$V = 510.05$ Å$^3$
Density (calc) = 3.380 g/cm$^3$

Figure of merit
$F_{30} = 127.7(0.0073,32)$

Reference
Schroeder, L. W. (1982). Private communication.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; temp. 26±1 °C
Internal standard Ag, a = 4.08651 Å

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.08 | 7 | 1 0 0 | 10.947 |
| 5.187 | 3 | 1 0 1 | 17.082 |
| 4.040 | 10 | 2 0 0 | 21.985 |
| 3.843 | 7 | 1 1 1 | 23.128 |
| 3.470 | 5 | 2 0 1 | 25.655 |
| 3.386 | 26 | 0 0 2 | 26.300 |
| 3.122 | 14 | 1 0 2 | 28.570 |
| 3.054 | 18 | 2 1 0 | 29.219 |
| 2.784 | 100 | 2 1 1 | 32.123 |
| 2.740 | 37 | 1 1 2 | 32.657 |
| 2.694 | 64 | 3 0 0 | 33.233 |
| 2.595 | 22 | 2 0 2 | 34.542 |
| 2.5018 | 18 | 3 0 1 | 35.865 |
| 2.3318 | 1 | 2 2 0 | 38.580 |
| 2.2664 | 6 | 2 1 2 | 39.738 |
| 2.2410 | 20 | 3 1 0 | 40.209 |
| 2.2061 | 3 | 2 2 1 | 40.873 |
| 2.1271 | 6 | 3 1 1 | 42.462 |
| 2.1073 | 2 | 3 0 2 | 42.882 |
| 2.0312 | 3 | 1 1 3 | 44.573 |
| 2.0200 | 2 | 4 0 0 | 44.834 |
| 1.9701 | 2 | 2 0 3 | 46.032 |
| 1.9358 | 3 | 4 0 1 | 46.897 |
| 1.9203 | 25 | 2 2 2 | 47.299 |
| 1.8680 | 12 | 3 1 2 | 48.707 |
| 1.8532 | 5 | 3 2 0 | 49.122 |
| 1.8143 | 23 | 2 1 3 | 50.246 |
| 1.7874 | 15 | 3 2 1 | 51.056 |
| 1.7628 | 15 | 4 1 0 | 51.821 |
| 1.7346 | 11 | 4 0 2 | 52.730 |
| 1.7060 | 2 | 4 1 1 | 53.684 |
| 1.6917 | 7 | 0 0 4 | 54.175 |
| 1.6256 | 7 | 3 2 2 | 56.569 |
| 1.6159 | 1 | 5 0 0 | 56.941 |
| 1.5900M | 2 | 1 1 4 | 57.954 |
| 1.5900M | | 3 1 3 | 57.954 |
| 1.5715 | 2 | 5 0 1 | 58.705 |
| 1.5637 | 1 | 4 1 2 | 59.026 |
| 1.5550 | 1 | 3 3 0 | 59.388 |
| 1.5266 | 5 | 4 2 0 | 60.606 |
| 1.5157 | 4 | 3 3 1 | 61.090 |
| 1.4893 | 2 | 4 2 1 | 62.292 |
| 1.4800 | 2 | 2 1 4 | 62.727 |
| 1.4580 | 9 | 5 0 2 | 63.785 |
| 1.4512 | 3 | 5 1 0 | 64.118 |
| 1.4324M | 9 | 3 0 4 | 65.065 |
| 1.4324M | | 3 2 3 | 65.065 |
| 1.4187 | 6 | 5 1 1 | 65.772 |
| 1.4123 | 2 | 3 3 2 | 66.105 |
| 1.3890 | 2 | 4 1 3 | 67.361 |
| 1.3468 | 1 | 6 0 0 | 69.771 |
| 1.3339 | 2 | 5 1 2 | 70.546 |
| 1.3285 | 1 | 4 3 0 | 70.879 |
| 1.3032 | 3 | 4 3 1 | 72.466 |
| 1.2936 | 3 | 5 2 0 | 73.094 |
| 1.2705 | 2 | 5 2 1 | 74.641 |
| 1.2640 | 2 | 4 2 3 | 75.094 |
| 1.2507 | 1 | 6 0 2 | 76.037 |
| 1.2366 | 5 | 4 3 2 | 77.061 |
| 1.2320 | 4 | 6 1 0 | 77.400 |
| 1.2202M | 6 | 4 1 4 | 78.290 |
| 1.2202M | | 5 1 3 | 78.290 |
| 1.2119 | 1 | 6 1 1 | 78.931 |
| 1.2084 | 4 | 5 2 2 | 79.204 |
| 1.1658 | 3 | 4 4 0 | 82.712 |
| 1.1542 | 1 | 5 3 0 | 83.729 |
| 1.1493 | 1 | 4 4 1 | 84.167 |
| 1.1446M | 2 | 3 3 4 | 84.593 |
| 1.1446M | | 4 3 3 | 84.593 |
| 1.1334 | 2 | 4 2 4 | 85.632 |
| 1.1223 | 1L | 5 2 3 | 86.685 |
| 1.1015 | 1 | 5 1 4 | 88.745 |
| 1.0921 | 5 | 5 3 2 | 89.713 |

# Calcium Zirconium Phosphate, $CaZr_4(PO_4)_6$

Synonym
Calcium zirconium orthophosphate

CAS registry no.
67972-87-6

Sample
The sample was made by heating a 1:4:6 molar mixture of $CaCO_3$, $ZrO_2$ and $(NH_4)_2HPO_4$ up to 500 °C. It was then reground and heated at 1300 °C overnight.

Color
Colorless

Structure
Rhombohedral, R⁂. The structure is similar to that of $NaZr_2(PO_4)_3$ (Chernorukov et al., 1978).

Crystallographic constants of this sample
(Hexagonal axes)
a = 8.7852(4) Å
c = 22.682(2)

c/a = 2.5819

Z = 3
V = 1516.06 Å$^3$
Density (calc) = 3.203 g/cm$^3$

Figure of merit
$F_{30}$ = 163.9(0.0045,41)

Reference
Chernorukov, N. G., Korshunov, I. A., and Prokof'eva, T. V. (1978). Sov. Phys. Crystallogr. Engl. Transl. 23, 475.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±5 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.556 | 3 | 0 0 3 | 11.702 |
| 7.208 | 4 | 1 0 1 | 12.269 |
| 6.316 | 22 | 0 1 2 | 14.010 |
| 4.546 | 69 | 1 0 4 | 19.512 |
| 4.392 | 82 | 1 1 0 | 20.204 |
| 3.896 | 6 | 0 1 5 | 22.808 |
| 3.798 | 100 | 1 1 3 | 23.402 |
| 3.607 | 1 | 2 0 2 | 24.663 |
| 3.1594 | 63 | 0 2 4 | 28.223 |
| 2.9140 | 3 | 2 0 5 | 30.656 |
| 2.8651 | 95 | 1 1 6 | 31.192 |
| 2.6559 | 5 | 0 1 8 | 33.720 |
| 2.5643 | 26 | 2 1 4 | 34.962 |
| 2.5355 | 44 | 3 0 0 | 35.373 |
| 2.4286 | 3 | 1 2 5 | 36.984 |
| 2.4040 | 2 | 3 0 3 | 37.377 |
| 2.2735 | 8 | 2 0 8 | 39.609 |
| 2.1965 | 6 | 2 2 0 | 41.060 |
| 2.1860 | 7 | 1 1 9 | 41.265 |
| 2.1734 | 4 | 1 0 10 | 41.515 |
| 2.1507 | 4 | 2 1 7 | 41.975 |
| 2.1062 | 12 | 3 0 6 | 42.906 |
| 2.0745 | 2 | 3 1 2 | 43.594 |
| 2.0191 | 25 | 1 2 8 | 44.854 |
| 1.9777 | 15 | 1 3 4 | 45.846 |
| 1.9483 | 8 | 0 2 10 | 46.578 |
| 1.9134 | 2 | 3 1 5 | 47.479 |
| 1.8989 | 32 | 2 2 6 | 47.863 |
| 1.8895 | 2 | 0 0 12 | 48.117 |
| 1.8760 | 5 | 0 4 2 | 48.487 |
| 1.8130 | 1 | 2 0 11 | 50.287 |
| 1.8033 | 1 | 4 0 4 | 50.576 |
| 1.7807 | 23 | 2 1 10 | 51.262 |
| 1.7679 | 5 | 1 3 7 | 51.660 |
| 1.7538 | 1 | 0 4 5 | 52.109 |
| 1.7358 | 1 | 1 1 12 | 52.691 |
| 1.7004 | 2 | 1 0 13 | 53.875 |
| 1.6924 | 12 | 3 1 8 | 54.150 |
| 1.6759 | 2 | 1 2 11 | 54.727 |
| 1.6679 | 16 | 3 2 4 | 55.013 |
| 1.6597 | 28 | 4 1 0 | 55.305 |
| 1.6286 | 2 | 2 3 5 | 56.455 |
| 1.6212 | 2 | 4 1 3 | 56.736 |
| 1.5840 | 7 | 0 1 14 | 58.196 |
| 1.5793 | 7 | 0 4 8 | 58.384 |

Calcium Zirconium Phosphate, $CaZr_4(PO_4)_6$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 5$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.5446 | 15 | 1 3 10 | 59.829 |
| 1.5366 | 2 | 3 2 7 | 60.173 |
| 1.5197 | 16 | 4 1 6 | 60.911 |
| 1.5159 | 1 | 3 0 12 | 61.079 |
| 1.4904 | 11 | 2 0 14 | 62.243 |
| 1.4865 | 8 | 2 3 8 | 62.424 |
| 1.4745 | 4 | 3 1 11 | 62.990 |
| 1.4694 | 6 | 0 5 4 | 63.233 |
| 1.4640 | 7 | 3 3 0 | 63.491 |
| 1.4572 | 7 | 4 0 10 | 63.825 |
| 1.4374 | 1 | 3 3 3 | 64.811 |
| 1.4298 | 3 | 1 1 15 | 65.198 |
| 1.4114 | 10 | 1 2 14 | 66.152 |
| 1.3935M | 5 | 2 4 4 | 67.114 |
| 1.3935M | | 1 0 16 | 67.114 |
| 1.3863 | 3 | 4 1 9 | 67.510 |
| 1.3832 | 3 | 3 2 10 | 67.682 |
| 1.3709 | 1 | 4 2 5 | 68.372 |
| 1.3648 | 4 | 3 3 6 | 68.720 |
| 1.3448 | 1L | 1 3 13 | 69.892 |
| 1.3284M | 9 | 5 1 4 | 70.883 |
| 1.3284M | | 0 2 16 | 70.883 |
| 1.3143M | 1L | 2 4 7 | 71.763 |
| 1.3143M | | 0 1 17 | 71.763 |
| 1.3085 | 1 | 1 5 5 | 72.127 |
| 1.2852M | 7 | 4 0 13 | 73.649 |
| 1.2852M | | 3 1 14 | 73.649 |
| 1.2822 | 1 | 4 2 8 | 73.851 |
| 1.2718 | 6 | 2 1 16 | 74.553 |
| 1.2682 | 3 | 6 0 0 | 74.803 |
| 1.2601 | 3 | 0 0 18 | 75.369 |
| 1.2430 | 1 | 3 4 2 | 76.587 |
| 1.2338M | 1 | 3 2 13 | 77.266 |
| 1.2338M | | 0 4 14 | 77.266 |
| 1.2217 | 2 | 4 3 4 | 78.175 |
| 1.2185 | 4 | 5 2 0 | 78.421 |
| 1.2147 | 4 | 2 4 10 | 78.711 |
| 1.2116 | 2 | 1 1 18 | 78.954 |
| 1.2025M | 1 | 5 2 3 | 79.669 |
| 1.2025M | | 6 0 6 | 79.669 |
| 1.1878 | 6 | 2 3 14 | 80.859 |
| 1.1706 | 1L | 5 1 10 | 82.305 |
| 1.1598 | 6 | 5 2 6 | 83.236 |
| 1.1446 | 3 | 3 4 8 | 84.598 |

# Cerium Oxide (Cerianite), $CeO_2$*

CAS registry no.
1306-38-3

Sample
This yttria-stabilized phase was prepared by Dragoo and Domingues (1982) from coprecipitation of the oxides. The powder was calcined at 620 °C and then formed into a billet without binder, isostatically pressed, and then hot-pressed in an alumina die for 30 minutes at 1350 °C with an applied stress of 28 MPa.

Color
Light gray yellowish brown

Structure
Cubic, Fm3m (225). Isostructural with fluorite, $CaF_2$. The structure of fluorite was determined by Bragg (1914).

Crystallographic constants of this sample
$a = 5.41134(12)$ Å

$Z = 4$
$V = 158.46$ Å$^3$
Density (calc) = 7.215 g/cm$^3$

Figure of merit
$F_{16} = 134.1(0.0075,16)$

*Comment
The true formula for this yttria-stabilized phase is $Ce_{0.914}Y_{0.086}O_{1.957}$. This sample was prepared to produce a high density ceramic.

References
Bragg, W. L. (1914). Proc. R. Soc. London, A89, 468.

Dragoo, A. L. and Domingues, L. P. (1982). J. Am. Ceram. Soc. 65, #5, 253.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 26.1 °C
Internal standard Ag, a = 4.08651 Å

| d(Å) | $I^{rel}$ $\sigma = \pm 1$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 3.123 | 100 | 1 1 1 | 28.555 |
| 2.706 | 30 | 2 0 0 | 33.082 |
| 1.9134 | 52 | 2 2 0 | 47.479 |
| 1.6318 | 42 | 3 1 1 | 56.335 |
| 1.5622 | 8 | 2 2 2 | 59.087 |
| 1.3531 | 8 | 4 0 0 | 69.402 |
| 1.2415 | 14 | 3 3 1 | 76.700 |
| 1.2101 | 8 | 4 2 0 | 79.070 |
| 1.1048 | 14 | 4 2 2 | 88.412 |
| 1.0415 | 11 | 5 1 1 | 95.397 |
| .9566 | 4 | 4 4 0 | 107.265 |
| .9147 | 13 | 5 3 1 | 114.730 |
| .9019 | 6 | 6 0 0 | 117.317 |
| .8556 | 9 | 6 2 0 | 128.393 |
| .8252 | 6 | 5 3 3 | 137.969 |
| .8158 | 5 | 6 2 2 | 141.566 |

# Cesium Hydrogen Phosphate, $CsH_5(PO_4)_2$

Synonym
Cesium pentahydrogen diphosphate

Sample
The sample was prepared by mixing an 85% solution of $H_3PO_4$ with $Cs_2CO_3$. The precipitate was washed with alcohol and dried in air one week.

Color
Colorless

Structure
Monoclinic, $P2_1/c$ (14) (Ferrari, 1956), confirmed by Norbert and André (1970).

Crystallographic constants of this sample

a = 10.8814(11) Å
b = 7.7717(8)
c = 9.5320(9)
β = 96.586(10)°

a/b = 1.4001
c/b = 1.2265

Z = 4
V = 800.77 Å$^3$
Density (calc) = 2.720 g/cm$^3$

Figure of merit
$F_{30}$ = 62.5(0.0098,49)

Additional pattern
PDF card 24-252 (Norbert, Univ. of Montpelier, Lab. de Chimie Min., C, 1971)

References
Ferrari, A., Nardelli, M., and Cingi, M. (1956). Gazz Chim. Ital. 86, 1174.

Norbert, A., and André, D. (1970). C. R. Séances Acad. Sci. Ser. C. 270, 1718.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.6 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.311 | 22 | 1 1 0 | 14.022 |
| 6.005 | 7 | 0 1 1 | 14.741 |
| 5.403 | 8 | 2 0 0 | 16.394 |
| 4.531 | 13 | -1 0 2 | 19.577 |
| 4.166M | 39 | -2 1 1 | 21.311 |
| 4.166M | | 1 0 2 | 21.311 |
| 3.918 | 37 | -1 1 2 | 22.678 |
| 3.879 | 40 | 2 1 1 | 22.909 |
| 3.785 | 37 | -2 0 2 | 23.485 |
| 3.672 | 52 | 1 1 2 | 24.217 |
| 3.595 | 20 | 0 2 1 | 24.744 |
| 3.458 | 13 | -1 2 1 | 25.743 |
| 3.404 | 24 | -2 1 2 | 26.160 |
| 3.369 | 44 | 1 2 1 | 26.435 |
| 3.271 | 100 | 3 1 0 | 27.244 |
| 3.094 | 8 | 2 1 2 | 28.828 |
| 3.038 | 5 | -3 0 2 | 29.379 |
| 3.004 | 4 | 0 2 2 | 29.715 |
| 2.951 | 5 | -1 2 2 | 30.262 |
| 2.923 | 17 | 0 1 3 | 30.555 |
| 2.902 | 3 | -1 1 3 | 30.791 |
| 2.841 | 4 | 1 2 2 | 31.460 |
| 2.832 | 7 | -3 1 2 | 31.569 |
| 2.751 | 11 | 1 1 3 | 32.525 |
| 2.721 | 7 | 3 0 2 | 32.892 |
| 2.711 | 11 | -2 2 2 | 33.013 |
| 2.701 | 8 | 4 0 0 | 33.138 |
| 2.603 | 12 | -3 2 1 | 34.421 |
| 2.569 | 7 | 3 1 2 | 34.891 |
| 2.548 | 14 | 2 2 2 | 35.196 |
| 2.535 | 4 | -4 1 1 | 35.376 |
| 2.499 | 20 | 0 3 1 | 35.912 |
| 2.493 | 18 | 3 2 1 | 36.002 |
| 2.472 | 6 | -4 0 2 | 36.320 |
| 2.451M | 4 | -1 3 1 | 36.636 |
| 2.451M | | 0 2 3 | 36.636 |
| 2.437 | 6 | -1 2 3 | 36.849 |
| 2.419 | 3 | 1 3 1 | 37.131 |
| 2.401 | 5 | 4 1 1 | 37.419 |
| 2.394 | 3 | -3 2 2 | 37.535 |
| 2.371 | 14 | -1 0 4 | 37.925 |
| 2.357 | 8 | -4 1 2 | 38.159 |
| 2.310 | 13 | -2 2 3 | 38.952 |
| 2.294 | 11 | -2 3 1 | 39.233 |
| 2.265M | 17 | -1 1 4 | 39.757 |
| 2.265M | | -2 0 4 | 39.757 |
| 2.242 | 22 | 2 3 1 | 40.199 |
| 2.218 | 5 | 4 2 0 | 40.644 |
| 2.175 | 5 | -2 1 4 | 41.486 |
| 2.1691 | 6 | 1 1 4 | 41.603 |
| 2.1626 | 6 | 5 0 0 | 41.732 |
| 2.1519 | 4 | 4 1 2 | 41.950 |
| 2.1147 | 3 | -3 2 3 | 42.724 |
| 2.1030 | 6 | 3 3 0 | 42.973 |
| 2.0828+ | 9 | -3 3 1 | 43.411 |
| 2.0828+ | | 5 1 0 | 43.411 |
| 2.0581 | 1 | -5 0 2 | 43.960 |
| 2.0232 | 3 | -1 2 4 | 44.758 |
| 2.0118 | 6 | 2 1 4 | 45.025 |
| 2.0026 | 9 | 0 3 3 | 45.244 |

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.9894M | 7 | -5 1 2 | 45.561 |
| 1.9894M | | 5 1 1 | 45.561 |
| 1.9531 | 4 | 1 2 4 | 46.457 |
| 1.9441 | 9 | 1 3 3 | 46.684 |
| 1.9396 | 8 | 4 2 2 | 46.799 |
| 1.9018 | 2 | -4 2 3 | 47.787 |
| 1.8882M | 4 | 5 2 0 | 48.154 |
| 1.8882M | | 4 1 3 | 48.154 |
| 1.8809M | 7 | 3 0 4 | 48.352 |
| 1.8809M | | -1 4 1 | 48.352 |
| 1.8668 | 5 | 1 4 1 | 48.741 |
| 1.8628 | 5 | -4 3 1 | 48.851 |
| 1.8478 | 1 | -1 1 5 | 49.275 |
| 1.8334M | 12 | -5 1 3 | 49.688 |
| 1.8334M | | 5 1 2 | 49.688 |
| 1.8285M | 7 | 3 1 4 | 49.830 |
| 1.8285M | | 2 4 0 | 49.830 |
| 1.8181M | 5 | -5 2 2 | 50.134 |
| 1.8181M | | 5 2 1 | 50.134 |
| 1.8072M | 7 | 4 3 1 | 50.459 |
| 1.8072M | | -3 3 3 | 50.459 |
| 1.8015 | 20 | 6 0 0 | 50.629 |
| 1.7554 | 2 | 6 1 0 | 52.058 |
| 1.7519 | 1L | -6 0 2 | 52.170 |
| 1.7403 | 2 | 4 2 3 | 52.542 |
| 1.7181 | 1L | -3 1 5 | 53.274 |
| 1.7085M | 1L | -6 1 2 | 53.598 |
| 1.7085M | | -1 2 5 | 53.598 |
| 1.7020M | 3 | 1 3 4 | 53.818 |
| 1.7020M | | 0 2 5 | 53.818 |
| 1.6985M | 6 | -3 4 1 | 53.938 |
| 1.6985M | | 3 3 3 | 53.938 |
| 1.6941M | 5 | 4 3 2 | 54.090 |
| 1.6941M | | 3 2 4 | 54.090 |
| 1.6840 | 1L | 2 4 2 | 54.443 |
| 1.6741 | 2 | -2 2 5 | 54.791 |
| 1.6671 | 4 | 3 4 1 | 55.041 |
| 1.6555 | 1 | 1 2 5 | 55.459 |
| 1.6506 | 3 | -1 4 3 | 55.637 |
| 1.6392 | 4 | -6 2 1 | 56.060 |

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.6344 | 9 | 6 2 0 | 56.238 |
| 1.6089 | 2 | -2 4 3 | 57.212 |
| 1.5777+ | 2 | 2 2 5 | 58.450 |
| 1.5777+ | | 4 4 0 | 58.450 |
| 1.5728 | 2 | -4 4 1 | 58.649 |
| 1.5558+ | 5 | -1 1 6 | 59.355 |
| 1.5558+ | | 4 3 3 | 59.355 |
| 1.5465 | 2 | 0 1 6 | 59.746 |
| 1.5389+ | 5 | -3 4 3 | 60.073 |
| 1.5389+ | | 1 5 0 | 60.073 |
| 1.5329M | 11 | -1 3 5 | 60.332 |
| 1.5329M | | -2 1 6 | 60.332 |
| 1.5247 | 4 | 5 3 2 | 60.690 |
| 1.5148M | 5 | 1 5 1 | 61.128 |
| 1.5148M | | 7 1 0 | 61.128 |
| 1.5121M | 3 | -4 2 5 | 61.249 |
| 1.5121M | | 5 0 4 | 61.249 |
| 1.4944M | 2 | 1 3 5 | 62.056 |
| 1.4944M | | 2 5 0 | 62.056 |
| 1.4823M | 1L | -6 3 1 | 62.622 |
| 1.4823M | | -2 5 1 | 62.622 |
| 1.4704+ | 8 | 3 4 3 | 63.185 |
| 1.4704+ | | -1 5 2 | 63.185 |
| 1.4558 | 1L | 1 5 2 | 63.893 |
| 1.4448+ | 2 | 5 4 0 | 64.436 |
| 1.4448+ | | 2 1 6 | 64.436 |
| 1.4408 | 3 | 6 3 1 | 64.639 |
| 1.4290 | 1 | 1 2 6 | 65.235 |
| 1.4121M | 1L | 5 4 1 | 66.119 |
| 1.4121M | | 2 5 2 | 66.119 |
| 1.3973M | 1L | 7 1 2 | 66.909 |
| 1.3973M | | 7 2 1 | 66.909 |
| 1.3939M | 1L | 0 5 3 | 67.095 |
| 1.3939M | | 6 2 3 | 67.095 |
| 1.3878 | 3 | 3 0 6 | 67.426 |
| 1.3742 | 2 | 1 5 3 | 68.185 |
| 1.3628 | 3 | 3 3 5 | 68.839 |

# Cesium Zirconium Phosphate, $CsZr_2(PO_4)_3$

Synonyms
Cesium zirconium orthophosphate
Cesium dizirconium tris(phosphate)

CAS registry no.
19527-88-9

Sample
The sample was prepared from a mixture of $(NH_4)_2HPO_4$, $Cs_2CO_3$ and $ZrO_2$ in molar ratios of 6:1:4. The mixture was heated for 2 hours at 500 °C, reground, and heated for 2 hours at 1000 °C. It was reground; a small amount of $Cs_2CO_3$ was added, and the mixture was heated at 900 °C for 16 hours.

Color
Colorless

Structure
Rhombohedral, $R\bar{3}c$ (167), (Matković et al., 1968).

Crystallographic constants of this sample (Hexagonal axes)
a = 8.5807(3) Å
c = 24.9654(13)

c/a = 2.9095

Z = 6
V = 1591.90 Å$^3$
Density (calc) = 3.757 g/cm$^3$

Figure of merit
$F_{30}$ = 157.5(0.0054,35)

Additional pattern
Roy et al. (1982)

References
Matković, B., Prodić, B., and Šljukić, M. (1968). Bull. Soc. Chim. Fr., 1777.

Roy, R., Vance, E. R., and Alamo, J. (1982). Mater. Res. Bull. 17, 585.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.390 | 1L | 0 1 2 | 13.848 |
| 4.781 | 1 | 1 0 4 | 18.544 |
| 4.291 | 73 | 1 1 0 | 20.685 |
| 4.161 | 7 | 0 0 6 | 21.338 |
| 3.814 | 32 | 1 1 3 | 23.306 |
| 3.562 | 7 | 2 0 2 | 24.980 |
| 3.193 | 5 | 0 2 4 | 27.924 |
| 2.9860 | 100 | 1 1 6 | 29.899 |
| 2.8765 | 10 | 0 1 8 | 31.066 |
| 2.7902 | 2 | 2 1 1 | 32.052 |
| 2.7400 | 8 | 1 2 2 | 32.655 |
| 2.5604 | 1L | 2 1 4 | 35.017 |
| 2.4766 | 23 | 3 0 0 | 36.242 |
| 2.4477 | 2 | 1 2 5 | 36.686 |
| 2.3892 | 6 | 2 0 8 | 37.617 |
| 2.3669 | 1L | 1 0 10 | 37.985 |
| 2.3291 | 2 | 1 1 9 | 38.626 |
| 2.2065 | 1L | 2 1 7 | 40.865 |
| 2.1453 | 8 | 2 2 0 | 42.085 |
| 2.1284 | 20 | 3 0 6 | 42.436 |
| 2.0877 | 6 | 1 2 8 | 43.304 |
| 2.0800 | 6 | 0 0 12 | 43.473 |
| 2.0547 | 1L | 1 3 1 | 44.035 |
| 2.0335 | 1L | 3 1 2 | 44.520 |
| 1.9575 | 1L | 1 3 4 | 46.347 |
| 1.9069 | 27 | 2 2 6 | 47.650 |
| 1.8721 | 8 | 1 1 12 | 48.593 |
| 1.8658 | 7 | 2 1 10 | 48.768 |
| 1.7842 | 2 | 1 3 7 | 51.154 |
| 1.7653 | 1L | 1 2 11 | 51.742 |
| 1.7340 | 3 | 0 1 14 | 52.748 |
| 1.7196 | 6 | 3 1 8 | 53.224 |
| 1.6971 | 1L | 2 2 9 | 53.989 |
| 1.6890 | 1L | 2 3 2 | 54.266 |
| 1.6453 | 1 | 3 2 4 | 55.831 |
| 1.6216 | 14 | 4 1 0 | 56.721 |
| 1.6077 | 6 | 2 0 14 | 57.258 |
| 1.5965 | 6 | 0 4 8 | 57.698 |
| 1.5930 | 16 | 3 0 12 | 57.836 |
| 1.5851 | 2 | 2 1 13 | 58.151 |
| 1.5521 | 1L | 1 1 15 | 59.511 |
| 1.5384 | 1L | 3 2 7 | 60.094 |
| 1.5262 | 1L | 3 1 11 | 60.627 |
| 1.5110 | 14 | 4 1 6 | 61.300 |
| 1.5056 | 10 | 1 2 14 | 61.543 |

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4935 | 4 | 2 2 12 | 62.099 |
| 1.4901 | 2 | 4 0 10 | 62.256 |
| 1.4765 | 1L | 5 0 2 | 62.895 |
| 1.4459 | 1L | 0 5 4 | 64.384 |
| 1.4304 | 4 | 3 3 0 | 65.167 |
| 1.4097 | 1L | 3 3 3 | 66.242 |
| 1.3525M | 4 | 3 3 6 | 69.434 |
| 1.3525M | | 4 2 5 | 69.434 |
| 1.3487 | 6 | 3 1 14 | 69.662 |
| 1.3419 | 1L | 5 0 8 | 70.066 |
| 1.3327 | 1L | 5 1 1 | 70.619 |
| 1.3269 | 1L | 1 5 2 | 70.977 |
| 1.3199 | 2 | 1 1 18 | 71.407 |
| 1.3148 | 1L | 2 2 15 | 71.730 |
| 1.3051 | 1 | 5 1 4 | 72.346 |
| 1.3017 | 1L | 1 2 17 | 72.566 |
| 1.2862 | 1L | 0 4 14 | 73.583 |
| 1.2789 | 4 | 4 1 12 | 74.073 |
| 1.2751 | 2 | 3 2 13 | 74.330 |
| 1.2501 | 1L | 5 1 7 | 76.080 |
| 1.2385 | 2 | 6 0 0 | 76.920 |
| 1.2322 | 5 | 2 3 14 | 77.385 |
| 1.2273 | 2 | 1 5 8 | 77.750 |
| 1.2100 | 1L | 3 0 18 | 79.081 |
| 1.1899M | 2 | 2 1 19 | 80.683 |
| 1.1899M | | 5 2 0 | 80.683 |
| 1.1870M | 3 | 6 0 6 | 80.921 |
| 1.1870M | | 3 4 5 | 80.921 |
| 1.1833 | 2 | 2 0 20 | 81.233 |
| 1.1784M | 2 | 3 3 12 | 81.641 |
| 1.1784M | | 5 2 3 | 81.641 |
| 1.1648 | 1L | 2 2 18 | 82.800 |
| 1.1507M | 1L | 1 5 11 | 84.044 |
| 1.1507M | | 3 2 16 | 84.044 |
| 1.1440 | 6 | 5 2 6 | 84.648 |
| 1.1377 | 2 | 3 4 8 | 85.226 |
| 1.1032 | 1L | 4 2 14 | 88.572 |
| 1.0972 | 1L | 4 3 10 | 89.182 |
| 1.0761M | 1L | 0 5 16 | 91.424 |
| 1.0761M | | 3 4 11 | 91.424 |
| 1.0724 | 1 | 4 4 0 | 91.823 |
| 1.0677 | 3 | 3 1 20 | 92.347 |
| 1.0642 | 2 | 6 0 12 | 92.746 |
| 1.0540 | 1L | 4 1 18 | 93.915 |
| 1.0439 | 1L | 2 4 16 | 95.104 |
| 1.0387 | 1 | 4 4 6 | 95.732 |
| 1.0361 | 2 | 0 4 20 | 96.056 |
| 1.0329 | 2 | 5 2 12 | 96.449 |
| 1.0295 | 1L | 6 2 1 | 96.869 |
| 1.0166 | 1L | 6 2 4 | 98.523 |
| 1.0143 | 1L | 5 1 16 | 98.834 |
| 1.0071 | 2 | 2 3 20 | 99.787 |
| 1.0052 | 2 | 0 7 8 | 100.054 |

# Chromium Tungsten Oxide, $CrWO_4$

Synonym
Chromium tungstate

CAS registry no.
56729-81-8

Sample
The sample was prepared from $Cr_2O_3$ and $WO_3$. The constituent oxides in a 1:2 molar ratio were blended by grinding in an agate mortar under acetone. The powders were heated in a tungsten metal tray in a controlled atmosphere furnace. Temperatures and partial pressures of oxygen were chosen from the work of Trumm (1979). The following heat treatments were satisfactory:

800 °C for 8 hours, at partial oxygen pressure $10^{-20}$ atm;
1000 °C for 8 hours, at partial oxygen pressure $10^{-20}$ atm;
1300 °C for 8 hours, at partial oxygen pressure $10^{-17}$ atm.

Traces of $Cr_2O_3$ and W metal were present as extra phases.

Color
Very dark greenish blue

Structure
Monoclinic, C2/m (12), distorted rutile type, isostructural with $AlWO_4$. The structure was determined by Vlasse et al. (1976).

Crystallographic constants of this sample
$a = 9.2708(6)$ Å
$b = 5.8282(3)$
$c = 4.6445(3)$
$\beta = 91.926(5)°$

$a/b = 1.5907$
$c/b = 0.7969$

$Z = 4$
$V = 250.81$ Å$^3$
Density (calc) = 7.941 g/cm$^3$

Figure of merit
$F_{30} = 78.9(0.0093,41)$

Additional patterns
PDF card 29-461 (Doumerc et al., 1975)
Trumm (1979)

References

Doumerc, J.-P., Pouchard, M., and Hagenmuller, P. (1975). C. R. Séances Acad. Sci. Ser. C 280, 1397.

Trumm, A. (1979). Neues Jahrb. Mineral. Monatsh., 267.

Vlasse, M., Doumerc, J.-P., Peshev, P., Chaminade, J.-P., and Pouchard, M. (1976). Rev. Chim. Miner. 13, 451.


$CuK\alpha_1$ $\lambda = 1.540598$ Å; temp. 26±1 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 4.934 | 2 | 1 | 1 | 0 | 17.964 |
| 4.637M | 64 | 0 | 0 | 1 | 19.124 |
| 4.637M | | 2 | 0 | 0 | 19.124 |
| 3.412 | 3 | -1 | 1 | 1 | 26.099 |
| 3.336 | 72 | -2 | 0 | 1 | 26.698 |
| 3.225 | 66 | 2 | 0 | 1 | 27.635 |
| 2.915 | 12 | 0 | 2 | 0 | 30.647 |
| 2.730 | 2 | 3 | 1 | 0 | 32.776 |
| 2.467M | 100 | 0 | 2 | 1 | 36.383 |
| 2.467M | | 2 | 2 | 0 | 36.383 |
| 2.321 | 26 | 0 | 0 | 2 | 38.771 |
| 2.316 | 24 | 4 | 0 | 0 | 38.860 |
| 2.1949 | 26 | -2 | 2 | 1 | 41.091 |
| 2.1623 | 2 | 2 | 2 | 1 | 41.740 |
| 2.1029 | 5 | -2 | 0 | 2 | 42.975 |
| 2.1014 | 3 | -4 | 0 | 1 | 43.007 |
| 2.0856 | 1L | 1 | 1 | 2 | 43.351 |
| 2.0468 | 15 | 2 | 0 | 2 | 44.215 |
| 1.9018 | 3 | 1 | 3 | 0 | 47.788 |
| 1.8151 | 11 | 0 | 2 | 2 | 50.223 |
| 1.8140 | 10 | 4 | 2 | 0 | 50.257 |
| 1.7945 | 1 | -3 | 1 | 2 | 50.840 |
| 1.7638 | 2 | -1 | 3 | 1 | 51.791 |
| 1.7552 | 1 | 1 | 3 | 1 | 52.064 |
| 1.7425 | 1L | 3 | 1 | 2 | 52.472 |
| 1.7052 | 38 | -2 | 2 | 2 | 53.710 |
| 1.6749M | 39 | 2 | 2 | 2 | 54.764 |
| 1.6749M | | 4 | 2 | 1 | 54.764 |
| 1.6679M | 26 | -5 | 1 | 1 | 55.010 |
| 1.6679M | | -4 | 0 | 2 | 55.010 |
| 1.6445 | 1 | 3 | 3 | 0 | 55.861 |
| 1.6332 | 1L | 5 | 1 | 1 | 56.281 |
| 1.6125 | 12 | 4 | 0 | 2 | 57.071 |
| 1.5591 | 2 | -3 | 3 | 1 | 59.217 |
| 1.5474 | 3 | 0 | 0 | 3 | 59.709 |
| 1.5441 | 3 | 6 | 0 | 0 | 59.851 |
| 1.5414 | 2 | 3 | 3 | 1 | 59.967 |
| 1.4828 | 7 | -2 | 0 | 3 | 62.598 |
| 1.4801 | 7 | -6 | 0 | 1 | 62.724 |
| 1.4759 | 3 | -1 | 3 | 2 | 62.923 |
| 1.4657 | 1 | 1 | 3 | 2 | 63.411 |
| 1.4570 | 8 | 0 | 4 | 0 | 63.833 |
| 1.4532 | 10 | 2 | 0 | 3 | 64.022 |
| 1.4506 | 8 | 6 | 0 | 1 | 64.150 |
| 1.4475 | 6 | -4 | 2 | 2 | 64.301 |

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4109 | 2 | 4 2 2 | 66.179 |
| 1.3902M | 4 | 0 4 1 | 67.298 |
| 1.3902M | | 2 4 0 | 67.298 |
| 1.3666 | 15 | 0 2 3 | 68.620 |
| 1.3644 | 15 | 6 2 0 | 68.748 |
| 1.3532 | 1L | -3 3 2 | 69.396 |
| 1.3410 | 1 | 5 3 0 | 70.120 |
| 1.3354 | 6 | -2 4 1 | 70.457 |
| 1.3278 | 7 | 2 4 1 | 70.921 |
| 1.3215 | 2 | -2 2 3 | 71.307 |
| 1.3199 | 2 | -6 2 1 | 71.410 |
| 1.3069 | 3 | -4 0 3 | 72.232 |
| 1.3004 | 4 | 2 2 3 | 72.648 |
| 1.2987 | 5 | 6 2 1 | 72.760 |
| 1.2799 | 1L | 5 3 1 | 74.006 |
| 1.2665 | 1 | 6 0 2 | 74.918 |
| 1.2338 | 6 | 0 4 2 | 77.267 |
| 1.2045 | 1L | -1 3 3 | 79.515 |
| 1.1978 | 1 | -2 4 2 | 80.049 |
| 1.1960 | 1 | 1 3 3 | 80.188 |
| 1.1925 | 7 | -4 2 3 | 80.477 |
| 1.1869M | 3 | 2 4 2 | 80.929 |
| 1.1869M | | 4 4 1 | 80.929 |
| 1.1737 | 1L | -5 3 2 | 82.034 |
| 1.1618 | 7 | 4 2 3 | 83.061 |
| 1.1583 | 6 | 8 0 0 | 83.365 |
| 1.1565 | 2 | 1 5 0 | 83.530 |
| 1.1490 | 1L | 5 3 2 | 84.194 |
| 1.1460 | 1L | 5 1 3 | 84.469 |
| 1.1439 | 1L | -7 1 2 | 84.659 |
| 1.1372 | 1 | -3 3 3 | 85.278 |
| 1.1347 | 1 | -2 0 4 | 85.505 |
| 1.1326 | 1 | -8 0 1 | 85.703 |
| 1.1233 | 1 | -1 5 1 | 86.589 |
| 1.1210 | 1L | 1 5 1 | 86.814 |
| 1.1169M | 2 | 3 3 3 | 87.207 |
| 1.1169M | | 2 0 4 | 87.207 |
| 1.1119 | 4 | -6 0 3 | 87.696 |
| 1.0974 | 1L | -4 4 2 | 89.165 |
| 1.0906 | 4 | 3 5 0 | 89.870 |
| 1.0810 | 3 | 4 4 2 | 90.886 |

# Cobalt Telluride, CoTe

CAS registry no.
12017-13-9

Sample
The sample was donated by CERAC/PURE, Inc., Butler, Wisc. The sample contained less than 5% $CoTe_2$ as a second phase.

Color
Very dark gray

Structure
Hexagonal, $P6_3/mmc$ (194). Isostructural with NiAs (Oftedal, 1927).

Crystallographic constants of this sample
$a = 3.89276(15)$ Å
$c = 5.3746(3)$

$Z = 2$
$V = 70.533$ Å$^3$
Density (calc) = 8.783 g/cm$^3$

Figure of merit
$F_{30} = 75.5(0.011,36)$

Additional pattern
Oftedal (1927)

Reference
Oftedal, I. (1927). Z. Phys. Chem. (Leipzig) 128, 135.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 26.4 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 3.369 | 2 | 1 0 0 | 26.436 |
| 2.856 | 100 | 1 0 1 | 31.295 |
| 2.688 | 10 | 0 0 2 | 33.310 |
| 2.101 | 45 | 1 0 2 | 43.007 |
| 1.9470 | 37 | 1 1 0 | 46.612 |
| 1.6082 | 16 | 2 0 1 | 57.239 |
| 1.5819 | 20 | 1 0 3 | 58.282 |
| 1.5768 | 18 | 1 1 2 | 58.486 |
| 1.4280 | 11 | 2 0 2 | 65.290 |
| 1.3433 | 4 | 0 0 4 | 69.981 |
| 1.2744 | 1L | 2 1 0 | 74.376 |
| 1.2484 | 1L | 1 0 4 | 76.197 |
| 1.2400 | 13 | 2 1 1 | 76.809 |
| 1.2278 | 7 | 2 0 3 | 77.718 |
| 1.1514 | 10 | 2 1 2 | 83.979 |
| 1.1236 | 6 | 3 0 0 | 86.561 |
| 1.1058 | 11 | 1 1 4 | 88.310 |
| 1.0384 | 5 | 2 1 3 | 95.775 |
| 1.0368 | 3 | 3 0 2 | 95.974 |
| 1.0240 | 3 | 1 0 5 | 97.564 |
| .9730 | 4 | 2 2 0 | 104.680 |
| .9246 | 2 | 2 1 4 | 112.841 |
| .9211 | 6 | 3 1 1 | 113.497 |
| .9149 | 2 | 2 2 2 | 114.692 |
| .9063 | 2 | 2 0 5 | 116.402 |
| .8957 | 2 | 0 0 6 | 118.624 |
| .8830 | 4 | 3 1 2 | 121.470 |
| .8657 | 4 | 1 0 6 | 125.699 |
| .8621 | 7 | 3 0 4 | 126.634 |
| .8327 | 2 | 4 0 1 | 135.370 |
| .8290 | 4 | 3 1 3 | 136.631 |

# Copper Chromium Oxide, $CuCr_2O_4$

Synonym
Copper chromite

CAS registry no.
12018-10-9

Sample
The sample was prepared by blending stoichiometric amounts of CuO and $Cr_2O_3$ and heating in a platinum boat in pure oxygen for extended periods at temperatures as high as 975 °C, with periodic grinding.

Color
Black

Structure
Tetragonal, $I\bar{4}2d$ (122). Distorted normal spinel. The structure was determined by Prince (1957).

Crystallographic constants of this sample
a = 6.0336(3) Å
c = 7.7824(6)

c/a = 1.2898

Z = 4
V = 283.31 $Å^3$
Density (calc) = 5.428 $g/cm^3$

Figure of merit
$F_{30}$ = 52.1(0.011,53)

Polymorphism
A cubic form was found at 580 °C by Ust'yantsev and Mar'evich (1973).

Additional pattern
PDF card 26-508 (Ust'yantsev and Mar'evich, 1973)

References
Prince, E. (1957). Acta Crystallogr. 10, 554.

Ust'yantsev, V. M. and Mar'evich, V. P. (1973). Inorg. Mater. (Engl. Trans.) 9, 306.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 24.8 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 4.765 | 11 | 1 0 1 | 18.606 |
| 3.018 | 23 | 2 0 0 | 29.573 |
| 2.877 | 34 | 1 1 2 | 31.065 |
| 2.550 | 100 | 2 1 1 | 35.160 |
| 2.385M | 67 | 2 0 2 | 37.693 |
| 2.385M | | 1 0 3 | 37.693 |
| 2.134 | 20 | 2 2 0 | 42.318 |
| 1.9463M | 8 | 3 0 1 | 46.629 |
| 1.9463M | | 0 0 4 | 46.629 |
| 1.8701 | 1 | 2 1 3 | 48.650 |
| 1.7135 | 13 | 3 1 2 | 53.428 |
| 1.6361 | 39 | 3 2 1 | 56.174 |
| 1.5897 | 9 | 3 0 3 | 57.967 |
| 1.5083 | 28 | 4 0 0 | 61.421 |
| 1.4376M | 35 | 4 1 1 | 64.797 |
| 1.4376M | | 2 2 4 | 64.797 |
| 1.4066M | 2 | 4 0 2 | 66.410 |
| 1.4066M | | 3 2 3 | 66.410 |
| 1.3491 | 3 | 4 2 0 | 69.637 |
| 1.3360 | 3 | 3 3 2 | 70.422 |
| 1.2745M | 14 | 4 2 2 | 74.368 |
| 1.2745M | | 4 1 3 | 74.368 |
| 1.2407 | 3 | 1 1 6 | 76.757 |
| 1.2310 | 4 | 3 0 5 | 77.475 |
| 1.1920 | 5 | 4 0 4 | 80.515 |
| 1.1320 | 2 | 5 1 2 | 85.763 |
| 1.1087 | 6 | 4 2 4 | 88.022 |
| 1.0941 | 7 | 4 3 3 | 89.507 |
| 1.0726 | 1 | 3 1 6 | 91.803 |
| 1.0662 | 7 | 4 1 5 | 92.514 |
| 1.0280 | 3 | 2 1 7 | 97.061 |
| 1.0056 | 1 | 6 0 0 | 99.987 |
| 1.0001 | 2 | 5 3 2 | 100.752 |
| .9840 | 3 | 6 1 1 | 103.044 |
| .9731 | 2 | 3 0 7 | 104.665 |
| .9536 | 4 | 4 3 5 | 107.766 |
| .9351 | 2 | 4 2 6 | 110.930 |
| .9260M | 3 | 3 2 7 | 112.584 |
| .9260M | | 2 0 8 | 112.584 |
| .8933 | 2 | 6 0 4 | 119.145 |
| .8856 | 4 | 5 4 3 | 120.863 |
| .8741 | 1 | 5 1 6 | 123.588 |

# Copper Iron Oxide, $CuFe_2O_4$

Synonym
Copper ferrite

CAS registry no.
12018-79-0

Sample
The sample was prepared by blending stoichiometric amounts of CuO and $Fe_2O_3$ and heating in a flowing atmosphere of pure oxygen for extended periods at temperatures as high as 975 °C, with periodic grinding. The sample contained traces of CuO and an unidentified phase.

Color
Olive black

Structure
Tetragonal, $I4_1/amd$ (141). It is a tetragonally distorted inverse spinel. The structure was determined by Prince and Treuting (1956). The "a" dimension given by Prince and Treuting was divided by $\sqrt{2}$ to make it conform to the body-centered space group.

Crystallographic constants of this sample
a = 5.8444(4) Å
c = 8.6304(10)

c/a = 1.4767

Z = 4
V = 294.79 $Å^3$
Density (calc) = 5.390 $g/cm^3$

Figure of merit
$F_{25}$ = 86.2(0.0097,30)

Polymorphism
A cubic phase has also been reported by Vervey and Heilman (1947).

Additional pattern
PDF card 6-545 (Weil et al., 1950)

References
Weil, L., Bertaut, F., and Bochirol, L. (1950). J. Phys. Rad. 11, 208.

Prince, E. and Treuting, R. G. (1956). Acta Crystallogr. 9, 1025.

Vervey, E. J. W. and Heilman, E. L. (1947). J. Chem. Phys. 15, 174.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26.1 °C
Internal standard Ag, a = 4.08651 Å

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 4.839 | 17 | 1 0 1 | 18.319 |
| 2.985 | 32 | 1 1 2 | 29.908 |
| 2.923 | 13 | 2 0 0 | 30.559 |
| 2.582 | 53 | 1 0 3 | 34.719 |
| 2.502 | 100 | 2 1 1 | 35.862 |
| 2.420 | 14 | 2 0 2 | 37.122 |
| 2.1580 | 11 | 0 0 4 | 41.826 |
| 2.0667 | 22 | 2 2 0 | 43.768 |
| 1.9345 | 1 | 2 1 3 | 46.930 |
| 1.7360 | 5 | 2 0 4 | 52.683 |
| 1.6990 | 10 | 3 1 2 | 53.923 |
| 1.6550 | 12 | 1 0 5 | 55.477 |
| 1.6134 | 11 | 3 0 3 | 57.035 |
| 1.5932 | 24 | 3 2 1 | 57.829 |
| 1.4922 | 40 | 2 2 4 | 62.158 |
| 1.4611 | 16 | 4 0 0 | 63.632 |
| 1.4119 | 1 | 3 2 3 | 66.127 |
| 1.3583 | 2 | 1 1 6 | 69.099 |
| 1.3118 | 2 | 3 3 2 | 71.920 |
| 1.3067 | 2 | 4 2 0 | 72.241 |
| 1.2922 | 5 | 3 0 5 | 73.184 |
| 1.2900 | 4 | 2 0 6 | 73.331 |
| 1.2713 | 9 | 4 1 3 | 74.586 |
| 1.2507 | 4 | 4 2 2 | 76.037 |
| 1.2098 | 5 | 4 0 4 | 79.094 |

# Copper Mercury Iodide, β-$Cu_2HgI_4$

Synonym
Cuprous mercuric tetraiodide

CAS registry no.
55945-38-5

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

Color
Vivid red

Structure
Tetragonal, $I\bar{4}2m$ (121). Pseudocubic, isostructural with $Ag_2HgI_4$ (Ketelaar, 1931). The structure of $Cu_2HgI_4$ was determined by Hahn et al. (1955).

Crystallographic constants of this sample
$a = 6.07802(15)$ Å
$c = 12.2540(4)$

$c/a = 2.0161$

$Z = 2$
$V = 452.69$ Å$^3$
Density (calc) = 6.128 g/cm$^3$

Figure of merit
$F_{30} = 113.4(0.0070,38)$

Polymorphism
β-$Cu_2HgI_4$ transforms to a cubic form above 90 °C (Ketelaar, 1934).

Additional patterns
PDF card 18-450 (Hahn et al., 1955)
Ketelaar (1931)

References
Hahn, H., Frank, G., and Klinger, W. (1955). Z. Anorg. Allg. Chem. 279, 271.

Ketelaar, J. A. A. (1931). Z. Kristallogr., 80, 190.

Ketelaar, J. A. A. (1934). Z. Kristallogr., 87, 440.

CuKα$_1$ λ = 1.540598 Å; mean T = 26±2 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.118 | 1L | 0 0 2 | 14.466 |
| 5.446 | 12 | 1 0 1 | 16.263 |
| 4.299 | 2 | 1 1 0 | 20.645 |
| 3.517 | 100 | 1 1 2 | 25.302 |
| 3.389 | 14 | 1 0 3 | 26.275 |
| 3.063 | 3 | 0 0 4 | 29.133 |
| 3.038 | 4 | 2 0 0 | 29.375 |
| 2.722 | 1L | 2 0 2 | 32.876 |
| 2.654 | 17 | 2 1 1 | 33.751 |
| 2.4945 | 1 | 1 1 4 | 35.974 |
| 2.2725 | 7 | 1 0 5 | 39.628 |
| 2.2623 | 7 | 2 1 3 | 39.813 |
| 2.1572 | 62 | 2 0 4 | 41.842 |
| 2.0418 | 1L | 0 0 6 | 44.328 |
| 2.0274 | 1L | 2 2 2 | 44.661 |
| 1.9985 | 6 | 3 0 1 | 45.341 |
| 1.8445 | 18 | 1 1 6 | 49.369 |
| 1.8338 | 30 | 3 1 2 | 49.675 |
| 1.8200 | 4 | 2 1 5 | 50.079 |
| 1.7591 | 2 | 2 2 4 | 51.939 |
| 1.6820 | 1L | 1 0 7 | 54.513 |
| 1.6698 | 1L | 3 2 1 | 54.945 |
| 1.6280 | 1L | 3 1 4 | 56.478 |
| 1.5580 | 5 | 3 2 3 | 59.261 |
| 1.5317 | 3 | 0 0 8 | 60.387 |
| 1.5194 | 5 | 4 0 0 | 60.924 |
| 1.4801 | 2 | 2 2 6 | 62.725 |
| 1.4716 | 2 | 2 1 7 | 63.125 |
| 1.4635 | 1L | 4 1 1 | 63.516 |
| 1.3996 | 10 | 3 1 6 | 66.783 |
| 1.3889 | 8 | 3 2 5 | 67.370 |
| 1.3863 | 3 | 4 1 3 | 67.512 |
| 1.3681 | 1 | 2 0 8 | 68.530 |
| 1.3610 | 1L | 4 0 4 | 68.942 |
| 1.3286 | 1L | 1 0 9 | 70.868 |
| 1.3245 | 2 | 3 0 7 | 71.121 |
| 1.2630 | 2 | 4 1 5 | 75.165 |
| 1.2472 | 6 | 2 2 8 | 76.287 |
| 1.2422 | 9 | 4 2 4 | 76.650 |
| 1.2173 | 1 | 2 1 9 | 78.513 |
| 1.2141 | 1 | 3 2 7 | 78.758 |
| 1.2096 | 1 | 4 3 1 | 79.107 |
| 1.1783 | 2 | 1 1 10 | 81.646 |
| 1.1728 | 3 | 3 3 6 | 82.112 |
| 1.1700 | 5 | 5 1 2 | 82.352 |

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.1650 | 2 | 4 3 3 | 82.784 |
| 1.1300 | 1 | 3 0 9 | 85.951 |
| 1.1275 | 1 | 4 1 7 | 86.190 |
| 1.1239 | 2 | 5 2 1 | 86.530 |
| 1.0960 | 1L | 1 0 11 | 89.313 |
| 1.0889 | 1 | 4 3 5 | 90.046 |
| 1.0788 | 2 | 4 0 8 | 91.130 |
| 1.0746 | 1 | 4 4 0 | 91.589 |
| 1.0463 | 1L | 3 3 8 | 94.816 |
| 1.0333 | 3 | 3 1 10 | 96.402 |
| 1.0308 | 2 | 2 1 11 | 96.714 |
| 1.0296 | 2 | 5 1 6 | 96.865 |
| 1.0275 | 2 | 5 3 2 | 97.119 |
| 1.0167 | 1L | 4 2 8 | 98.521 |
| 1.0141 | 1L | 4 4 4 | 98.857 |
| 1.0001 | 1L | 4 1 9 | 100.748 |
| .9985 | 1L | 4 3 7 | 100.972 |
| .9959 | 1L | 6 1 1 | 101.328 |
| .9706 | 1 | 6 1 3 | 105.059 |
| .9681 | 1 | 2 0 12 | 105.447 |
| .9619 | 1 | 6 0 4 | 106.418 |
| .9610 | 1L | 6 2 0 | 106.565 |
| .9486 | 1L | 5 2 7 | 108.595 |
| .9313 | 1 | 3 3 10 | 111.617 |
| .9294 | 1 | 3 2 11 | 111.946 |
| .9285 | 1 | 5 3 6 | 112.118 |
| .9254 | 1 | 6 1 5 | 112.696 |
| .9246 | 1L | 5 4 3 | 112.836 |
| .9102 | 1 | 4 2 10 | 115.631 |
| .9068 | 1L | 4 3 9 | 116.302 |
| .9036 | 1L | 6 3 1 | 116.966 |
| .9018 | 1L | 3 1 12 | 117.343 |

# Europium Oxide, $Eu_2O_3$

Synonym
Europium sesquioxide

CAS registry no.
1308-96-9

Sample
The sample was obtained from American Potash and Chemical Corp., Research Division, West Chicago, IL. It was heated at 1000 °C for 5 days.

Color
Colorless

Structure
Cubic, Ia3 (206). Its structure was determined by Zachariasen (1928).

Crystallographic constants of this sample
a = 10.8683(2) Å

Z = 16
V = 1283.76 Å$^3$
Density (calc) = 7.283 g/cm$^3$

Figure of merit
$F_{30}$ = 125.6 (0.0075,32)

Polymorphism
There is a monoclinic modification formed above 1075 °C (Roth and Schneider, 1960) and a hexagonal form was found at 2330 °C (Foëx and Traverse, 1966).

Additional patterns
PDF card 12-393 (General Electric, ANP Dept., Cincinnati, OH)
PDF card 32-380 (Ferguson, I. and Hughes, UK Atomic Energy Authority. See UKAEA Report ND-R-150 (S). Gives a as 1/2 of value used here.)

References
Foëx, M. and Traverse, J. P. (1966). Bull. Soc. Fr. Minéral. Cristallogr. 89, 184.

Roth, R. S. and Schneider, S. J. (1960). J. Res. Nat. Bur. Stand. 64A, 309.

Zachariasen, W. H. (1928). Skr. Nor. Vidensk. Akad., Kl. 1: Mat-Naturvidensk. Kl. 1, 4.

CuK$\alpha_1$ $\lambda$ = 1.540598 Å; temp. 26±1 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 4.436 | 8 | 2 1 1 | 19.998 |
| 3.138 | 100 | 2 2 2 | 28.422 |
| 2.904 | 2 | 3 2 1 | 30.760 |
| 2.718 | 34 | 4 0 0 | 32.927 |
| 2.5624 | 6 | 4 1 1 | 34.990 |
| 2.4314 | 1 | 4 2 0 | 36.940 |
| 2.3174 | 5 | 3 3 2 | 38.829 |
| 2.2193 | 1L | 4 2 2 | 40.619 |
| 2.1319 | 8 | 4 3 1 | 42.363 |
| 1.9844 | 3 | 5 2 1 | 45.683 |
| 1.9215 | 43 | 4 4 0 | 47.267 |
| 1.8641 | 2 | 4 3 3 | 48.815 |
| 1.8116 | 1L | 6 0 0 | 50.326 |
| 1.7632 | 6 | 6 1 1 | 51.809 |
| 1.7186 | 1 | 6 2 0 | 53.257 |
| 1.6772 | 4 | 5 4 1 | 54.682 |
| 1.6387 | 31 | 6 2 2 | 56.078 |
| 1.6027 | 6 | 6 3 1 | 57.453 |
| 1.5688 | 6 | 4 4 4 | 58.813 |
| 1.5372 | 2 | 5 4 3 | 60.144 |
| 1.5072 | 1 | 6 4 0 | 61.473 |
| 1.4794 | 3 | 7 2 1 | 62.756 |
| 1.4527 | 1 | 6 4 2 | 64.045 |
| 1.3803 | 2 | 6 5 1 | 67.844 |
| 1.3586 | 4 | 8 0 0 | 69.081 |
| 1.3379 | 3 | 7 4 1 | 70.303 |
| 1.3181 | 2 | 8 2 0 | 71.521 |
| 1.2990 | 2 | 6 5 3 | 72.737 |
| 1.2809 | 1 | 6 6 0 | 73.939 |
| 1.2636 | 3 | 8 3 1 | 75.124 |
| 1.2468 | 8 | 6 6 2 | 76.312 |
| 1.2152 | 6 | 8 4 0 | 78.678 |
| 1.2002 | 1L | 8 3 3 | 79.855 |
| 1.1860 | 1L | 8 4 2 | 81.010 |
| 1.1722 | 2 | 7 6 1 | 82.164 |
| 1.1457 | 2 | 8 5 1 | 84.498 |
| 1.1211 | 2 | 9 3 2 | 86.801 |
| 1.1093 | 5 | 8 4 4 | 87.963 |
| 1.0981 | 2 | 9 4 1 | 89.095 |
| 1.0870 | 1 | 8 6 0 | 90.255 |

Europium Oxide, $Eu_2O_3$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 1$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.0763 | 1L | 10 | 1 | 1 | 91.403 |
| 1.0658 | 3 | 10 | 2 | 0 | 92.559 |
| 1.0558 | 1L | 9 | 4 | 3 | 93.708 |
| 1.0458 | 5 | 10 | 2 | 2 | 94.877 |
| 1.0363 | 2 | 10 | 3 | 1 | 96.025 |
| 1.0179 | 2 | 8 | 7 | 1 | 98.355 |
| 1.0091 | 2 | 10 | 4 | 0 | 99.519 |
| 1.0006 | 2 | 9 | 6 | 1 | 100.679 |
| .9922 | 2 | 10 | 4 | 2 | 101.863 |
| .9840 | 2 | 8 | 7 | 3 | 103.035 |
| .9683 | 2 | 10 | 5 | 1 | 105.413 |
| .9605 | 2 | 8 | 8 | 0 | 106.631 |
| .9460 | 1L | 8 | 8 | 2 | 109.028 |
| .9389 | 1 | 11 | 3 | 2 | 110.258 |
| .9319 | 1L | 10 | 6 | 0 | 111.508 |
| .9251 | 1 | 11 | 4 | 1 | 112.744 |
| .9184 | 3 | 10 | 6 | 2 | 114.006 |
| .9120 | 1L | 9 | 6 | 5 | 115.271 |
| .9056 | 2 | 12 | 0 | 0 | 116.560 |
| .8995 | 2 | 9 | 8 | 1 | 117.817 |
| .8933 | 1 | 12 | 2 | 0 | 119.143 |
| .8873 | 1 | 10 | 7 | 1 | 120.487 |
| .8815 | 2 | 12 | 2 | 2 | 121.824 |
| .8757 | 1 | 12 | 3 | 1 | 123.201 |
| .8646 | 2 | 11 | 6 | 1 | 125.990 |
| .8592 | 2 | 12 | 4 | 0 | 127.408 |
| .8539 | 1 | 12 | 3 | 3 | 128.860 |
| .8486 | 3 | 10 | 8 | 0 | 130.381 |
| .8435 | 2 | 11 | 6 | 3 | 131.901 |
| .8384 | 2 | 10 | 8 | 2 | 133.482 |
| .8336 | 1 | 12 | 5 | 1 | 135.053 |

# Europium Oxide, $Eu_2O_3$

Synonym
Europium sesquioxide

CAS registry no.
1308-96-9

Sample
The sample was obtained from American Potash and Chemical Corp., Research Division, West Chicago, IL. It was heated to 1250 °C for 3 hours to convert it to the monoclinic form.

Color
Colorless

Structure
Monoclinic, Roth and Schneider (1960). Its aspect C*/* was assumed to be the same as that of $Sm_2O_3$ determined by Douglass and Staritzky (1956).

Crystallographic constants of this sample

a = 14.1126(12) Å
b = 3.6025(3)
c = 8.8089(4)
β = 100.050(6)°

a/b = 3.9174
c/b = 2.4452

Z = 6
V = 440.98 Å$^3$
Density (calc) = 7.951 g/cm$^3$

Figure of merit
$F_{30}$ = 62.1(0.0070,69)

Polymorphism
There is a cubic form existing below 1050 °C, Roth and Schneider (1960). A hexagonal form was found at 2330 °C, Foëx and Traverse (1966).

Additional pattern
PDF card 12-384 (General Electric ANP Dept., Cincinnati, OH)

References


Douglass, R. M. and Staritzky, E. (1956). Anal. Chem. 28, 552.

Foëx, M. and Traverse, J. P. (1966). Bull. Soc. Fr. Mineral Crystallogr. 89, 184.

Roth, R. S. and Schneider, S. J. (1960). J. Res. Natl. Bur. Stand. 64A, 309.


$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.3 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.953 | 4 | -2 0 1 | 14.869 |
| 5.014 | 1L | 2 0 1 | 17.676 |
| 4.003 | 8 | -2 0 2 | 22.192 |
| 3.419 | 18 | 2 0 2 | 26.042 |
| 3.187 | 83 | 1 1 1 | 27.971 |
| 3.046 | 85 | 4 0 1 | 29.297 |
| 2.977 | 87 | -4 0 2 | 29.996 |
| 2.891 | 58 | 0 0 3 | 30.906 |
| 2.844 | 89 | 3 1 0 | 31.432 |
| 2.778 | 100 | -1 1 2 | 32.196 |
| 2.662 | 4 | 1 1 2 | 33.642 |
| 2.5179 | 2 | 2 0 3 | 35.628 |
| 2.3162 | 16 | 6 0 0 | 38.850 |
| 2.2756 | 6 | -1 1 3 | 39.571 |
| 2.2072 | 26 | -5 1 1 | 40.852 |
| 2.1800M | 9 | -2 0 4 | 41.385 |
| 2.1800M | | 1 1 3 | 41.385 |
| 2.1459M | 56 | 6 0 1 | 42.072 |
| 2.1459M | | -3 1 3 | 42.072 |
| 2.0662 | 1 | 5 1 1 | 43.778 |
| 2.0534 | 1L | 4 0 3 | 44.064 |
| 1.9739 | 2 | 2 0 4 | 45.940 |
| 1.9267 | 56 | 3 1 3 | 47.132 |
| 1.8804 | 4 | -5 1 3 | 48.366 |
| 1.8614 | 4 | 5 1 2 | 48.892 |
| 1.8213 | 3 | -3 1 4 | 50.042 |
| 1.8014 | 32 | 0 2 0 | 50.632 |
| 1.7635M | 17 | 0 2 1 | 51.799 |
| 1.7635M | | -8 0 1 | 51.799 |
| 1.7425 | 1L | -6 0 4 | 52.472 |
| 1.7061 | 39 | -7 1 2 | 53.679 |
| 1.6729 | 19 | -4 0 5 | 54.834 |
| 1.6635M | 17 | -5 1 4 | 55.168 |
| 1.6635M | | 0 2 2 | 55.168 |
| 1.6563 | 34 | 7 1 1 | 55.429 |
| 1.6443 | 7 | 5 1 3 | 55.868 |
| 1.6410 | 7 | 3 1 4 | 55.993 |
| 1.6178 | 4 | 2 0 5 | 56.866 |
| 1.5939 | 4 | 2 2 2 | 57.801 |
| 1.5809 | 18 | -1 1 5 | 58.322 |
| 1.5569 | 6 | -3 1 5 | 59.308 |
| 1.5504 | 23 | 4 2 1 | 59.580 |
| 1.5412 | 24 | -4 2 2 | 59.975 |
| 1.5289 | 18 | 0 2 3 | 60.507 |
| 1.5232M | 14 | 8 0 2 | 60.758 |

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.5232M | | -2 | 2 | 3 | 60.758 |
| 1.4882 | 9 | -8 | 0 | 4 | 62.345 |
| 1.4673 | 3 | -2 | 0 | 6 | 63.332 |
| 1.4648M | 4 | 2 | 2 | 3 | 63.456 |
| 1.4648M | | -5 | 1 | 5 | 63.456 |
| 1.4459 | 6 | 0 | 0 | 6 | 64.384 |
| 1.4218 | 5 | 6 | 2 | 0 | 65.610 |
| 1.3961M | 3 | -6 | 2 | 2 | 66.975 |
| 1.3961M | | -10 | 0 | 2 | 66.975 |
| 1.3796 | 3 | 6 | 2 | 1 | 67.881 |
| 1.3683 | 3 | 2 | 0 | 6 | 68.519 |
| 1.3635 | 4 | -9 | 1 | 3 | 68.797 |
| 1.3488 | 3 | -3 | 1 | 6 | 69.654 |
| 1.3362 | 8 | 10 | 0 | 1 | 70.406 |
| 1.3341M | 7 | -7 | 1 | 5 | 70.535 |
| 1.3341M | | -6 | 2 | 3 | 70.535 |
| 1.3308 | 4 | 2 | 2 | 4 | 70.739 |
| 1.3156 | 2 | 1 | 1 | 6 | 71.681 |
| 1.2652 | 8 | 7 | 1 | 4 | 75.008 |
| 1.2600 | 10 | -8 | 2 | 1 | 75.373 |
| 1.2574 | 8 | -2 | 2 | 5 | 75.558 |
| 1.2405 | 6 | 4 | 2 | 4 | 76.770 |
| 1.2363 | 7 | 3 | 1 | 6 | 77.081 |
| 1.2258 | 10 | -4 | 2 | 5 | 77.862 |
| 1.2083 | 8 | -11 | 1 | 1 | 79.215 |
| 1.2044 | 4 | -8 | 2 | 3 | 79.521 |
| 1.1967M | 1 | -9 | 1 | 5 | 80.136 |
| 1.1967M | | 1 | 3 | 0 | 80.136 |
| 1.1829 | 5 | 1 | 3 | 1 | 81.266 |
| 1.1628+ | 9 | 8 | 2 | 2 | 82.977 |
| 1.1628+ | | -6 | 2 | 5 | 82.977 |
| 1.1579M | 7 | 12 | 0 | 0 | 83.402 |
| 1.1579M | | -1 | 3 | 2 | 83.402 |
| 1.1474 | 8 | -8 | 2 | 4 | 84.345 |
| 1.1401 | 3 | 6 | 0 | 6 | 85.005 |
| 1.1378 | 3 | -2 | 2 | 6 | 85.223 |
| 1.1351 | 1 | -3 | 3 | 2 | 85.471 |
| 1.1327 | 1 | 8 | 0 | 5 | 85.694 |
| 1.1274 | 6 | 0 | 2 | 6 | 86.196 |
| 1.1258 | 7 | -11 | 1 | 4 | 86.351 |
| 1.1091 | 3 | 9 | 1 | 4 | 87.980 |
| 1.1040M | 10 | 11 | 1 | 2 | 88.492 |
| 1.1040M | | -8 | 0 | 7 | 88.492 |
| 1.1010 | 6 | -2 | 0 | 8 | 88.798 |
| 1.0951 | 4 | -3 | 3 | 3 | 89.398 |
| 1.0903 | 3 | -4 | 0 | 8 | 89.902 |
| 1.0871 | 3 | 10 | 0 | 4 | 90.243 |

# Hafnium Oxide, $HfO_2$

CAS registry no.
12055-23-1

Sample
A commercial sample was heated at 1450 °C for 96 hours, then at 1550 °C for 48 hours.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14), isostructural with $ZrO_2$ (Geller and Corenzwit, 1953). The structure of $ZrO_2$ was redetermined by McCullough and Trueblood (1959) and Adams and Rogers (1959).

Crystallographic constants of this sample
a = 5.2851(2) Å
b = 5.1819(2)
c = 5.1157(2)
β = 99.259(3)°

a/b = 1.0199
c/b = 0.9872

Z = 4
V = 138.28 Å$^3$
Density (calc) = 10.111 g/cm$^3$

Figure of merit
$F_{30}$ = 129.1(0.0061,38)

Polymorphism
Hafnium oxide has been reported to exist in 3 other polymorphic phases. Curtis, Doney, and Johnson (1954) report a tetragonal phase. Ruh et al. (1968) and Ruh and Corfield (1970) report inversion temperatures of the tetragonal to the cubic phase. Bocquillon et al. (1968) report an orthorhombic phase.

Additional pattern
PDF card 6-318 (Geller and Corenzwit, 1953)

References

Adams, J. and Rogers, M. D. (1959). Acta Crystallogr. 12, 951.

Bocquillon, G., Susse, C., and Vodar, B. (1968). Rev. Int. Hautes Temp. Refract. 5, 247.

Curtis, C. E., Doney, L. M., and Johnson, J. R. (1954). J. Am. Ceram. Soc. 37, 458.

Geller, S. and Corenzwit, E. (1953). Anal. Chem. 25, 1774.

McCullough, J. D. and Trueblood, K. N. (1959). Acta Crystallogr. 12, 507.

Ruh, R. and Corfield, P. W. R. (1970). J. Am. Ceram. Soc. 53, No. 3, 126.

Ruh, R., Garrett, H. J., Domagala, R. F., and Tallan, N. M. (1968). J. Am. Ceram. Soc. 51, No. 1, 23.


CuKα$_1$ λ = 1.540598 Å; mean T = 25.4 °C
Internal standards Ag, a = 4.08651 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.051 | 6 | 0 0 1 | 17.544 |
| 3.677 | 16 | 1 1 0 | 24.185 |
| 3.616 | 12 | 0 1 1 | 24.597 |
| 3.147 | 100 | -1 1 1 | 28.336 |
| 2.823 | 78 | 1 1 1 | 31.665 |
| 2.6080 | 25 | 2 0 0 | 34.358 |
| 2.5907 | 20 | 0 2 0 | 34.595 |
| 2.5244 | 23 | 0 0 2 | 35.534 |
| 2.4870 | 7 | -2 0 1 | 36.086 |
| 2.3204 | 9 | 1 2 0 | 38.776 |
| 2.3050 | 1 | 0 2 1 | 39.046 |
| 2.2690 | 1L | 0 1 2 | 39.691 |
| 2.2423 | 2 | -2 1 1 | 40.185 |
| 2.2010 | 15 | -1 1 2 | 40.971 |
| 2.1792 | 5 | 2 0 1 | 41.401 |
| 2.1678 | 5 | -1 2 1 | 41.628 |
| 2.0088 | 5 | 2 1 1 | 45.096 |
| 1.9803 | 7 | -2 0 2 | 45.783 |
| 1.8494 | 3 | -2 1 2 | 49.230 |
| 1.8379 | 18 | 2 2 0 | 49.559 |
| 1.8079 | 23 | 0 2 2 | 50.436 |
| 1.7936 | 12 | -2 2 1 | 50.868 |
| 1.7727 | 6 | -1 2 2 | 51.513 |
| 1.6834M | 12 | 2 0 2 | 54.461 |
| 1.6834M | | 0 0 3 | 54.461 |
| 1.6673 | 1 | 2 2 1 | 55.032 |
| 1.6483 | 13 | 3 1 0 | 55.722 |
| 1.6431 | 10 | -3 1 1 | 55.914 |
| 1.6342 | 9 | 0 3 1 | 56.246 |
| 1.6006+ | 9 | 0 1 3 | 57.535 |
| 1.6006+ | | -1 1 3 | 57.535 |
| 1.5833 | 7 | -1 3 1 | 58.225 |
| 1.5732 | 5 | -2 2 2 | 58.635 |
| 1.5370 | 9 | 1 3 1 | 60.155 |
| 1.5306 | 9 | -2 0 3 | 60.433 |
| 1.5009 | 6 | 3 1 1 | 61.759 |
| 1.4881 | 8 | -3 1 2 | 62.350 |
| 1.4687 | 11 | 1 1 3 | 63.265 |
| 1.4439 | 2 | 3 2 0 | 64.484 |
| 1.4401M | 3 | 2 3 0 | 64.676 |
| 1.4401M | | -3 2 1 | 64.676 |
| 1.4252 | 1 | 0 3 2 | 65.433 |
| 1.4184 | 3 | -2 3 1 | 65.784 |
| 1.4118M | 9 | 2 2 2 | 66.133 |
| 1.4118M | | 0 2 3 | 66.133 |
| 1.4083 | 4 | -1 3 2 | 66.318 |
| 1.3537 | 3 | 2 3 1 | 69.367 |
| 1.3414 | 1 | 3 2 1 | 70.094 |
| 1.3325 | 1 | -3 2 2 | 70.634 |
| 1.3181M | 4 | 1 2 3 | 71.520 |

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.3181M | | -2 2 3 | 71.520 |
| 1.3149 | 5 | -4 0 1 | 71.721 |
| 1.3041 | 1 | 4 0 0 | 72.410 |
| 1.3017 | 2 | -2 3 2 | 72.565 |
| 1.2955 | 2 | 0 4 0 | 72.967 |
| 1.2927 | 1 | 3 1 2 | 73.151 |
| 1.2795M | 1 | 2 1 3 | 74.033 |
| 1.2795M | | -3 1 3 | 74.033 |
| 1.2624 | 2 | 0 0 4 | 75.203 |
| 1.2574 | 4 | 1 4 0 | 75.560 |
| 1.2378 | 3 | -1 1 4 | 76.967 |
| 1.2315 | 1L | -1 4 1 | 77.437 |
| 1.2254 | 2 | 3 3 0 | 77.899 |
| 1.2230 | 2 | -3 3 1 | 78.079 |
| 1.2162 | 1 | 4 0 1 | 78.599 |
| 1.2086 | 1L | -4 1 2 | 79.188 |
| 1.2056+ | 3 | 2 3 2 | 79.428 |
| 1.2056+ | | 0 3 3 | 79.428 |
| 1.1866 | 1L | 3 2 2 | 80.953 |
| 1.1839 | 1L | 4 1 1 | 81.179 |
| 1.1766 | 1 | 2 2 3 | 81.794 |
| 1.1727 | 3 | -4 2 1 | 82.125 |
| 1.1651 | 1L | 4 2 0 | 82.776 |
| 1.1613 | 3 | 3 3 1 | 83.108 |
| 1.1551 | 3 | -3 3 2 | 83.653 |
| 1.1525 | 2 | 0 4 2 | 83.887 |
| 1.1458M | 3 | 1 3 3 | 84.485 |
| 1.1458M | | -2 3 3 | 84.485 |
| 1.1432 | 3 | -1 4 2 | 84.724 |
| 1.1348 | 2 | 0 2 4 | 85.498 |
| 1.1218 | 1 | -4 0 3 | 86.736 |
| 1.1136 | 1L | 2 4 1 | 87.534 |
| 1.1085 | 2 | 1 4 2 | 88.036 |
| 1.1009 | 3 | 4 2 1 | 88.804 |
| 1.0970 | 3 | 3 1 3 | 89.206 |
| 1.0894 | 1 | 4 0 2 | 89.992 |
| 1.0854 | 3 | -3 1 4 | 90.423 |
| 1.0771 | 1 | 1 2 4 | 91.317 |
| 1.0706 | 1 | 2 0 4 | 92.023 |
| 1.0492 | 2 | 2 3 3 | 94.472 |

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.0407 | 1 | 4 3 0 | 95.490 |
| 1.0390 | 2 | 3 4 0 | 95.699 |
| 1.0376 | 1 | -3 4 1 | 95.868 |
| 1.0297 | 2 | -4 2 3 | 96.851 |
| 1.0267+ | 3 | 2 4 2 | 97.228 |
| 1.0267+ | | 0 4 3 | 97.228 |
| 1.0256 | 1 | -1 3 4 | 97.367 |
| 1.0228 | 3 | 5 1 0 | 97.723 |
| 1.0191 | 1L | 0 3 4 | 98.198 |
| 1.0153 | 2 | 0 5 1 | 98.701 |
| 1.0098 | 2 | 0 0 5 | 99.423 |
| 1.0091 | 1 | -4 3 2 | 99.527 |
| 1.0045 | 3 | -5 1 2 | 100.147 |
| .9973 | 1L | -2 0 5 | 101.138 |
| .9943 | 2 | 4 3 1 | 101.556 |
| .9895 | 2 | 2 2 4 | 102.247 |
| .9778 | 1L | -5 2 1 | 103.962 |
| .9588M | 1L | 4 0 3 | 106.909 |
| .9588M | | 0 5 2 | 106.909 |
| .9565 | 1 | -2 5 1 | 107.278 |
| .9466 | 2 | 1 1 5 | 108.921 |
| .9409M | 3 | -4 3 3 | 109.903 |
| .9409M | | 0 2 5 | 109.903 |
| .9359 | 2 | 2 5 1 | 110.790 |
| .9337 | 3 | -3 3 4 | 111.173 |
| .9306 | 3 | -2 2 5 | 111.727 |
| .9297 | 3 | 3 4 2 | 111.898 |
| .9245 | 2 | -3 4 3 | 112.861 |
| .9228 | 2 | -4 4 1 | 113.187 |
| .9189 | 1 | 4 4 0 | 113.914 |
| .9182 | 1L | -2 5 2 | 114.060 |
| .8998 | 1 | 5 1 2 | 117.765 |
| .8992 | 1 | 4 2 3 | 117.882 |
| .8929M | 2 | 3 2 4 | 119.242 |
| .8929M | | 5 3 0 | 119.242 |

# Iron Niobium Oxide, $Fe(NbO_3)_2$

Synonyms
Iron niobate
Ferrous niobate

CAS registry no.
12022-59-2

Sample
The sample was prepared according to the paper by Turnock (1966). Stoichiometric amounts of $Fe_2O_3$ and $Nb_2O_5$ were mixed and heated in a platinum boat (presaturated with Fe by heating a sample of $FeNb_2O_6$ under the same conditions as in the synthesis). Two heatings in the 1130-1160 °C range in a controlled atmosphere with the partial pressure of oxygen less than or equal to $10^{-14}$ atm. The sample contains a trace of $NbO_2$.

Color
Black

Structure
Orthorhombic, Pcan (60). It has the columbite structure, solved by Sturdivant (1930). The structure was qualitatively done by Brandt (1943).

Crystallographic constants of this sample
a = 5.7350(3) Å
b = 14.2688(7)
c = 5.0504(3)

a/b = 0.4019
c/b = 0.3539

Z = 4
V = 413.29 $Å^3$
Density (calc) = 5.427 g/$cm^3$

Figure of merit
$F_{30}$ = 49.3(0.0086,71)

Additional pattern
PDF card 31-644 (Husson, et al., 1977)

References
Brandt, K. (1943). Ark. Kemi Mineral. Geol. 17a, No. 15.

Husson, E., Repelin, Y., Nguyen, Q. D., and Brusset, H. (1977). Mater. Res. Bull. 12, 1199.

Sturdivant, J. H. (1930). Z. Kristallogr. 68, 239.

Turnock, A. C. (1966). J. Am. Ceram. Soc. 49, 177.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26.8 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.14 | 4 | 0 2 0 | 12.394 |
| 5.319 | 1 | 1 1 0 | 16.655 |
| 3.661M | 38 | 1 1 1 | 24.290 |
| 3.661M | | 1 3 0 | 24.290 |
| 3.567 | 5 | 0 4 0 | 24.944 |
| 2.965 | 100 | 1 3 1 | 30.118 |
| 2.868 | 11 | 2 0 0 | 31.164 |
| 2.662 | 1 | 2 2 0 | 33.642 |
| 2.526 | 14 | 0 0 2 | 35.510 |
| 2.495 | 14 | 2 0 1 | 35.972 |
| 2.379M | 7 | 0 2 2 | 37.790 |
| 2.379M | | 0 6 0 | 37.790 |
| 2.354 | 1L | 2 2 1 | 38.196 |
| 2.2302 | 4 | 0 3 2 | 40.411 |
| 2.2088 | 8 | 2 3 1 | 40.820 |
| 2.0790 | 10 | 1 3 2 | 43.495 |
| 2.0613 | 2 | 0 4 2 | 43.887 |
| 2.0438 | 2 | 2 4 1 | 44.283 |
| 1.9212 | 1L | 1 7 0 | 47.274 |
| 1.8952M | 8 | 2 0 2 | 47.964 |
| 1.8952M | | 3 1 0 | 47.964 |
| 1.8307M | 8 | 2 2 2 | 49.765 |
| 1.8307M | | 2 6 0 | 49.765 |
| 1.7957M | 2 | 1 5 2 | 50.805 |
| 1.7957M | | 1 7 1 | 50.805 |
| 1.7740M | 14 | 3 1 1 | 51.471 |
| 1.7740M | | 3 3 0 | 51.471 |
| 1.7315 | 17 | 0 6 2 | 52.829 |
| 1.7211 | 22 | 2 6 1 | 53.175 |
| 1.6738M | 2 | 2 4 2 | 54.801 |
| 1.6738M | | 3 3 1 | 54.801 |
| 1.6052 | 1L | 1 1 3 | 57.355 |
| 1.5294M | 14 | 1 3 3 | 60.485 |
| 1.5294M | | 1 7 2 | 60.485 |
| 1.5155M | 1L | 3 1 2 | 61.101 |
| 1.5155M | | 3 5 1 | 61.101 |
| 1.4821 | 5 | 2 6 2 | 62.631 |
| 1.4625 | 12 | 1 9 1 | 63.563 |
| 1.4517M | 18 | 2 0 3 | 64.094 |
| 1.4517M | | 3 3 2 | 64.094 |
| 1.4338 | 2 | 4 0 0 | 64.995 |
| 1.4271 | 1L | 0 10 0 | 65.337 |
| 1.4231 | 1L | 2 2 3 | 65.544 |
| 1.3946 | 1 | 3 7 0 | 67.056 |
| 1.3792 | 5 | 4 0 1 | 67.905 |

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.3445+ | 1L | 2 4 3 | 69.907 |
| 1.3445+ | | 3 5 2 | 69.907 |
| 1.3380 | 1L | 2 9 1 | 70.299 |
| 1.3072 | 1 | 1 9 2 | 72.210 |
| 1.2864 | 1L | 4 4 1 | 73.571 |
| 1.2776 | 1L | 2 10 0 | 74.161 |
| 1.2659 | 1L | 1 7 3 | 74.960 |
| 1.2626M | 1 | 3 8 1 | 75.191 |
| 1.2626M | | 0 0 4 | 75.191 |
| 1.2422M | 1L | 0 10 2 | 76.647 |
| 1.2422M | | 4 1 2 | 76.647 |
| 1.2390 | 2 | 2 6 3 | 76.883 |
| 1.2204+ | 2 | 3 9 0 | 78.275 |
| 1.2204+ | | 0 3 4 | 78.275 |
| 1.2060 | 1L | 4 3 2 | 79.391 |
| 1.1932 | 6 | 4 6 1 | 80.416 |
| 1.1901 | 3 | 0 4 4 | 80.671 |
| 1.1862 | 1 | 3 9 1 | 80.992 |
| 1.1554M | 1 | 2 0 4 | 83.625 |
| 1.1554M | | 3 5 3 | 83.625 |
| 1.1400 | 1L | 2 10 2 | 85.014 |
| 1.1314M | 3 | 1 9 3 | 85.821 |
| 1.1314M | | 1 11 2 | 85.821 |
| 1.1152+ | 3 | 3 10 1 | 87.377 |
| 1.1152+ | | 0 6 4 | 87.377 |
| 1.1042 | 1L | 4 6 2 | 88.466 |
| 1.0987 | 4 | 3 9 2 | 89.028 |
| 1.0915 | 1 | 4 0 3 | 89.782 |
| 1.0887 | 2 | 5 3 1 | 90.066 |
| 1.0789 | 1L | 4 2 3 | 91.122 |
| 1.0779 | 1L | 1 13 0 | 91.230 |
| 1.0758 | 1 | 0 12 2 | 91.453 |
| 1.0733+ | 1 | 0 7 4 | 91.729 |
| 1.0733+ | | 2 12 1 | 91.729 |
| 1.0542 | 1L | 1 13 1 | 93.892 |
| 1.0507 | 1L | 3 1 4 | 94.302 |
| 1.0438 | 1L | 4 4 3 | 95.117 |
| 1.0414+ | 1L | 5 1 2 | 95.408 |
| 1.0414+ | | 5 5 1 | 95.408 |
| 1.0394 | 1 | 2 6 4 | 95.656 |
| 1.0287 | 2 | 3 3 4 | 96.980 |
| 1.0201 | 2 | 5 3 2 | 98.076 |
| 1.0176 | 1 | 2 10 3 | 98.402 |
| 1.0073 | 1 | 2 12 2 | 99.758 |
| .9996 | 1L | 5 7 0 | 100.816 |
| .9920 | 3 | 4 6 3 | 101.886 |
| .9879M | 1 | 3 9 3 | 102.473 |
| .9879M | | 3 11 2 | 102.473 |

# Iron Niobium Oxide, $Fe_4Nb_2O_9$

Synonym
Iron niobate

Sample
The sample was prepared by blending $Fe^2Nb_2O_6$ with $Fe_2O_3$ in the appropriate molar ratio. The mixture was heated in an iron boat at 1160 °C for 8 hours, in a controlled atmosphere with the partial pressure of oxygen less than or equal to $10^{-16}$ atm. The product was essentially single phase and contained only a trace of $Fe^2Nb_2O_6$ as a second phase.

Color
Colorless

Structure
Hexagonal, P6/***, Z = 2, isostructural with $Co_4Nb_2O_9$ (Bertaut et al., 1960).

Crystallographic constants of this sample
a = 5.2253(2) Å
c = 14.2070(8)

c/a = 2.7189

Z = 2
V = 335.94 Å$^3$
Density (calc) = 5.469 g/cm$^3$

Figure of merit
$F_{30}$ = 46.6(0.0097,66)

Reference
Bertaut, F., Corliss, L., and Forrat, F. (1960). C. R. Hebd. Séances Acad. Sci. 251, 1733.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 27.6 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.12 | 1 | 0 0 2 | 12.428 |
| 4.524 | 20 | 1 0 0 | 19.605 |
| 3.818 | 23 | 1 0 2 | 23.282 |
| 3.553 | 2 | 0 0 4 | 25.040 |
| 2.793 | 100 | 1 0 4 | 32.019 |
| 2.611 | 72 | 1 1 0 | 34.314 |
| 2.368 | 3 | 0 0 6 | 37.961 |
| 2.287 | 12 | 1 1 3 | 39.369 |
| 2.263 | 2 | 2 0 0 | 39.801 |
| 2.1557 | 2 | 2 0 2 | 41.873 |
| 2.1045 | 2 | 1 1 4 | 42.941 |
| 2.0979 | 2 | 1 0 6 | 43.083 |
| 1.9084 | 29 | 2 0 4 | 47.612 |
| 1.7753 | 4 | 0 0 8 | 51.432 |
| 1.7540 | 31 | 1 1 6 | 52.101 |
| 1.7108 | 2 | 2 1 0 | 53.520 |
| 1.6630 | 3 | 2 1 2 | 55.187 |
| 1.6530 | 7 | 1 0 8 | 55.552 |
| 1.6362 | 1 | 2 0 6 | 56.172 |
| 1.5413 | 23 | 2 1 4 | 59.972 |
| 1.5087 | 21 | 3 0 0 | 61.405 |
| 1.4684 | 2 | 1 1 8 | 63.279 |
| 1.3973 | 3 | 2 0 8 | 66.911 |
| 1.3886 | 3 | 3 0 4 | 67.385 |
| 1.3555 | 8 | 1 0 10 | 69.261 |
| 1.3065 | 4 | 2 2 0 | 72.255 |
| 1.2721 | 2 | 3 0 6 | 74.531 |
| 1.2594 | 1 | 2 2 3 | 75.419 |
| 1.2553 | 1L | 3 1 0 | 75.704 |
| 1.2360 | 2 | 3 1 2 | 77.103 |
| 1.2322 | 3 | 2 1 8 | 77.388 |
| 1.2032 | 4 | 2 0 10 | 79.617 |
| 1.1835 | 6 | 3 1 4 | 81.216 |
| 1.1496 | 1 | 3 0 8 | 84.143 |
| 1.1440 | 4 | 2 2 6 | 84.655 |
| 1.1316 | 1L | 4 0 0 | 85.800 |
| 1.0929M | 4 | 2 1 10 | 89.626 |
| 1.0929M | | 0 0 13 | 89.626 |
| 1.0781 | 2 | 4 0 4 | 91.206 |
| 1.0522 | 1L | 2 2 8 | 94.120 |
| 1.0270 | 1L | 3 2 2 | 97.185 |
| 1.0251 | 1 | 3 1 8 | 97.426 |
| .9965 | 3 | 3 2 4 | 101.247 |
| .9903 | 2 | 1 0 14 | 102.129 |
| .9875 | 4 | 4 1 0 | 102.524 |
| .9541 | 1 | 4 0 8 | 107.679 |
| .9508 | 1 | 3 2 6 | 108.215 |
| .9460 | 1 | 1 1 14 | 109.033 |
| .9407 | 3 | 3 1 10 | 109.944 |
| .9260 | 2 | 2 0 14 | 112.582 |
| .9114 | 3 | 4 1 6 | 115.386 |
| .8962 | 1L | 3 2 8 | 118.532 |
| .8849M | 1L | 4 0 10 | 121.021 |
| .8849M | | 3 0 13 | 121.021 |
| .8770 | 1L | 5 0 4 | 122.887 |
| .8727 | 2 | 2 1 14 | 123.940 |
| .8709 | 3 | 3 3 0 | 124.382 |
| .8629 | 1L | 4 1 8 | 126.414 |

# Iron Silicate (Fayalite), $Fe_2SiO_4$

Synonym
Ferrous orthosilicate

Sample
The sample was prepared by grinding together equimolar parts of $Fe_2O_3$ and $SiO_2$ under acetone. After drying, the specimen was transferred to a high purity iron boat. It was heated twice for 8 hours each time in a controlled atmosphere with the partial pressure of oxygen less than or equal to $10^{-20}$ atm, first at 1110 °C and then at 1150 °C.

Color
Grayish olive

Structure
Orthorhombic, Pmnb (62). The structure was determined by Rinne et al. (1924) and an indexing error was corrected by Bragg and Brown (1926).

Crystallographic constants of this sample
a = 6.0902(5) Å
b = 10.4805(8)
c = 4.8215(5)

a/b = 0.5811
c/b = 0.4600

Z = 4
V = 307.75 Å$^3$
Density (calc) = 4.398 g/cm$^3$

Figure of merit
$F_{30}$ = 70.4(0.010,44)

Polymorphism
Fayalite is converted to a cubic form with spinel structure at high pressure and temperature (Ringwood, 1958).

Additional patterns
PDF card 20-1139 (Feier, British Museum (Natural History), London)
PDF card 31-649 (Smith et al., Penn State U., University Park, PA) calculated pattern

References

Bragg, W. L. and Brown, G. B. (1926). Z. Kristallogr. 63, 538.

Ringwood, A. E. (1958). Geochim. Cosmochim. Acta, 15, 18.

Rinne, F., Leonhardt, J., and Hentschel, H. (1924). Z. Kristallogr. 59, 548.


CuK$\alpha_1$ $\lambda$ = 1.540598 Å; temp. 26±1 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.242 | 6 | 0 2 0 | 16.901 |
| 4.380 | 9 | 0 1 1 | 20.257 |
| 3.974 | 11 | 1 2 0 | 22.353 |
| 3.783 | 7 | 1 0 1 | 23.496 |
| 3.556 | 55 | 1 1 1 | 25.019 |
| 3.064 | 6 | 1 2 1 | 29.123 |
| 3.046 | 7 | 2 0 0 | 29.295 |
| 2.829 | 86 | 0 3 1 | 31.599 |
| 2.633 | 32 | 2 2 0 | 34.020 |
| 2.619 | 23 | 0 4 0 | 34.205 |
| 2.565 | 45 | 1 3 1 | 34.952 |
| 2.500 | 100 | 2 1 1 | 35.893 |
| 2.407 | 25 | 1 4 0 | 37.331 |
| 2.351 | 10 | 0 1 2 | 38.259 |
| 2.311 | 23 | 2 2 1 | 38.949 |
| 2.303 | 21 | 0 4 1 | 39.073 |
| 2.193 | 9 | 1 1 2 | 41.134 |
| 2.1532 | 7 | 1 4 1 | 41.923 |
| 2.0723 | 8 | 2 3 1 | 43.643 |
| 1.9855M | 5 | 2 4 0 | 45.655 |
| 1.9855M | | 0 3 2 | 45.655 |
| 1.9220 | 5 | 0 5 1 | 47.253 |
| 1.8418 | 12 | 3 1 1 | 49.446 |
| 1.8327 | 10 | 1 5 1 | 49.709 |
| 1.7781 | 79 | 2 2 2 | 51.343 |
| 1.7735 | 65 | 0 4 2 | 51.486 |
| 1.7624 | 6 | 3 2 1 | 51.834 |
| 1.7032 | 13 | 1 4 2 | 53.779 |
| 1.6789 | 15 | 1 6 0 | 54.621 |
| 1.6496 | 17 | 3 3 1 | 55.674 |
| 1.6253 | 17 | 2 5 1 | 56.581 |
| 1.6044 | 9 | 3 4 0 | 57.386 |
| 1.5885 | 6 | 0 1 3 | 58.014 |
| 1.5367M | 11 | 0 2 3 | 60.166 |
| 1.5367M | | 1 1 3 | 60.166 |
| 1.5331 | 10 | 2 4 2 | 60.326 |
| 1.5225M | 26 | 4 0 0 | 60.789 |
| 1.5225M | | 3 4 1 | 60.789 |
| 1.5151 | 31 | 2 6 0 | 61.115 |
| 1.4896M | 3 | 1 2 3 | 62.276 |

Iron Silicate (Fayalite), $Fe_2SiO_4$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.4896M | | 3 | 2 | 2 | 62.276 |
| 1.4602 | 9 | 0 | 3 | 3 | 63.679 |
| 1.4383 | 2 | 4 | 1 | 1 | 64.765 |
| 1.4300 | 15 | 0 | 7 | 1 | 65.186 |
| 1.4201 | 8 | 1 | 3 | 3 | 65.698 |
| 1.4085 | 10 | 2 | 1 | 3 | 66.311 |
| 1.3962 | 3 | 3 | 5 | 1 | 66.971 |
| 1.3778 | 6 | 1 | 6 | 2 | 67.986 |
| 1.3719 | 9 | 2 | 2 | 3 | 68.315 |
| 1.3408 | 13 | 4 | 3 | 1 | 70.130 |
| 1.3365 | 12 | 1 | 4 | 3 | 70.386 |
| 1.3240 | 5 | 3 | 6 | 0 | 71.156 |
| 1.3165M | 3 | 4 | 4 | 0 | 71.624 |
| 1.3165M | | 2 | 3 | 3 | 71.624 |
| 1.2868 | 6 | 4 | 0 | 2 | 73.542 |
| 1.2832 | 6 | 2 | 6 | 2 | 73.780 |
| 1.2699 | 1L | 4 | 4 | 1 | 74.686 |
| 1.2507 | 2 | 3 | 1 | 3 | 76.032 |
| 1.2478M | 3 | 3 | 5 | 2 | 76.241 |
| 1.2478M | | 1 | 5 | 3 | 76.241 |
| 1.2053 | 5 | 0 | 0 | 4 | 79.446 |
| 1.2034 | 3 | 2 | 8 | 0 | 79.601 |
| 1.1935 | 1 | 4 | 5 | 1 | 80.395 |
| 1.1855 | 4 | 3 | 3 | 3 | 81.045 |
| 1.1830 | 3 | 0 | 6 | 3 | 81.258 |
| 1.1763 | 8 | 2 | 5 | 3 | 81.818 |
| 1.1737M | 7 | 2 | 7 | 2 | 82.037 |
| 1.1737M | | 5 | 1 | 1 | 82.037 |
| 1.1673 | 1 | 2 | 8 | 1 | 82.581 |
| 1.1606M | 4 | 1 | 6 | 3 | 83.168 |
| 1.1606M | | 3 | 6 | 2 | 83.168 |
| 1.1556 | 6 | 4 | 4 | 2 | 83.611 |
| 1.1512 | 4 | 0 | 8 | 2 | 84.004 |
| 1.1355 | 5 | 3 | 4 | 3 | 85.430 |
| 1.1311 | 1 | 1 | 8 | 2 | 85.848 |
| 1.1188 | 4 | 5 | 3 | 1 | 87.020 |
| 1.1143 | 3 | 2 | 1 | 4 | 87.467 |
| 1.0992 | 2 | 4 | 1 | 3 | 88.981 |
| 1.0959 | 13 | 2 | 2 | 4 | 89.319 |
| 1.0811M | 2 | 5 | 1 | 2 | 90.875 |
| 1.0811M | | 4 | 2 | 3 | 90.875 |
| 1.0767M | 2 | 2 | 8 | 2 | 91.355 |
| 1.0767M | | 5 | 4 | 1 | 91.355 |

# Iron Titanium Oxide (Ulvöspinel), $Fe_2TiO_4$

Synonym
Iron titanate

CAS registry no.
12434-86-5

Sample
The sample was prepared from stoichiometric amounts of $Fe_2O_3$ and $TiO_2$, blended in an agate mortar. The mixture was dried and transferred to a high-purity iron boat for heat treatments. All heatings were done in a controlled atmosphere at an oxygen partial pressure of $10^{-18}$ atmosphere or lower. Three heatings, 1140 °C for 8 hours, 1150 °C for 8 hours, and 1200 °C for 8 hours were sufficient to yield a single phase, well crystallized product.

Color
Dark gray

Structure
Cubic, Fd3m (227), isostructural with spinel, $MgAl_2O_4$ (Barth and Posnjak, 1932). The structure was refined by Forster and Hall (1965) by neutron diffraction methods.

Crystallographic constants of this sample
$a = 8.53520(12)$ Å

$Z = 8$
$V = 621.786$ Å$^3$
Density (calc) = 4.777 g/cm$^3$

Figure of merit
$F_{30} = 124.2(0.0069,35)$

Additional patterns
PDF card 24-537 (Ashworth, Dept. of Geology, Univ. of Durham, U.K.)
Forster and Hall (1965)
Pouillard (1950)

References

Barth, T. F. W. and Posnjak, E. (1932). Z. Kristallogr. 82, 325.

Forster, R. H. and Hall, E. O. (1965). Acta Crystallogr. 18, 857.

Pouillard, E. (1950). Ann. Chim. Paris 5, 164.


$CuK\alpha_1$ $\lambda = 1.540598$ Å; temp. 26±1 °C
Internal standards W, $a = 3.16524$ Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 4.924 | 8 | 1 1 1 | 18.002 |
| 3.018 | 33 | 2 2 0 | 29.573 |
| 2.573 | 100 | 3 1 1 | 34.837 |
| 2.4640 | 6 | 2 2 2 | 36.434 |
| 2.1339 | 19 | 4 0 0 | 42.321 |
| 1.7419 | 10 | 4 2 2 | 52.490 |
| 1.6426 | 33 | 5 1 1 | 55.932 |
| 1.5089 | 39 | 4 4 0 | 61.395 |
| 1.4427 | 1 | 5 3 1 | 64.545 |
| 1.3495 | 3 | 6 2 0 | 69.615 |
| 1.3016 | 7 | 5 3 3 | 72.572 |
| 1.2867 | 3 | 6 2 2 | 73.551 |
| 1.2318 | 2 | 4 4 4 | 77.413 |
| 1.1952 | 1L | 7 1 1 | 80.255 |
| 1.1406 | 3 | 6 4 2 | 84.960 |
| 1.1111 | 8 | 7 3 1 | 87.782 |
| 1.0669 | 2 | 8 0 0 | 92.435 |
| 1.0059 | 1 | 6 6 0 | 99.948 |
| .9856 | 5 | 7 5 1 | 102.805 |
| .9792 | 2 | 6 6 2 | 103.754 |
| .9543 | 2 | 8 4 0 | 107.649 |
| .9369 | 1L | 7 5 3 | 110.606 |
| .9099 | 1L | 6 6 4 | 115.689 |
| .8947 | 4 | 9 3 1 | 118.843 |
| .8711 | 10 | 8 4 4 | 124.332 |
| .8578 | 1L | 7 7 1 | 127.778 |
| .8370 | 2 | 10 2 0 | 133.953 |
| .8251 | 4 | 7 7 3 | 138.003 |
| .8212 | 2 | 10 2 2 | 139.428 |
| .7959 | 1L | 9 5 3 | 150.838 |

# Lanthanum Boride, $LaB_6$

CAS registry no.
12008-21-8

Sample
The sample from Koch-Light Laboratories, Colnbrook Bucks, England was donated by H. Göbel, Munich, Germany.

Color
Purplish black

Structure
Cubic, Pm3m (221), isostructural with $CaB_6$. The structure was determined by von Stackelburg and Neumann (1932).

Crystallographic constants of this sample
$a = 4.15690(5)$ Å

$Z = 1$
$V = 71.830$ Å$^3$
Density (calc) = 4.711 g/cm$^3$

Figure of merit
$F_{24} = 180.5(0.0055,24)$

Additional pattern
PDF card 6-0401 (American Electro Metal Corp., Yonkers, NY)

Reference
Stackelburg, von, M. and Neumann, F. (1932). Z. Phys. Chem. (Leipzig) B19, 314.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 25.9 °C
Internal standards Ag, a = 4.08651 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ $\sigma = \pm 5$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 4.158 | 54 | 1 0 0 | 21.354 |
| 2.939 | 100 | 1 1 0 | 30.387 |
| 2.3998 | 41 | 1 1 1 | 37.445 |
| 2.0780 | 22 | 2 0 0 | 43.517 |
| 1.8586 | 46 | 2 1 0 | 48.969 |
| 1.6969 | 24 | 2 1 1 | 53.995 |
| 1.4697 | 8 | 2 2 0 | 63.218 |
| 1.3853 | 23 | 3 0 0 | 67.564 |
| 1.3143 | 16 | 3 1 0 | 71.757 |
| 1.2533 | 10 | 3 1 1 | 75.849 |
| 1.2000 | 2 | 2 2 2 | 79.869 |
| 1.1529 | 6 | 3 2 0 | 83.849 |
| 1.1110 | 13 | 3 2 1 | 87.793 |
| 1.0393 | 2 | 4 0 0 | 95.665 |
| 1.0082 | 8 | 4 1 0 | 99.640 |
| .9798 | 7 | 4 1 1 | 103.656 |
| .9536 | 3 | 3 3 1 | 107.755 |
| .9295 | 4 | 4 2 0 | 111.940 |
| .9071 | 9 | 4 2 1 | 116.250 |
| .8862 | 3 | 3 3 2 | 120.725 |
| .8485 | 3 | 4 2 2 | 130.416 |
| .8314 | 3 | 5 0 0 | 135.794 |
| .8152 | 10 | 5 1 0 | 141.773 |
| .8000 | 6 | 5 1 1 | 148.670 |

# Lithium Thorium Molybdenum Oxide, $Li_4Th_7(MoO_4)_{16}$

Synonym
Lithium thorium molybdate

Sample
One mole of $Li_2MoO_4$, 3.5 moles of $ThO_2$ and 7 moles of $MoO_3$ were heated at 700 °C for 21 hours.

Color
Colorless

Structure
Cubic, I*3* Martel and Roth (1981). Apparently isostructural with cubic phase in the system lithium thorium tungsten oxide, Finch and Clark (1965).

Crystallographic constants of this sample
a = 14.4504(3) Å

Z = 2
V = 3017.5 Å$^3$
Density (calc) = 4.635 g/cm$^3$

Figure of merit
$F_{30}$ = 108.8(0.0073,38)

References
Finch, C. B. and Clark, G. W. (1965). J. Appl. Phys. 36, 2143.

Martel, L. C. and Roth, R. C. (1981). Am. Ceram. Soc. Bull. 60, 376.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.894 | 15 | 2 1 1 | 15.018 |
| 5.104 | 59 | 2 2 0 | 17.361 |
| 4.571 | 1L | 3 1 0 | 19.402 |
| 3.862 | 68 | 3 2 1 | 23.010 |
| 3.611 | 94 | 4 0 0 | 24.635 |
| 3.231 | 37 | 4 2 0 | 27.582 |
| 3.081 | 100 | 3 3 2 | 28.954 |
| 2.950 | 75 | 4 2 2 | 30.269 |
| 2.834 | 10 | 5 1 0 | 31.544 |
| 2.638 | 26 | 5 2 1 | 33.954 |
| 2.5561 | 34 | 4 4 0 | 35.079 |
| 2.4786 | 5 | 5 3 0 | 36.213 |
| 2.3433 | 8 | 6 1 1 | 38.383 |
| 2.2851 | 23 | 6 2 0 | 39.401 |
| 2.2306 | 19 | 5 4 1 | 40.404 |
| 2.1304 | 20 | 6 3 1 | 42.393 |
| 2.0862 | 5 | 4 4 4 | 43.336 |
| 2.0435 | 22 | 5 5 0 | 44.290 |
| 2.0037 | 6 | 6 4 0 | 45.218 |
| 1.9661 | 56 | 7 2 1 | 46.131 |
| 1.9308 | 43 | 6 4 2 | 47.025 |
| 1.8972 | 17 | 7 3 0 | 47.911 |
| 1.8350 | 67 | 7 3 2 | 49.642 |
| 1.8061 | 16 | 8 0 0 | 50.492 |
| 1.7787 | 20 | 7 4 1 | 51.325 |
| 1.7524 | 7 | 8 2 0 | 52.152 |
| 1.7270 | 15 | 6 5 3 | 52.979 |
| 1.7031 | 14 | 6 6 0 | 53.782 |
| 1.6797 | 30 | 7 5 0 | 54.592 |
| 1.6151 | 11 | 8 4 0 | 56.972 |
| 1.5956 | 3 | 9 1 0 | 57.732 |
| 1.5583 | 40 | 7 6 1 | 59.249 |
| 1.5407 | 8 | 6 6 4 | 59.997 |
| 1.5231 | 20 | 9 3 0 | 60.761 |
| 1.4905 | 15 | 9 3 2 | 62.237 |
| 1.4750 | 2 | 8 4 4 | 62.963 |
| 1.4598 | 10 | 7 7 0 | 63.696 |
| 1.4450 | 5 | 8 6 0 | 64.428 |
| 1.4312 | 2 | 10 1 1 | 65.123 |
| 1.4169 | 11 | 10 2 0 | 65.865 |
| 1.4036 | 3 | 9 4 3 | 66.571 |
| 1.3774 | 25 | 10 3 1 | 68.006 |
| 1.3533 | 7 | 8 7 1 | 69.386 |
| 1.3415 | 4 | 10 4 0 | 70.091 |
| 1.3299 | 26 | 10 3 3 | 70.791 |
| 1.3192 | 4 | 10 4 2 | 71.455 |
| 1.3082 | 11 | 11 1 0 | 72.149 |
| 1.2872 | 16 | 10 5 1 | 73.517 |
| 1.2771 | 3 | 8 8 0 | 74.196 |
| 1.2673 | 10 | 11 3 0 | 74.864 |
| 1.2482 | 15 | 11 3 2 | 76.215 |
| 1.2390 | 5 | 10 6 0 | 76.879 |
| 1.2299 | 14 | 11 4 1 | 77.555 |
| 1.2126 | 14 | 9 6 5 | 78.873 |
| 1.2041 | 3 | 12 0 0 | 79.543 |
| 1.1960 | 21 | 11 5 0 | 80.195 |
| 1.1878 | 5 | 12 2 0 | 80.856 |
| 1.1797 | 9 | 11 5 2 | 81.528 |
| 1.1723 | 4 | 12 2 2 | 82.158 |
| 1.1643 | 8 | 12 3 1 | 82.846 |
| 1.1497 | 11 | 11 6 1 | 84.131 |
| 1.1354 | 6 | 9 9 0 | 85.445 |
| 1.1283 | 2 | 10 8 0 | 86.107 |
| 1.1216 | 15 | 11 6 3 | 86.756 |
| 1.1150 | 2 | 10 8 2 | 87.396 |
| 1.1083 | 8 | 11 7 0 | 88.055 |
| 1.0956 | 5 | 11 7 2 | 89.350 |
| 1.0893 | 1 | 12 4 4 | 90.010 |
| 1.0832 | 5 | 13 3 0 | 90.658 |
| 1.0772 | 4 | 12 6 0 | 91.302 |
| 1.0712 | 4 | 11 6 5 | 91.959 |
| 1.0655 | 1 | 12 6 2 | 92.601 |
| 1.0597 | 12 | 11 8 1 | 93.260 |

# Lithium Thorium Tungsten Oxide, $Li_4Th_7(WO_4)_{16}$

Synonym
Lithium thorium tungstate

Sample
$Li_2WO_4$ was prepared by reacting $Li_2CO_3$ and $WO_3$ in equimolar proportions at 700 °C for 24 hours to form $Li_2WO_4$. Then $Li_2WO_4$, $ThO_2$, and $WO_3$ in the molar ratios of 1:3.5:7 were ground together under acetone, heated in gold to 700 °C for 48 hours with regrinding every 24 hours, then heated a further 16 hours at 700 °C, reground and heated at 750 °C for 21 hours.

Color
Colorless

Structure
Cubic, I*3*. Finch and Clark (1965) referred to a body-centered cubic phase of this approximate composition.

Crystallographic constants of this sample
$a = 14.4969(4)$ Å

$Z = 2$
$V = 3046.7$ Å$^3$
Density (calc) = 6.124 g/cm$^3$

Figure of merit
$F_{30} = 159.6(0.0049,38)$

Reference
Finch, C. B. and Clark, G. W. (1965). J. Appl. Phys. 36, 2143.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 26.0 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.920 | 8 | 2 1 1 | 14.952 |
| 5.127 | 10 | 2 2 0 | 17.281 |
| 4.586 | 7 | 3 1 0 | 19.340 |
| 3.875 | 68 | 3 2 1 | 22.931 |
| 3.625 | 80 | 4 0 0 | 24.540 |
| 3.242 | 50 | 4 2 0 | 27.489 |
| 3.091 | 100 | 3 3 2 | 28.860 |
| 2.9593 | 44 | 4 2 2 | 30.175 |
| 2.8430 | 15 | 5 1 0 | 31.441 |
| 2.6465 | 19 | 5 2 1 | 33.843 |
| 2.5625 | 24 | 4 4 0 | 34.988 |
| 2.3518 | 14 | 6 1 1 | 38.239 |
| 2.2922 | 4 | 6 2 0 | 39.273 |
| 2.2376 | 10 | 5 4 1 | 40.272 |
| 2.1378 | 30 | 6 3 1 | 42.240 |
| 2.0931 | 1 | 4 4 4 | 43.187 |
| 2.0500 | 13 | 5 5 0 | 44.142 |
| 2.0103 | 12 | 6 4 0 | 45.062 |
| 1.9725 | 53 | 7 2 1 | 45.973 |
| 1.9369 | 28 | 6 4 2 | 46.868 |
| 1.9031 | 18 | 7 3 0 | 47.751 |
| 1.8412 | 61 | 6 5 1 | 49.463 |
| 1.8122 | 16 | 8 0 0 | 50.310 |
| 1.7844 | 13 | 7 4 1 | 51.148 |
| 1.7582 | 12 | 8 2 0 | 51.969 |
| 1.7327 | 20 | 6 5 3 | 52.790 |
| 1.7088 | 9 | 8 2 2 | 53.588 |
| 1.6853 | 35 | 7 5 0 | 54.395 |
| 1.6417 | 1L | 7 5 2 | 55.967 |
| 1.6210 | 9 | 8 4 0 | 56.746 |
| 1.5634 | 40 | 7 6 1 | 59.038 |
| 1.5455 | 5 | 6 6 4 | 59.792 |
| 1.5280 | 11 | 9 3 0 | 60.548 |
| 1.4954 | 13 | 9 3 2 | 62.011 |
| 1.4794 | 1 | 8 4 4 | 62.756 |
| 1.4645 | 6 | 7 7 0 | 63.471 |
| 1.4499 | 7 | 8 6 0 | 64.184 |
| 1.4354 | 1 | 10 1 1 | 64.910 |
| 1.4215 | 9 | 10 2 0 | 65.624 |
| 1.4082 | 4 | 9 5 0 | 66.324 |
| 1.3823 | 29 | 10 3 1 | 67.733 |
| 1.3579 | 5 | 8 7 1 | 69.123 |
| 1.3460 | 5 | 10 4 0 | 69.819 |
| 1.3347 | 28 | 9 6 1 | 70.498 |
| 1.3235 | 3 | 10 4 2 | 71.183 |

Lithium Thorium Tungsten Oxide, $Li_4Th_7(WO_4)_{16}$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.3125 | 11 | 11 | 1 | 0 | 71.874 |
| 1.2913 | 13 | 10 | 5 | 1 | 73.241 |
| 1.2814 | 2 | 8 | 8 | 0 | 73.902 |
| 1.2716 | 9 | 11 | 3 | 0 | 74.567 |
| 1.2525 | 14 | 9 | 7 | 2 | 75.909 |
| 1.2431 | 5 | 10 | 6 | 0 | 76.580 |
| 1.2342 | 8 | 11 | 4 | 1 | 77.239 |
| 1.2165 | 14 | 9 | 6 | 5 | 78.571 |
| 1.2082 | 13 | 12 | 0 | 0 | 79.219 |
| 1.1999 | 17 | 11 | 5 | 0 | 79.876 |
| 1.1917 | 6 | 12 | 2 | 0 | 80.542 |
| 1.1839 | 7 | 10 | 7 | 1 | 81.182 |
| 1.1760 | 3 | 12 | 2 | 2 | 81.842 |
| 1.1682 | 7 | 12 | 3 | 1 | 82.504 |
| 1.1534 | 8 | 11 | 6 | 1 | 83.803 |
| 1.1390 | 3 | 12 | 3 | 3 | 85.113 |
| 1.1319 | 3 | 10 | 8 | 0 | 85.771 |
| 1.1252 | 16 | 9 | 9 | 2 | 86.409 |
| 1.1185 | 1 | 10 | 8 | 2 | 87.056 |
| 1.1118 | 4 | 11 | 7 | 0 | 87.713 |
| 1.0989 | 3 | 13 | 2 | 1 | 89.006 |
| 1.0926 | 2 | 12 | 4 | 4 | 89.656 |
| 1.0864 | 5 | 13 | 3 | 0 | 90.312 |
| 1.0803 | 5 | 12 | 6 | 0 | 90.962 |
| 1.0745 | 3 | 10 | 9 | 1 | 91.601 |
| 1.0686 | 1 | 12 | 6 | 2 | 92.255 |
| 1.0628 | 9 | 11 | 8 | 1 | 92.902 |

# Lithium Titanium Oxide, $Li_2Ti_3O_7$

Synonym
Lithium titanate

Sample
The sample was obtained from J. C. Mikkelson of Xerox Palo Alto Research Center, Palo Alto, CA.

Color
Colorless

Structure
Orthorhombic, Pbnm (62). Its ramsdellite-like structure was qualitatively determined by Lundberg and Andersson (1964).

Crystallographic constants of this sample

a = 5.0182(4) Å
b = 9.5523(8)
c = 2.9455(3)

a/b = 0.5253
c/b = 0.3084

Z = 1
V = 141.19 Å$^3$
Density (calc) = 3.170 g/cm$^3$

Figure of merit
$F_{30}$ = 62.0(0.012,42)

Reference
Lundberg, M. and Andersson, S. (1964). Acta Chem. Scand. 18, 817.

CuK$\alpha_1$ $\lambda$ = 1.540598 Å; temp. 26±1 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ σ = ±4 | hkℓ | 2θ(°) |
|---|---|---|---|
| 4.777 | 3 | 0 2 0 | 18.561 |
| 4.440 | 100 | 1 1 0 | 19.982 |
| 3.461 | 9 | 1 2 0 | 25.721 |
| 2.688 | 46 | 1 3 0 | 33.303 |
| 2.541 | 3 | 1 0 1 | 35.291 |
| 2.507M | 24 | 2 0 0 | 35.790 |
| 2.507M | | 0 2 1 | 35.790 |
| 2.457 | 23 | 1 1 1 | 36.543 |
| 2.388 | 2 | 0 4 0 | 37.637 |
| 2.243 | 32 | 1 2 1 | 40.179 |
| 2.222 | 3 | 2 2 0 | 40.569 |
| 2.156 | 6 | 1 4 0 | 41.861 |
| 1.9857 | 13 | 1 3 1 | 45.651 |
| 1.9707 | 12 | 2 3 0 | 46.017 |
| 1.8554 | 3 | 0 4 1 | 49.060 |
| 1.7733 | 32 | 2 2 1 | 51.494 |
| 1.7301 | 21 | 2 4 0 | 52.878 |
| 1.6382 | 9 | 2 3 1 | 56.095 |
| 1.5923 | 1L | 0 6 0 | 57.863 |
| 1.5792 | 3 | 3 2 0 | 58.389 |
| 1.5265 | 17 | 1 5 1 | 60.612 |
| 1.4917 | 2 | 2 4 1 | 62.179 |
| 1.4814 | 7 | 3 3 0 | 62.663 |
| 1.4729 | 7 | 0 0 2 | 63.067 |
| 1.4540 | 5 | 3 0 1 | 63.981 |
| 1.4380 | 14 | 3 1 1 | 64.782 |
| 1.4001 | 10 | 0 6 1 | 66.760 |
| 1.3976 | 9 | 1 1 2 | 66.895 |
| 1.3913 | 2 | 3 2 1 | 67.236 |
| 1.3697 | 2 | 3 4 0 | 68.444 |
| 1.3444 | 2 | 2 6 0 | 69.916 |
| 1.3233 | 1 | 3 3 1 | 71.198 |
| 1.3168 | 4 | 1 7 0 | 71.605 |
| 1.2914 | 6 | 1 3 2 | 73.235 |
| 1.2703 | 1 | 2 0 2 | 74.658 |
| 1.2589M | 3 | 2 1 2 | 75.451 |
| 1.2589M | | 3 5 0 | 75.451 |
| 1.2440 | 3 | 4 1 0 | 76.519 |
| 1.2418 | 3 | 3 4 1 | 76.678 |
| 1.2230 | 1 | 2 6 1 | 78.078 |
| 1.2162 | 1L | 1 4 2 | 78.601 |
| 1.1940 | 1 | 0 8 0 | 80.354 |
| 1.1798 | 2 | 2 3 2 | 81.523 |
| 1.1617 | 1 | 1 8 0 | 83.074 |
| 1.1573 | 1 | 3 5 1 | 83.457 |
| 1.1530 | 2 | 3 6 0 | 83.837 |
| 1.1458 | 2 | 4 1 1 | 84.485 |
| 1.1216M | 6 | 4 2 1 | 86.750 |
| 1.1216M | | 2 4 2 | 86.750 |
| 1.1103M | 1 | 4 4 0 | 87.861 |
| 1.1103M | | 2 7 1 | 87.861 |
| 1.1069 | 2 | 0 8 1 | 88.200 |
| 1.0979 | 1L | 3 1 2 | 89.108 |
| 1.0849 | 1 | 4 3 1 | 90.469 |
| 1.0781 | 2 | 2 8 0 | 91.201 |
| 1.0769 | 2 | 3 2 2 | 91.332 |
| 1.0740 | 2 | 3 6 1 | 91.648 |
| 1.0575M | 3 | 2 5 2 | 93.511 |
| 1.0575M | | 3 7 0 | 93.511 |
| 1.0488 | 1 | 4 5 0 | 94.522 |
| 1.0444 | 2 | 3 3 2 | 95.051 |
| 1.0392 | 1L | 4 4 1 | 95.673 |
| 1.0124 | 2 | 2 8 1 | 99.082 |
| .9982 | 1 | 5 1 0 | 101.013 |

# Magnesium Manganese Zinc Iron Sulfate Hydroxide Hydrate, Zincobotryogen, $(Zn,Mg,Mn)Fe(SO_4)_2(OH)\cdot 7H_2O$

Sample
The specimen from the northern border of the Tsadam Basin, China was obtained by E. C. T. Chao of the U.S. Geological Survey.

Chemical analysis
$SO_3$-36.03, $Fe_2O_3$-18.34, MgO-2.50, FeO-0.85, MnO-1.75, ZnO-11.77, $H_2O$+29.13, minor $H_2O$-$Na_2O$; this corresponds to the formula $(Zn_{0.59}Mg_{0.26}Mn_{0.10}Fe_{0.05})Fe^{+3}(SO_4)_2(OH)\cdot 7H_2O$ (Kwanchih et al., 1964).

Color
Deep orange

Optical data
Biaxial(+). $N_\alpha$ = 1.542, $N_\beta$ = 1.551, $N_\gamma$ = 1.587. 2V = 54° (calc.) Ibid.

Structure
Monoclinic, $P2_1/n$ (14). The structure was determined by Süsse (1968).

Crystallographic constants of this sample
a = 10.523(2) Å
b = 17.841(3)
c = 7.137(2)
β = 100.11(2)°

a/b = 0.5898
c/b = 0.4000

Z = 4
V = 1310.10 Å$^3$
Density (calc) = 2.237 g/cm$^3$

Figure of merit
$F_{30}$ = 44.6(0.011,61)

Additional pattern
Kwanchih et al. (1964)

References
Kwanchih, T., et al. (1964). Ti Chih K'o Hsueh (Geol. Sci.), No. 11, 313.

Süsse, von P. (1968). Acta Crystallogr., Sect. B, 24, 760.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.7 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±4 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.96 | 100 | 1 1 0 | 9.860 |
| 6.76 | 8 | 1 2 0 | 13.090 |
| 6.354 | 58 | -1 0 1 | 13.926 |
| 5.990 | 8 | -1 1 1 | 14.778 |
| 5.525 | 36 | 0 2 1 | 16.030 |
| 5.395 | 28 | 1 0 1 | 16.419 |
| 5.163M | 75 | 1 1 1 | 17.162 |
| 5.163M | | 1 3 0 | 17.162 |
| 4.613 | 17 | 1 2 1 | 19.226 |
| 4.538 | 29 | 0 3 1 | 19.544 |
| 4.480 | 23 | 2 2 0 | 19.800 |
| 4.456 | 26 | 0 4 0 | 19.910 |
| 4.425 | 29 | -2 1 1 | 20.049 |
| 4.340 | 40 | -1 3 1 | 20.447 |
| 4.095 | 53 | 1 4 0 | 21.684 |
| 3.905 | 27 | 2 3 0 | 22.753 |
| 3.766 | 41 | 0 4 1 | 23.603 |
| 3.655 | 9 | -1 4 1 | 24.333 |
| 3.541 | 41 | 2 2 1 | 25.128 |
| 3.451 | 25 | -1 1 2 | 25.792 |
| 3.389 | 32 | 3 1 0 | 26.278 |
| 3.343 | 19 | -3 0 1 | 26.640 |
| 3.267 | 26 | 0 2 2 | 27.277 |
| 3.219 | 51 | 3 2 0 | 27.689 |
| 3.181M | 17 | 0 5 1 | 28.030 |
| 3.181M | | -2 0 2 | 28.030 |
| 3.112M | 14 | 1 1 2 | 28.664 |
| 3.112M | | -1 5 1 | 28.664 |
| 3.027M | 61 | -1 3 2 | 29.485 |
| 3.027M | | 0 3 2 | 29.485 |
| 2.987 | 16 | 3 3 0 | 29.894 |
| 2.905 | 12 | 3 0 1 | 30.750 |
| 2.867 | 7 | 3 1 1 | 31.172 |
| 2.858 | 6 | 1 6 0 | 31.269 |
| 2.813 | 24 | -2 5 1 | 31.787 |
| 2.803 | 31 | -2 3 2 | 31.907 |
| 2.762M | 52 | -1 4 2 | 32.384 |
| 2.762M | | 3 2 1 | 32.384 |
| 2.732 | 13 | 3 4 0 | 32.752 |
| 2.695M | 13 | 2 0 2 | 33.210 |
| 2.695M | | -1 6 1 | 33.210 |
| 2.673 | 15 | -3 4 1 | 33.502 |
| 2.609 | 8 | 3 3 1 | 34.349 |
| 2.594 | 11 | -3 2 2 | 34.554 |
| 2.580M | 14 | 2 2 2 | 34.747 |
| 2.580M | | 1 4 2 | 34.747 |
| 2.563 | 12 | 4 1 0 | 34.987 |
| 2.555 | 12 | -4 1 1 | 35.090 |
| 2.487 | 28 | 4 2 0 | 36.080 |
| 2.480M | 28 | 3 5 0 | 36.190 |

Magnesium Manganese Zinc Iron Sulfate Hydroxide Hydrate, Zincobotryogen, $(Zn,Mg,Mn)Fe(SO_4)_2(OH)\cdot 7H_2O$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 2.480M | | -4 | 2 | 1 | 36.190 |
| 2.439 | 10 | -3 | 5 | 1 | 36.815 |
| 2.432 | 8 | 3 | 4 | 1 | 36.926 |
| 2.396 | 10 | 0 | 7 | 1 | 37.512 |
| 2.368M | 23 | -4 | 3 | 1 | 37.963 |
| 2.368M | | 1 | 5 | 2 | 37.963 |
| 2.294 | 5 | -1 | 2 | 3 | 39.237 |
| 2.284M | 10 | -4 | 0 | 2 | 39.414 |
| 2.284M | | 4 | 1 | 1 | 39.414 |
| 2.271+ | 7 | -2 | 1 | 3 | 39.659 |
| 2.271+ | | -1 | 6 | 2 | 39.659 |
| 2.255 | 9 | 3 | 6 | 0 | 39.947 |
| 2.229M | 12 | 0 | 8 | 0 | 40.440 |
| 2.229M | | 4 | 2 | 1 | 40.440 |
| 2.180M | 7 | 1 | 8 | 0 | 41.392 |
| 2.180M | | 0 | 3 | 3 | 41.392 |
| 2.172 | 20 | -2 | 6 | 2 | 41.537 |
| 2.134 | 9 | -4 | 3 | 2 | 42.322 |
| 2.097M | 14 | -1 | 4 | 3 | 43.106 |
| 2.097M | | 4 | 5 | 0 | 43.106 |
| 2.092 | 14 | -4 | 5 | 1 | 43.217 |
| 2.0776 | 18 | 3 | 6 | 1 | 43.526 |
| 2.0611M | 22 | -3 | 2 | 3 | 43.891 |
| 2.0611M | | 1 | 8 | 1 | 43.891 |
| 2.0241 | 8 | 3 | 4 | 2 | 44.738 |
| 2.0032M | 7 | -2 | 8 | 1 | 45.229 |
| 2.0032M | | -3 | 6 | 2 | 45.229 |
| 1.9857 | 11 | 1 | 7 | 2 | 45.651 |
| 1.9580M | 6 | 0 | 5 | 3 | 46.333 |
| 1.9580M | | 2 | 2 | 3 | 46.333 |
| 1.9521 | 7 | 4 | 6 | 0 | 46.481 |
| 1.9473 | 7 | 1 | 9 | 0 | 46.604 |
| 1.9275M | 10 | -5 | 1 | 2 | 47.110 |
| 1.9275M | | -2 | 5 | 3 | 47.110 |
| 1.9241 | 11 | -4 | 5 | 2 | 47.200 |
| 1.9179 | 11 | 4 | 1 | 2 | 47.360 |
| 1.8999M | 9 | 2 | 3 | 3 | 47.837 |
| 1.8999M | | 5 | 0 | 1 | 47.837 |
| 1.8841 | 10 | -1 | 8 | 2 | 48.264 |
| 1.8598 | 11 | 1 | 9 | 1 | 48.935 |
| 1.8557M | 12 | -1 | 6 | 3 | 49.050 |
| 1.8557M | | -3 | 8 | 1 | 49.050 |
| 1.8296 | 7 | 2 | 4 | 3 | 49.799 |
| 1.8242 | 9 | -2 | 8 | 2 | 49.955 |
| 1.8195+ | 13 | -4 | 3 | 3 | 50.093 |
| 1.8195+ | | -2 | 9 | 1 | 50.093 |
| 1.8144M | 16 | -2 | 6 | 3 | 50.243 |
| 1.8144M | | -4 | 7 | 1 | 50.243 |

# Magnesium Silicate (Clinoenstatite), $MgSiO_3$

Synonym
Magnesium metasilicate

CAS registry no.
13776-74-4

Sample
The sample was prepared by solid state reaction of basic magnesium carbonate and $SiO_2$. After an overnight calcine at 850 °C, the sample was heated at temperatures in the 1450 °C to 1500 °C range for about 4 days with daily regrindings.

Color
Colorless

Structure
Monoclinic, $P2_1/c$ (14). The structure was determined by Morimoto et al. (1960).

Crystallographic constants of this sample
a = 9.6061(10) Å
b = 8.8185(8)
c = 5.1710(5)
β = 108.289(10)°

a/b = 1.0893
c/b = 0.5864

Z = 8
V = 415.92 Å$^3$
Density (calc) = 3.206 g/cm$^3$

Figure of merit
$F_{30}$ = 56.7(0.010,52)

Polymorphism
There has been and still is considerable controversy. The present view is that there is a stable high temperature form, orthorhombic protoenstatite and a stable low temperature form, orthorhombic enstatite. Protoenstatite on cooling reversibly transforms into metastable monoclinic clinoenstatite.

Additional patterns
PDF card 19-769 Stephenson et al. (1966)
Smyth (1974)


References
Morimoto, N., Appleman, D. E., and Evans, H. T. (1960). Z. Kristallogr. 114, 120.

Smyth, J. R. (1974). Am. Mineral. 59, 345.

Stephenson, D. A., Sclar, C. B., and Smith, J. V. (1966). Mineral. Mag. 35, 838.


$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26±2 °C
Internal standard Ag, a = 4.08651 Å

| d(Å) | $I^{rel}$ σ = ±4 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.341 | 1 | 1 1 0 | 13.955 |
| 4.410 | 9 | 0 2 0 | 20.119 |
| 4.372 | 3 | -1 1 1 | 20.296 |
| 4.293 | 8 | 0 1 1 | 20.673 |
| 4.048 | 1L | 2 1 0 | 21.937 |
| 3.530 | 4 | 1 1 1 | 25.206 |
| 3.316 | 8 | -1 2 1 | 26.863 |
| 3.280 | 30 | 0 2 1 | 27.162 |
| 3.170 | 47 | 2 2 0 | 28.125 |
| 3.041 | 4 | 3 0 0 | 29.350 |
| 2.976 | 69 | -2 2 1 | 30.000 |
| 2.874 | 100 | 3 1 0 | 31.094 |
| 2.798 | 3 | 1 3 0 | 31.956 |
| 2.769 | 2 | 2 1 1 | 32.308 |
| 2.582 | 2 | -1 0 2 | 34.716 |
| 2.539 | 23 | -1 3 1 | 35.323 |
| 2.523 | 19 | 0 3 1 | 35.555 |
| 2.516 | 17 | -2 0 2 | 35.659 |
| 2.472 | 13 | 2 3 0 | 36.319 |
| 2.455 | 35 | 0 0 2 | 36.570 |
| 2.433 | 14 | 2 2 1 | 36.916 |
| 2.375 | 11 | -2 3 1 | 37.847 |
| 2.280 | 4 | 4 0 0 | 39.483 |
| 2.209 | 9 | 4 1 0 | 40.815 |
| 2.204M | 9 | 0 4 0 | 40.921 |
| 2.204M | | 1 0 2 | 40.921 |
| 2.1443M | 6 | 0 2 2 | 42.107 |
| 2.1443M | | 1 4 0 | 42.107 |
| 2.1380 | 5 | 1 1 2 | 42.237 |
| 2.1166 | 26 | -3 3 1 | 42.684 |
| 2.0901 | 5 | -4 2 1 | 43.253 |
| 2.0359 | 3 | -3 2 2 | 44.465 |
| 2.0247 | 6 | 4 2 0 | 44.722 |
| 2.0193 | 10 | -1 4 1 | 44.849 |
| 2.0114 | 9 | 0 4 1 | 45.035 |
| 1.9862 | 6 | 2 4 0 | 45.639 |
| 1.9655 | 4 | -4 1 2 | 46.148 |
| 1.9349 | 8 | -2 4 1 | 46.921 |
| 1.9238 | 5 | 2 0 2 | 47.206 |
| 1.9135 | 2 | 1 4 1 | 47.476 |
| 1.8847 | 2 | 0 3 2 | 48.249 |
| 1.8737 | 2 | -5 1 1 | 48.549 |
| 1.8455 | 3 | -4 3 1 | 49.339 |
| 1.8085 | 2 | -3 3 2 | 50.420 |
| 1.8038 | 1 | 3 3 1 | 50.560 |
| 1.7862M | 9 | -3 4 1 | 51.095 |
| 1.7862M | | 5 1 0 | 51.095 |
| 1.7640M | 7 | 2 2 2 | 51.784 |
| 1.7640M | | 1 3 2 | 51.784 |
| 1.7586M | 8 | 2 4 1 | 51.955 |

Magnesium Silicate (Clinoenstatite), $MgSiO_3$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.7586M | | -5 | 2 | 1 | 51.955 |
| 1.7311 | 7 | 1 | 5 | 0 | 52.844 |
| 1.7112 | 2 | 4 | 2 | 1 | 53.506 |
| 1.6763M | 1 | -1 | 4 | 2 | 54.713 |
| 1.6763M | | -1 | 1 | 3 | 54.713 |
| 1.6713 | 2 | 3 | 0 | 2 | 54.890 |
| 1.6595 | 5 | 0 | 5 | 1 | 55.315 |
| 1.6480 | 5 | -3 | 1 | 3 | 55.733 |
| 1.6412 | 7 | 3 | 1 | 2 | 55.983 |
| 1.6273 | 2 | -5 | 2 | 2 | 56.504 |
| 1.6054 | 30 | -5 | 3 | 1 | 57.347 |
| 1.5920 | 4 | -1 | 2 | 3 | 57.875 |
| 1.5852 | 5 | 4 | 4 | 0 | 58.147 |
| 1.5702 | 1 | 4 | 3 | 1 | 58.755 |
| 1.5608 | 1 | -4 | 1 | 3 | 59.146 |
| 1.5340M | 1L | 0 | 2 | 3 | 60.284 |
| 1.5340M | | 5 | 1 | 1 | 60.284 |
| 1.5257 | 9 | 3 | 5 | 0 | 60.648 |
| 1.5201 | 7 | 6 | 0 | 0 | 60.896 |
| 1.4857 | 10 | -2 | 3 | 3 | 62.459 |
| 1.4757 | 10 | -1 | 3 | 3 | 62.933 |
| 1.4695 | 11 | 0 | 6 | 0 | 63.229 |
| 1.4571M | 2 | -3 | 3 | 3 | 63.829 |
| 1.4571M | | -1 | 5 | 2 | 63.829 |
| 1.4507 | 1 | 1 | 6 | 0 | 64.145 |
| 1.4448M | 1 | 1 | 2 | 3 | 64.436 |
| 1.4448M | | -2 | 5 | 2 | 64.436 |
| 1.4401 | 1 | -6 | 2 | 2 | 64.675 |
| 1.4320 | 3 | 0 | 5 | 2 | 65.085 |
| 1.4084 | 1 | 0 | 6 | 1 | 66.316 |
| 1.4049 | 1 | 5 | 4 | 0 | 66.503 |
| 1.3981 | 2 | -3 | 5 | 2 | 66.865 |
| 1.3952 | 2 | 4 | 5 | 0 | 67.021 |
| 1.3762 | 11 | 5 | 3 | 1 | 68.074 |
| 1.3568M | 6 | -2 | 4 | 3 | 69.182 |
| 1.3568M | | 1 | 3 | 3 | 69.182 |
| 1.3381 | 2 | -7 | 0 | 2 | 70.294 |
| 1.3351C | 2 | -3 | 4 | 3 | 70.474 |
| 1.3233 | 3 | 3 | 6 | 0 | 71.195 |
| 1.3233 | 3 | 6 | 1 | 1 | 71.195 |
| 1.3139M | 1 | 0 | 4 | 3 | 71.787 |
| 1.3139M | | -5 | 3 | 3 | 71.787 |
| 1.2888 | 2 | 7 | 1 | 0 | 73.411 |
| 1.2867 | 2 | -3 | 0 | 4 | 73.548 |
| 1.2776M | 2 | -2 | 1 | 4 | 74.161 |
| 1.2776M | | -1 | 6 | 2 | 74.161 |
| 1.2696 | 3 | 3 | 1 | 3 | 74.706 |
| 1.2680 | 2 | 5 | 5 | 0 | 74.819 |
| 1.2609 | 5 | 0 | 6 | 2 | 75.309 |
| 1.2579 | 3 | -4 | 0 | 4 | 75.519 |

# Magnesium Silicate (Forsterite), $Mg_2SiO_4$

Synonym
Magnesium orthosilicate

CAS registry no.
10034-94-3

Sample
$MgCO_3$ and $SiO_2$ were mixed in a 2:1 molar ratio and heated at 800 °C overnight, 1300 °C for 21 hours, 1500 °C for 25 hours, and 1525 °C for 24 hours with intermittent grinding. There was a trace of MgO in the sample.

Color
Colorless

Structure
Orthorhombic, Pmnb (62). The structure was solved by Rinne et al. (1924).

Crystallographic constants of this sample
a = 5.9817(5) Å
b = 10.1978(8)
c = 4.7553(3)

a/b = 0.5866
c/b = 0.4663

Z = 4
V = 290.07 Å$^3$
Density (calc) = 3.222 g/cm$^3$

Figure of merit
$F_{30}$ = 113.8(0.0068,39)

Additional patterns
PDF card 7-74 (Gillery, Coll. of Min. Ind., Penn. State University, University Park, PA)

Swanson and Tatge (1951)

References
Rinne, F. (1924). Z. Kristallogr. 59, 230.

Rinne, F., Leonhardt, J., and Hentschel, H. (1924) ibid 59, 548.

Swanson, H. E. and Tatge, E. (1953). Natl. Bur. Stand. (U.S.) Circ. 539, Vol. 1, p. 83.

CuK$\alpha_1$ $\lambda$ = 1.540598 Å; mean T = 26±2 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±4 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.102 | 22 | 0 2 0 | 17.367 |
| 4.307 | 4 | 0 1 1 | 20.603 |
| 3.881 | 76 | 1 2 0 | 22.895 |
| 3.722 | 25 | 1 0 1 | 23.887 |
| 3.496 | 26 | 1 1 1 | 25.458 |
| 3.477 | 22 | 0 2 1 | 25.601 |
| 3.006 | 14 | 1 2 1 | 29.691 |
| 2.991 | 18 | 2 0 0 | 29.852 |
| 2.765 | 66 | 0 3 1 | 32.348 |
| 2.5097 | 83 | 1 3 1 | 35.748 |
| 2.4567 | 100 | 2 1 1 | 36.547 |
| 2.3456 | 13 | 1 4 0 | 38.344 |
| 2.3150 | 13 | 0 1 2 | 38.870 |
| 2.2673 | 57 | 2 2 1 | 39.722 |
| 2.2470 | 37 | 0 4 1 | 40.096 |
| 2.1589 | 23 | 1 1 2 | 41.807 |
| 2.0303 | 7 | 2 3 1 | 44.593 |
| 1.9479 | 6 | 0 3 2 | 46.589 |
| 1.9407 | 5 | 2 4 0 | 46.772 |
| 1.8744 | 8 | 0 5 1 | 48.531 |
| 1.8608 | 3 | 2 0 2 | 48.908 |
| 1.8569 | 2 | 3 2 0 | 49.018 |
| 1.8388 | 1L | 3 0 1 | 49.533 |
| 1.8299 | 1 | 2 1 2 | 49.789 |
| 1.8090 | 4 | 3 1 1 | 50.405 |
| 1.7886 | 5 | 1 5 1 | 51.020 |
| 1.7483 | 73 | 2 2 2 | 52.285 |
| 1.7386 | 24 | 0 4 2 | 52.598 |
| 1.7294 | 6 | 3 2 1 | 52.899 |
| 1.6698 | 16 | 1 4 2 | 54.944 |
| 1.6347 | 15 | 1 6 0 | 56.226 |
| 1.6173 | 17 | 3 3 1 | 56.886 |
| 1.6008 | 2 | 0 6 1 | 57.527 |
| 1.5884 | 4 | 2 5 1 | 58.020 |
| 1.5708 | 11 | 3 4 0 | 58.733 |
| 1.5666 | 8 | 0 1 3 | 58.906 |
| 1.5323 | 2 | 1 0 3 | 60.357 |
| 1.5144 | 10 | 1 1 3 | 61.146 |
| 1.5111 | 9 | 3 1 2 | 61.295 |
| 1.5032 | 11 | 2 4 2 | 61.651 |

Magnesium Silicate (Forsterite), $Mg_2SiO_4$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4990 | 20 | 1 5 2 | 61.845 |
| 1.4954 | 30 | 4 0 0 | 62.008 |
| 1.4780 | 33 | 2 6 0 | 62.825 |
| 1.4674 | 3 | 1 2 3 | 63.328 |
| 1.4638 | 3 | 3 2 2 | 63.505 |
| 1.4365 | 4 | 0 3 3 | 64.853 |
| 1.4111 | 2 | 2 6 1 | 66.172 |
| 1.3968 | 13 | 1 3 3 | 66.934 |
| 1.3930M | 14 | 3 3 2 | 67.143 |
| 1.3930M | | 0 7 1 | 67.143 |
| 1.3874 | 9 | 2 1 3 | 67.448 |
| 1.3748 | 2 | 2 5 2 | 68.155 |
| 1.3657 | 1L | 3 5 1 | 68.668 |
| 1.3505 | 22 | 2 2 3 | 69.553 |
| 1.3465 | 15 | 0 4 3 | 69.793 |
| 1.3155 | 11 | 4 3 1 | 71.685 |
| 1.3131 | 9 | 1 4 3 | 71.838 |
| 1.2937 | 5 | 3 6 0 | 73.085 |
| 1.2661 | 2 | 4 0 2 | 74.950 |
| 1.2627 | 1 | 2 7 1 | 75.185 |
| 1.2561 | 3 | 4 1 2 | 75.651 |
| 1.2515 | 1 | 0 5 3 | 75.975 |
| 1.2477 | 3 | 3 6 1 | 76.246 |
| 1.2448 | 3 | 4 4 1 | 76.456 |
| 1.2411 | 3 | 3 0 3 | 76.726 |
| 1.2317 | 1 | 3 1 3 | 77.420 |
| 1.2276 | 2 | 2 4 3 | 77.732 |
| 1.2228 | 2 | 3 5 2 | 78.089 |
| 1.2160 | 1L | 1 7 2 | 78.615 |
| 1.2060 | 1L | 1 8 1 | 79.391 |

# Potassium Barium Niobium Oxide, $KBa_2(NbO_3)_5$

Synonym
Potassium barium niobate

CAS registry no.
12400-06-5

Sample
The sample was made by heating a mixture of $KNbO_3$, $BaCO_3$, and $Nb_2O_5$ at temperatures up to 1340 °C for 56 hours with intermediate grindings.

Color
Colorless

Structure
Tetragonal, P4bm (100). Tungsten bronze structure (Giess et al., 1969).

Crystallographic constants of this sample
a = 12.5407(5) Å
c = 4.0210(3)

c/a = 0.3206

Z = 2
V = 632.38 Å$^3$
Density (calc) = 5.348 g/cm$^3$

Figure of merit
$F_{30}$ = 104.2(0.0082,35)

Additional pattern
PDF card 28-375 (Giess et al., 1969)

Reference
Giess, E. A., Scott, B. A., Burns, G., O'Kane, D. F., and Segmüller, A. (1969). J. Am. Ceram. Soc. 52, 276.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26±2 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±4 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.87 | 1 | 1 1 0 | 9.968 |
| 6.279 | 1L | 2 0 0 | 14.093 |
| 5.609 | 1 | 2 1 0 | 15.787 |
| 4.433 | 1L | 2 2 0 | 20.014 |
| 4.021 | 13 | 0 0 1 | 22.086 |
| 3.967 | 4 | 3 1 0 | 22.394 |
| 3.664 | 1 | 1 1 1 | 24.274 |
| 3.479 | 29 | 3 2 0 | 25.585 |
| 3.386 | 3 | 2 0 1 | 26.303 |
| 3.269 | 59 | 2 1 1 | 27.255 |
| 3.136 | 9 | 4 0 0 | 28.440 |
| 3.042 | 68 | 4 1 0 | 29.332 |
| 2.981 | 23 | 2 2 1 | 29.955 |
| 2.957 | 15 | 3 3 0 | 30.204 |
| 2.824 | 100 | 3 1 1 | 31.661 |
| 2.804 | 36 | 4 2 0 | 31.889 |
| 2.631 | 16 | 3 2 1 | 34.052 |
| 2.474 | 4 | 4 0 1 | 36.280 |
| 2.427 | 1 | 4 1 1 | 37.013 |
| 2.3811 | 1 | 3 3 1 | 37.750 |
| 2.3291 | 9 | 5 2 0 | 38.626 |
| 2.3015 | 1 | 4 2 1 | 39.108 |
| 2.2167 | 2 | 4 4 0 | 40.669 |
| 2.1506 | 17 | 5 3 0 | 41.976 |
| 2.0981 | 2 | 5 1 1 | 43.079 |
| 2.0901 | 3 | 6 0 0 | 43.252 |
| 2.0616 | 1 | 6 1 0 | 43.880 |
| 2.0100 | 25 | 0 0 2 | 45.069 |
| 1.9823 | 15 | 6 2 0 | 45.734 |
| 1.9581 | 1 | 5 4 0 | 46.332 |
| 1.9416 | 1 | 4 4 1 | 46.748 |
| 1.8963 | 4 | 5 3 1 | 47.934 |
| 1.8690 | 8 | 6 3 0 | 48.678 |
| 1.8544 | 14 | 6 0 1 | 49.088 |
| 1.7785 | 21 | 6 2 1 | 51.332 |
| 1.7733 | 27 | 5 5 0 | 51.492 |
| 1.7606 | 18 | 5 4 1 | 51.892 |
| 1.7404 | 7 | 3 2 2 | 52.540 |
| 1.7225 | 2 | 7 2 0 | 53.127 |
| 1.6951 | 9 | 6 3 1 | 54.056 |
| 1.6770 | 20 | 4 1 2 | 54.687 |
| 1.6622 | 4 | 3 3 2 | 55.217 |
| 1.6464 | 2 | 7 3 0 | 55.792 |
| 1.6339 | 11 | 4 2 2 | 56.256 |
| 1.6226 | 26 | 5 5 1 | 56.684 |
| 1.6058 | 1L | 6 5 0 | 57.332 |
| 1.5837 | 4 | 7 2 1 | 58.209 |
| 1.5677 | 1 | 8 0 0 | 58.858 |
| 1.5553 | 3 | 7 4 0 | 59.375 |
| 1.5206 | 12 | 8 2 0 | 60.871 |
| 1.4912 | 1 | 6 5 1 | 62.202 |
| 1.4780 | 3 | 6 6 0 | 62.825 |
| 1.4680 | 12 | 8 3 0 | 63.300 |
| 1.4578 | 2 | 7 5 0 | 63.793 |
| 1.4509 | 3 | 7 4 1 | 64.134 |
| 1.4117 | 5 | 6 2 2 | 66.139 |
| 1.4018 | 1 | 8 4 0 | 66.665 |
| 1.3847 | 2 | 9 1 0 | 67.597 |
| 1.3787 | 3 | 8 3 1 | 67.931 |
| 1.3690 | 6 | 6 3 2 | 68.480 |
| 1.3298 | 7 | 5 5 2 | 70.795 |
| 1.3239 | 2 | 8 4 1 | 71.162 |
| 1.3095 | 1 | 9 1 1 | 72.067 |
| 1.3034 | 2 | 2 1 3 | 72.453 |
| 1.2886 | 1 | 7 6 1 | 73.421 |
| 1.2830 | 1 | 2 2 3 | 73.796 |
| 1.2735 | 2 | 9 4 0 | 74.442 |
| 1.2700 | 3 | 3 1 3 | 74.680 |
| 1.2668 | 2 | 7 7 0 | 74.900 |

# Potassium Strontium Niobium Oxide, $KSr_2(NbO_3)_5$

Synonym
Potassium strontium niobate

CAS registry no.
12358-94-0

Sample
The sample was made by heating $KNbO_3$, $SrCO_3$, and $Nb_2O_5$ at 850 °C for 18 hours, at 1300 °C for 18 hours, and at 1340 °C for 20 hours.

Color
Colorless

Structure
Tetragonal, P4bm (100). Tungsten bronze structure (Giess et al., 1969).

Crystallographic constants of this sample
a = 12.461(1) Å
c = 3.9431(8)

c/a = 0.3164

Z = 2
V = 612.27 $Å^3$
Density (calc) = 4.984 $g/cm^3$

Figure of merit
$F_{30}$ = 49.1(0.012,50)

Reference
Giess, E. A., Scott, B. A., Burns, G., O'Kane, D. F., and Segmüller, A. (1969). J. Am. Ceram. Soc. 52, 276.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26±2 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.82 | 2 | 1 1 0 | 10.025 |
| 6.24 | 5 | 2 0 0 | 14.189 |
| 5.578 | 2 | 2 1 0 | 15.876 |
| 3.944M | 34 | 0 0 1 | 22.527 |
| 3.944M | | 3 1 0 | 22.527 |
| 3.602 | 4 | 1 1 1 | 24.700 |
| 3.458 | 37 | 3 2 0 | 25.745 |
| 3.219 | 43 | 2 1 1 | 27.687 |
| 3.116 | 12 | 4 0 0 | 28.627 |
| 3.023 | 52 | 4 1 0 | 29.521 |
| 2.939M | 25 | 2 2 1 | 30.392 |
| 2.939M | | 3 3 0 | 30.392 |
| 2.788M | 100 | 3 1 1 | 32.077 |
| 2.788M | | 4 2 0 | 32.077 |
| 2.600 | 20 | 3 2 1 | 34.472 |
| 2.446M | 2 | 4 0 1 | 36.711 |
| 2.446M | | 5 1 0 | 36.711 |
| 2.399 | 1 | 4 1 1 | 37.454 |
| 2.356 | 2 | 3 3 1 | 38.176 |
| 2.315 | 3 | 5 2 0 | 38.875 |
| 2.202 | 1 | 4 4 0 | 40.960 |
| 2.137 | 8 | 5 3 0 | 42.252 |
| 2.077M | 3 | 5 1 1 | 43.539 |
| 2.077M | | 6 0 0 | 43.539 |
| 2.048 | 3 | 6 1 0 | 44.179 |
| 1.9709M | 36 | 0 0 2 | 46.014 |
| 1.9709M | | 6 2 0 | 46.014 |
| 1.9468 | 6 | 5 4 0 | 46.616 |
| 1.9229M | 1 | 1 1 2 | 47.231 |
| 1.9229M | | 4 4 1 | 47.231 |
| 1.8786M | 1 | 2 0 2 | 48.414 |
| 1.8786M | | 5 3 1 | 48.414 |
| 1.8576M | 12 | 2 1 2 | 48.998 |
| 1.8576M | | 6 3 0 | 48.998 |
| 1.8375 | 8 | 6 0 1 | 49.568 |
| 1.7625+ | 20 | 6 2 1 | 51.831 |
| 1.7625+ | | 5 5 0 | 51.831 |
| 1.7452 | 10 | 5 4 1 | 52.385 |
| 1.7288 | 1L | 6 4 0 | 52.918 |
| 1.7127 | 6 | 3 2 2 | 53.456 |
| 1.6805 | 7 | 6 3 1 | 54.563 |
| 1.6656 | 1 | 4 0 2 | 55.093 |
| 1.6513 | 12 | 4 1 2 | 55.613 |
| 1.6377 | 2 | 3 3 2 | 56.116 |
| 1.6090M | 31 | 4 2 2 | 57.206 |

| d(Å) | $I^{rel}$ $\sigma = \pm 1$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.6090M | | 5 5 1 | 57.206 |
| 1.5961 | 1L | 6 5 0 | 57.714 |
| 1.5698 | 1 | 7 2 1 | 58.771 |
| 1.5459M | 2 | 4 3 2 | 59.774 |
| 1.5459M | | 7 4 0 | 59.774 |
| 1.5350 | 1L | 5 1 2 | 60.241 |
| 1.5110M | 6 | 7 3 1 | 61.299 |
| 1.5110M | | 8 2 0 | 61.299 |
| 1.5008 | 1 | 5 2 2 | 61.764 |
| 1.4785 | 1L | 6 5 1 | 62.798 |
| 1.4684 | 3 | 6 6 0 | 63.281 |
| 1.4583 | 4 | 8 3 0 | 63.768 |
| 1.4490M | 3 | 5 3 2 | 64.229 |
| 1.4490M | | 8 0 1 | 64.229 |
| 1.4389 | 1 | 7 4 1 | 64.736 |
| 1.4298 | 1L | 6 0 2 | 65.194 |
| 1.3935M | 7 | 6 2 2 | 67.114 |
| 1.3935M | | 8 4 0 | 67.114 |
| 1.3848 | 1L | 5 4 2 | 67.594 |
| 1.3758M | 1L | 6 6 1 | 68.097 |
| 1.3758M | | 9 1 0 | 68.097 |
| 1.3677 | 4 | 8 3 1 | 68.556 |
| 1.3599 | 1 | 7 5 1 | 69.002 |
| 1.3520M | 4 | 6 3 2 | 69.468 |
| 1.3520M | | 9 2 0 | 69.468 |
| 1.3207 | 1L | 8 5 0 | 71.358 |
| 1.3137+ | 6 | 5 5 2 | 71.795 |
| 1.3137+ | | 8 4 1 | 71.795 |

# Potassium Titanium Phosphate, $KTi_2(PO_4)_3$

Synonym
Potassium titanium orthophosphate

CAS registry no.
30622-41-4

Sample
The sample was made by heating a mixture of $KH_2PO_4$, $TiO_2$ (anatase) and $(NH_4)_2HPO_4$ up to 1000 °C for 2 days.

Color
Colorless

Structure
Rhombohedral, R**. Isostructural with many other similar double phosphates (Masse, 1970).

Crystallographic constants of this sample (Hexagonal axes)
a = 8.3582(5) Å
c = 23.086(2)

c/a = 2.7621

Z = 6
V = 1396.71 Å$^3$
Density (calc) = 2.995 g/cm$^3$

Figure of merit
$F_{30}$ = 83.0(0.0070,52)

Polymorphism
Masse et al. (1972) reported a cubic form of $KTi_2(PO_4)_3$.

Additional pattern
PDF card 25-691 (Masse, 1970)

References
Masse, R. (1970). Bull. Soc. Fr. Mineral. Crystallogr. 93, 500.

Masse, R., Durif, A., Guitel, J.-C., and Tordjman, I. (1972). Bull. Soc. Fr. Mineral. Crystallogr. 95, 47.

CuK$\alpha_1$ $\lambda$ = 1.540598 Å; mean T = 26±2 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.131 | 8 | 0 1 2 | 14.435 |
| 4.514 | 9 | 1 0 4 | 19.653 |
| 4.178 | 42 | 1 1 0 | 21.248 |
| 3.846 | 1 | 0 0 6 | 23.109 |
| 3.672 | 100 | 1 1 3 | 24.218 |
| 3.452 | 5 | 2 0 2 | 25.790 |
| 3.065 | 24 | 0 2 4 | 29.110 |
| 2.830 | 80 | 1 1 6 | 31.587 |
| 2.716 | 11 | 2 1 1 | 32.951 |
| 2.681 | 5 | 0 1 8 | 33.398 |
| 2.662 | 6 | 1 2 2 | 33.643 |
| 2.4129 | 16 | 3 0 0 | 37.234 |
| 2.3541 | 2 | 1 2 5 | 38.200 |
| 2.2562 | 2 | 2 0 8 | 39.926 |
| 2.1986 | 4 | 1 0 10 | 41.019 |
| 2.1866 | 8 | 1 1 9 | 41.253 |
| 2.1050 | 2 | 2 1 7 | 42.931 |
| 2.0438 | 11 | 3 0 6 | 44.284 |
| 2.0166 | 3 | 2 2 3 | 44.912 |
| 1.9850 | 6 | 1 2 8 | 45.668 |
| 1.9468 | 2 | 0 2 10 | 46.616 |
| 1.9233 | 3 | 0 0 12 | 47.221 |
| 1.8964 | 2 | 1 3 4 | 47.931 |
| 1.8363 | 22 | 2 2 6 | 49.605 |
| 1.7880 | 1 | 0 4 2 | 51.038 |
| 1.7642 | 8 | 2 1 10 | 51.779 |
| 1.7266 | 2 | 4 0 4 | 52.992 |
| 1.7149 | 6 | 1 3 7 | 53.382 |
| 1.6651 | 1L | 1 2 11 | 55.113 |
| 1.6481 | 6 | 3 1 8 | 55.728 |
| 1.6202 | 1 | 2 2 9 | 56.774 |
| 1.6081 | 1L | 0 1 14 | 57.243 |
| 1.5955 | 1 | 3 2 4 | 57.737 |
| 1.5797 | 11 | 4 1 0 | 58.369 |
| 1.5627 | 1 | 2 3 5 | 59.065 |
| 1.5474 | 2 | 4 1 3 | 59.711 |
| 1.5332 | 4 | 0 4 8 | 60.319 |
| 1.5150 | 6 | 1 3 10 | 61.123 |
| 1.5043 | 10 | 3 0 12 | 61.602 |
| 1.5005 | 9 | 2 0 14 | 61.776 |
| 1.4832 | 1 | 3 2 7 | 62.577 |
| 1.4611 | 7 | 4 1 6 | 63.636 |
| 1.4511 | 2 | 3 1 11 | 64.124 |
| 1.4442 | 1 | 1 1 15 | 64.466 |
| 1.4244 | 2 | 4 0 10 | 65.476 |
| 1.4123 | 3 | 1 2 14 | 66.108 |
| 1.4044 | 1L | 0 5 4 | 66.528 |
| 1.3928 | 2 | 3 3 0 | 67.154 |
| 1.3708 | 1L | 3 3 3 | 68.377 |

# Potassium Zinc Phosphate, $KZnPO_4$

Synonym
Potassium zinc orthophosphate

CAS registry no.
13826-55-6

Sample
The sample was prepared by heating $KH_2PO_4$ and ZnO at 800 °C for 2 days. After grinding and sieving, it was held at 800 °C overnight.

Color
Colorless

Structure
Hexagonal, $P6_3/*$ (Averbuch-Pouchot and Durif, 1973).

Crystallographic constants of this sample
a = 18.1626(12) Å
c = 8.5066(11)

c/a = 0.4684

Z = 24
V = 2430.20 $Å^3$
Density (calc) = 3.2702 $g/cm^3$

Figure of merit
$F_{30}$ = 57.4(0.0093,56)

Additional patterns
PDF card 20-1447 (Salutsky and Steiger, 1964)
PDF card 20-1448 (Frazier et al., 1966)
PDF card 25-1342 (Averbuch-Pouchot and Durif, 1973)
Barbou des Courières and Simonot-Grange (1979)
Grins and Nygren (1982)

References


Averbuch-Pouchot, M. T. and Durif, A. (1973). Mat. Res. Bull. 8, 353.

Barbou des Courieres, T. and Simonot-Grange, M.-H. (1979). Mat. Res. Bull. 14, 1419.

Grins, J. and Nygren, M. (1982). Mat. Res. Bull. 17, 895.

Frazier, A. W., Smith, J. P., and Lehr, J. R. (1966). J. Agric. Food Chem. 14, 522.

Salutsky, M. L. and Steiger, R. P. (1964). J. Agric. Food Chem. 12, 6.


$CuK\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C
Internal standard Ag, a = 4.08651 Å

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 9.08 | 1L | 1 1 0 | 9.738 |
| 6.203 | 13 | 1 1 1 | 14.268 |
| 4.537 | 16 | 2 2 0 | 19.549 |
| 4.252 | 34 | 0 0 2 | 20.873 |
| 4.004 | 19 | 2 2 1 | 22.183 |
| 3.884 | 1 | 3 1 1 | 22.881 |
| 3.852 | 2 | 1 1 2 | 23.072 |
| 3.609 | 1 | 3 2 0 | 24.651 |
| 3.567 | 1 | 4 0 1 | 24.941 |
| 3.436 | 1 | 4 1 0 | 25.912 |
| 3.320 | 1 | 3 2 1 | 26.834 |
| 3.302 | 3 | 3 0 2 | 26.982 |
| 3.182 | 34 | 4 1 1 | 28.020 |
| 3.103 | 100 | 2 2 2 | 28.743 |
| 3.045 | 1L | 3 1 2 | 29.303 |
| 2.972 | 3 | 4 2 0 | 30.040 |
| 2.851 | 2 | 3 3 1 | 31.349 |
| 2.824 | 2 | 5 1 0 | 31.660 |
| 2.750 | 1 | 3 2 2 | 32.528 |
| 2.706 | 12 | 1 1 3 | 33.073 |
| 2.671 | 1L | 4 1 2 | 33.522 |
| 2.621 | 60 | 6 0 0 | 34.177 |
| 2.558 | 1 | 2 1 3 | 35.047 |
| 2.518 | 2 | 5 2 0 | 35.626 |
| 2.505 | 11 | 6 0 1 | 35.823 |
| 2.465 | 3 | 3 3 2 | 36.422 |
| 2.436 | 3 | 4 2 2 | 36.869 |
| 2.416 | 8 | 5 2 1 | 37.191 |
| 2.405 | 10 | 2 2 3 | 37.368 |
| 2.377 | 2 | 3 1 3 | 37.818 |
| 2.354 | 1 | 5 1 2 | 38.202 |
| 2.309 | 1L | 6 1 1 | 38.972 |
| 2.299 | 1 | 4 0 3 | 39.153 |
| 2.2313M | 2 | 6 0 2 | 40.391 |
| 2.2313M | | 3 2 3 | 40.391 |
| 2.2095 | 1 | 4 3 2 | 40.807 |
| 2.1932 | 9 | 4 4 1 | 41.125 |
| 2.1868 | 10 | 4 1 3 | 41.250 |
| 2.1665 | 2 | 5 2 2 | 41.655 |
| 2.1259 | 6 | 0 0 4 | 42.488 |
| 2.1144 | 1 | 6 2 1 | 42.731 |
| 2.0696M | 4 | 1 1 4 | 43.702 |
| 2.0696M | | 3 3 3 | 43.702 |
| 2.0028+ | 9 | 4 4 2 | 45.238 |
| 2.0028+ | | 2 1 4 | 45.238 |
| 1.9815 | 1 | 6 3 0 | 45.752 |
| 1.9705 | 2 | 3 0 4 | 46.023 |
| 1.9251M | 4 | 2 2 4 | 47.173 |
| 1.9251M | | 6 0 3 | 47.173 |
| 1.9112M | 1 | 3 1 4 | 47.537 |

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.9112M | | 4 3 3 | 47.537 |
| 1.8832 | 10 | 5 2 3 | 48.289 |
| 1.8705M | 1 | 7 1 2 | 48.639 |
| 1.8705M | | 4 0 4 | 48.639 |
| 1.8162 | 1 | 5 5 0 | 50.191 |
| 1.8076 | 1L | 4 1 4 | 50.445 |
| 1.8038 | 1L | 6 4 0 | 50.561 |
| 1.7994 | 1L | 8 1 1 | 50.693 |
| 1.7959 | 1 | 6 3 2 | 50.798 |
| 1.7759 | 3 | 5 5 1 | 51.411 |
| 1.7718 | 5 | 4 4 3 | 51.540 |
| 1.7603 | 1 | 5 3 3 | 51.900 |
| 1.7400 | 2 | 3 3 4 | 52.554 |
| 1.7286M | 1 | 4 2 4 | 52.926 |
| 1.7286M | | 6 2 3 | 52.926 |
| 1.7160 | 2 | 8 2 0 | 53.345 |
| 1.7117 | 1 | 9 0 1 | 53.489 |
| 1.6822 | 10 | 8 2 1 | 54.504 |
| 1.6787 | 12 | 7 1 3 | 54.628 |
| 1.6510 | 3 | 6 0 4 | 55.622 |
| 1.6307 | 1L | 7 4 0 | 56.376 |
| 1.6245M | 1 | 5 2 4 | 56.610 |
| 1.6245M | | 6 3 3 | 56.610 |
| 1.6183M | 1 | 6 5 1 | 56.846 |
| 1.6183M | | 3 0 5 | 56.846 |
| 1.6016 | 3 | 7 4 1 | 57.494 |
| 1.5978 | 3 | 8 3 0 | 57.647 |
| 1.5915M | 14 | 8 2 2 | 57.896 |
| 1.5915M | | 6 1 4 | 57.896 |
| 1.5522 | 2 | 4 4 4 | 59.508 |
| 1.5443M | 1 | 5 3 4 | 59.843 |
| 1.5443M | | 8 1 3 | 59.843 |
| 1.5297 | 2 | 5 5 3 | 60.470 |
| 1.5243M | 7 | 9 2 1 | 60.710 |
| 1.5243M | | 4 1 5 | 60.710 |
| 1.5138 | 7 | 6 6 0 | 61.177 |
| 1.5019 | 1 | 7 3 3 | 61.712 |
| 1.4888 | 1 | 7 1 4 | 62.313 |
| 1.4836M | 1 | 7 5 1 | 62.556 |
| 1.4836M | | 3 3 5 | 62.556 |
| 1.4708 | 4 | 10 1 1 | 63.165 |
| 1.4684 | 2 | 8 2 3 | 63.282 |
| 1.4543 | 1 | 9 3 0 | 63.965 |
| 1.4501 | 1 | 6 3 4 | 64.175 |
| 1.4330 | 1 | 9 3 1 | 65.032 |

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4261M | 3 | 6 6 2 | 65.386 |
| 1.4261M | | 7 2 4 | 65.386 |
| 1.4183 | 1 | 0 0 6 | 65.794 |
| 1.4141 | 2 | 7 4 3 | 66.010 |
| 1.4101M | 4 | 11 0 1 | 66.222 |
| 1.4101M | | 5 2 5 | 66.222 |
| 1.3757+ | 1 | 6 4 4 | 68.102 |
| 1.3757+ | | 10 0 3 | 68.102 |
| 1.3610M | 2 | 4 4 5 | 68.941 |
| 1.3610M | | 7 3 4 | 68.941 |
| 1.3504 | 1 | 9 0 4 | 69.558 |

# Rubidium Hydrogen Phosphate, $RbH_2PO_4$

Synonym
Rubidium dihydrogen orthophosphate

CAS registry no.
13774-16-8

Sample
The sample was made by adding $Rb_2CO_3$ to an 85% solution of $H_3PO_4$. The precipitate was washed with alcohol.

Color
Colorless

Structure
Tetragonal, $I\bar{4}2d$ (122). The structure was determined by Al-Karaghouli et al. (1978). Isostructural with $KH_2PO_4$.

Crystallographic constants of this sample
a = 7.6080(3) Å
c = 7.2979(6)

c/a = 0.9592

Z = 4
V = 422.42 $Å^3$
Density (calc) = 2.869 $g/cm^3$

Figure of merit
$F_{30}$ = 90.5(0.011,31)

Additional patterns
PDF card 30-1064 (Smith et al., 1979) (calculated pattern)
Nirsha et al. (1981)

References
Al-Karaghouli, A. R., Abdul-Wahab, B., Ajaj, E., and Sequeira, A. (1978). Acta Crystallogr. B34, 1040.

Nirsha, B. M., Budinitsa, E. N., Efremov, V. A., Zhadanov, B. V., Olikova, V. A., and Fakeer, A. A. (1981). Russ. J. Inorg. Chem. 26, 1560.

Smith, D. E. (1979). Ann. Report to Joint Committee on Powder Diffraction Standards.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.7 °C
Internal standards Ag, a = 4.08651 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.262 | 2 | 1 0 1 | 16.837 |
| 3.803 | 100 | 2 0 0 | 23.375 |
| 3.083 | 15 | 2 1 1 | 28.934 |
| 3.020 | 67 | 1 1 2 | 29.555 |
| 2.689 | 24 | 2 2 0 | 33.292 |
| 2.633 | 2 | 2 0 2 | 34.018 |
| 2.405 | 10 | 3 1 0 | 37.353 |
| 2.396 | 19 | 3 0 1 | 37.509 |
| 2.317 | 7 | 1 0 3 | 38.835 |
| 2.0265 | 15 | 3 2 1 | 44.682 |
| 2.0090 | 45 | 3 1 2 | 45.092 |
| 1.9790 | 8 | 2 1 3 | 45.815 |
| 1.9022 | 5 | 4 0 0 | 47.775 |
| 1.8248 | 1L | 0 0 4 | 49.938 |
| 1.7892 | 6 | 4 1 1 | 51.001 |
| 1.7009 | 12 | 4 2 0 | 53.858 |
| 1.6862 | 1L | 4 0 2 | 54.365 |
| 1.6447 | 7 | 2 0 4 | 55.854 |
| 1.6100 | 10 | 3 3 2 | 57.170 |
| 1.5941 | 2 | 3 2 3 | 57.790 |
| 1.5411 | 1L | 4 2 2 | 59.977 |
| 1.5095 | 6 | 2 2 4 | 61.367 |
| 1.4921 | 1 | 5 1 0 | 62.160 |
| 1.4892 | 1 | 4 3 1 | 62.295 |
| 1.4702 | 1L | 4 1 3 | 63.192 |
| 1.4532 | 1L | 3 1 4 | 64.022 |
| 1.4331 | 4 | 1 0 5 | 65.029 |
| 1.3870 | 2 | 5 2 1 | 67.472 |
| 1.3807 | 9 | 5 1 2 | 67.820 |
| 1.3451 | 4 | 4 4 0 | 69.873 |
| 1.3418 | 3 | 2 1 5 | 70.071 |
| 1.3166 | 7 | 4 0 4 | 71.618 |
| 1.3049 | 1L | 5 3 0 | 72.360 |
| 1.2896 | 1 | 4 3 3 | 73.355 |
| 1.2680 | 2 | 6 0 0 | 74.816 |
| 1.2441 | 7 | 4 2 4 | 76.506 |
| 1.2327 | 1 | 6 1 1 | 77.347 |
| 1.2284 | 7 | 5 3 2 | 77.669 |
| 1.2217 | 1L | 5 2 3 | 78.173 |
| 1.2029 | 4 | 6 2 0 | 79.637 |
| 1.2002 | 2 | 3 2 5 | 79.856 |
| 1.1976 | 1L | 6 0 2 | 80.059 |
| 1.1864 | 1 | 1 1 6 | 80.973 |
| 1.1730 | 1L | 5 4 1 | 82.093 |
| 1.1447 | 1L | 4 1 5 | 84.584 |
| 1.1124 | 1L | 6 1 3 | 87.647 |
| 1.0855 | 4 | 3 1 6 | 90.407 |
| 1.0827 | 4 | 4 4 4 | 90.711 |
| 1.0677 | 1 | 5 4 3 | 92.355 |
| 1.0551 | 2 | 6 4 0 | 93.790 |
| 1.0413 | 3 | 6 0 4 | 95.423 |
| 1.0344 | 1L | 7 2 1 | 96.257 |
| 1.0321 | 4 | 5 5 2 | 96.550 |
| 1.0279 | 1 | 6 3 3 | 97.075 |

# Rubidium Phosphate, $RbPO_3$

Synonym
Rubidium metaphosphate

Sample
The sample was prepared by heating $RbH_2PO_4$ at 250 °C for 17 hours.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14). The structure of $RbPO_3$ was determined by Corbridge (1956) and refined by Cruickshank (1964).

Crystallographic constants of this sample
a = 12.1221(14) Å
b = 4.2307(5)
c = 6.4773(9)
β = 95.980(11)°

a/b = 2.8652
c/b = 1.5310

Z = 4
V = 330.38 Å$^3$
Density (calc) = 3.306 g/cm$^3$

Figure of merit
$F_{30}$ = 123.3(0.0055,44)

Additional patterns
Majling et al. (1979) (calculated pattern)
Nirsha et al. (1981)


References
Corbridge, D. E. C. (1956). Acta Crystallogr. 9, 308.

Cruickshank, D. W. J. (1964). Acta Crystallogr. 17, 681.

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

Nirsha, B. M., Gudinitsa, E. N., Efremov, V. A., Zhadanov, B. V., Olikova, V. A., and Fakeev, A. A. (1981). Russ. J. Inorg. Chem. 26, 1560.


$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.6 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.025 | 1 | 2 0 0 | 14.690 |
| 5.944 | 1 | -1 0 1 | 14.891 |
| 3.994 | 8 | 1 1 0 | 22.241 |
| 3.582 | 31 | -3 0 1 | 24.839 |
| 3.536 | 19 | 0 1 1 | 25.164 |
| 3.463 | 68 | 2 1 0 | 25.704 |
| 3.447 | 50 | -1 1 1 | 25.822 |
| 3.342 | 13 | 1 1 1 | 26.651 |
| 3.260 | 72 | 3 0 1 | 27.338 |
| 3.220 | 72 | 0 0 2 | 27.681 |
| 3.129 | 100 | -2 1 1 | 28.501 |
| 3.014 | 24 | 4 0 0 | 29.617 |
| 2.976 | 55 | 2 1 1 | 30.003 |
| 2.914 | 10 | 3 1 0 | 30.657 |
| 2.5832 | 7 | 3 1 1 | 34.698 |
| 2.5623 | 8 | 0 1 2 | 34.991 |
| 2.4550 | 40 | 4 1 0 | 36.572 |
| 2.4326 | 37 | -2 1 2 | 36.922 |
| 2.3613 | 6 | -4 1 1 | 38.079 |
| 2.3398 | 6 | -5 0 1 | 38.443 |
| 2.3253 | 6 | -4 0 2 | 38.692 |
| 2.2918 | 13 | 2 1 2 | 39.281 |
| 2.2325 | 3 | 4 1 1 | 40.369 |
| 2.0946M | 26 | 5 1 0 | 43.155 |
| 2.0946M | | 4 0 2 | 43.155 |
| 2.0829 | 12 | 1 2 0 | 43.409 |
| 2.0773 | 11 | 1 0 3 | 43.533 |
| 2.0474 | 8 | -5 1 1 | 44.202 |
| 2.0369 | 8 | -4 1 2 | 44.442 |
| 2.0094M | 28 | 0 2 1 | 45.083 |
| 2.0094M | | 6 0 0 | 45.083 |
| 1.9958 | 1 | 2 2 0 | 45.406 |
| 1.9815 | 3 | -3 0 3 | 45.753 |
| 1.9408 | 1 | 5 1 1 | 46.769 |
| 1.9253 | 3 | -2 2 1 | 47.167 |
| 1.9153 | 4 | 0 1 3 | 47.430 |
| 1.8892 | 3 | 2 2 1 | 48.125 |
| 1.8716 | 15 | 3 2 0 | 48.607 |
| 1.8340 | 1 | -5 1 2 | 49.670 |
| 1.8157 | 5 | 6 1 0 | 50.206 |
| 1.7909M | 9 | -6 1 1 | 50.951 |
| 1.7909M | | -6 0 2 | 50.951 |
| 1.7779M | 2 | 2 1 3 | 51.350 |
| 1.7744M | 1 | 3 2 1 | 51.460 |
| 1.7637 | 1L | -1 2 2 | 51.793 |
| 1.7351 | 2 | 1 2 2 | 52.712 |
| 1.7086 | 3 | -7 0 1 | 53.595 |
| 1.6976 | 4 | -4 2 1 | 53.971 |
| 1.6937 | 4 | -5 0 3 | 54.103 |
| 1.6874 | 6 | 5 1 2 | 54.323 |
| 1.6706 | 4 | 2 2 2 | 54.915 |

## Rubidium Strontium Niobium Oxide, $RbSr_2(NbO_3)_5$

Synonym
Rubidium strontium niobate

Sample
The sample was prepared by heating $Rb_2CO_3$, $SrCO_3$, and $Nb_2O_5$ at 900 °C overnight, followed by heating at 1275 °C overnight with intermediate grindings.

Color
Colorless

Structure
Tetragonal, P4bm (100). Tungsten bronze type (Giess et al., 1969).

Crystallographic constants of this sample
a = 12.5127(7) Å
c = 3.9600(4)

c/a = 0.3165

Z = 2
V = 620.01 Å$^3$
Density (calc) = 5.172 g/cm$^3$

Figure of merit
$F_{30}$ = 75.7(0.0076,52)

Reference
Giess, E. A., Scott, B. A., Burns, G., O'Kane, D. F., and Segmüller, A. (1969). J. Am. Ceram. Soc. 52, 276.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26±2 °C
Internal standards Ag, a = 4.08651 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.86 | 1 | 1 1 0 | 9.971 |
| 6.263 | 3 | 2 0 0 | 14.129 |
| 3.961M | 22 | 0 0 1 | 22.428 |
| 3.961M | | 3 1 0 | 22.428 |
| 3.616 | 3 | 1 1 1 | 24.601 |
| 3.472 | 29 | 3 2 0 | 25.638 |
| 3.346 | 1 | 2 0 1 | 26.620 |
| 3.233 | 51 | 2 1 1 | 27.564 |
| 3.129 | 8 | 4 0 0 | 28.506 |
| 3.036 | 54 | 4 1 0 | 29.400 |
| 2.951 | 26 | 2 2 1 | 30.260 |
| 2.799M | 100 | 3 1 1 | 31.952 |
| 2.799M | | 4 2 0 | 31.952 |
| 2.610 | 17 | 3 2 1 | 34.327 |
| 2.455 | 2 | 4 0 1 | 36.574 |
| 2.4097 | 1 | 4 1 1 | 37.285 |
| 2.3233 | 5 | 5 2 0 | 38.727 |
| 2.2846 | 1 | 4 2 1 | 39.409 |
| 2.2110 | 1 | 4 4 0 | 40.779 |
| 2.1461 | 10 | 5 3 0 | 42.069 |
| 2.0851 | 3 | 6 0 0 | 43.361 |
| 1.9796 | 33 | 0 0 2 | 45.799 |
| 1.9538 | 2 | 5 4 0 | 46.440 |
| 1.9314 | 2 | 4 4 1 | 47.009 |
| 1.8867 | 3 | 5 3 1 | 48.193 |
| 1.8653 | 10 | 6 3 0 | 48.781 |
| 1.8455 | 8 | 6 0 1 | 49.340 |
| 1.7696M | 20 | 6 2 1 | 51.609 |
| 1.7696M | | 5 5 0 | 51.609 |
| 1.7524 | 11 | 5 4 1 | 52.154 |
| 1.7197 | 6 | 3 2 2 | 53.223 |
| 1.6874 | 7 | 6 3 1 | 54.323 |
| 1.6729 | 2 | 4 0 2 | 54.834 |
| 1.6583 | 14 | 4 1 2 | 55.356 |
| 1.6433 | 3 | 7 3 0 | 55.906 |
| 1.6158 | 29 | 5 5 1 | 56.943 |
| 1.5766 | 2 | 7 2 1 | 58.495 |
| 1.5520 | 2 | 7 4 0 | 59.516 |
| 1.5415 | 1L | 5 1 2 | 59.961 |
| 1.5173 | 6 | 8 2 0 | 61.018 |
| 1.5069 | 1 | 5 2 2 | 61.486 |
| 1.4849 | 1 | 6 5 1 | 62.500 |
| 1.4750M | 3 | 4 4 2 | 62.967 |
| 1.4750M | | 6 6 0 | 62.967 |
| 1.4646 | 5 | 8 3 0 | 63.465 |
| 1.4551 | 5 | 5 3 2 | 63.925 |
| 1.4452 | 1 | 7 4 1 | 64.420 |
| 1.4359 | 1L | 6 0 2 | 64.883 |
| 1.3994M | 5 | 6 2 2 | 66.797 |
| 1.3994M | | 8 4 0 | 66.797 |
| 1.3907 | 1 | 5 4 2 | 67.272 |
| 1.3736 | 4 | 8 3 1 | 68.219 |
| 1.3654 | 2 | 7 5 1 | 68.685 |
| 1.3577 | 5 | 6 3 2 | 69.133 |
| 1.3263 | 1 | 8 5 0 | 71.015 |
| 1.3194M | 7 | 7 1 2 | 71.441 |
| 1.3194M | | 8 4 1 | 71.441 |
| 1.2846 | 2 | 2 1 3 | 73.689 |
| 1.2705 | 2 | 9 4 0 | 74.645 |
| 1.2646 | 3 | 7 3 2 | 75.051 |

# Sodium Antimony Fluoride, $NaSbF_4$

Synonyms
Sodium fluoantimonite
Sodium antimony tetrafluoride

Sample
The sample was from Harshaw Chemical Co., Cleveland, Ohio. There were a number of impurity lines, the strongest being at d = 3.20, 4.91, and 4.20 with relative intensities of 5, 6, and 12, respectively. Because of the impurity, the intensities may be somewhat in error.

Color
Colorless

Optical data
Biaxial (-) $N_\alpha = 1.475$, $N_\beta = 1.521$, $N_\gamma = 1.540$. 2V is about 75° (Byström et al., 1953)

Structure
Monoclinic, $P2_1$ (4). The structure of $NaSbF_4$ was determined by Byström et al. (1953). The authors gave the space group as $P2_1$ or $P2_1/a$. $P2_1$ indexed our data more completely than $P2_1/a$.

Crystallographic constants of this sample
a = 8.5749(12) Å
b = 5.5299(10)
c = 8.0703(9)
β = 94.089(14)°

Z = 4
V = 381.71 $Å^3$
Density (calc) = 3.841 $g/cm^3$

Figure of merit
$F_{30} = 68.2(0.0088,50)$

Reference
Byström, A., Bäcklund, S., and Wilhelmi, K.-A. (1953). Ark. Kemi 6, 77.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26.5 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.05 | 22 | 0 0 1 | 10.983 |
| 4.643 | 21 | 1 1 0 | 19.100 |
| 4.554 | 93 | 0 1 1 | 19.475 |
| 4.273 | 19 | 2 0 0 | 20.771 |
| 4.092 | 8 | -1 1 1 | 21.702 |
| 4.022 | 59 | 0 0 2 | 22.083 |
| 3.959 | 2 | 1 1 1 | 22.440 |
| 3.890 | 23 | -2 0 1 | 22.840 |
| 3.669 | 47 | 2 0 1 | 24.239 |
| 3.381 | 100 | 2 1 0 | 26.338 |
| 3.254 | 94 | 0 1 2 | 27.383 |
| 3.184 | 16 | -2 1 1 | 28.004 |
| 3.041 | 21 | -2 0 2 | 29.345 |
| 2.985 | 3 | 1 1 2 | 29.907 |
| 2.832 | 9 | 2 0 2 | 31.571 |
| 2.765 | 10 | 0 2 0 | 32.349 |
| 2.747 | 3 | -3 0 1 | 32.573 |
| 2.684 | 9 | 0 0 3 | 33.361 |
| 2.666 | 3 | -2 1 2 | 33.590 |
| 2.631M | 6 | 1 2 0 | 34.049 |
| 2.631M | | 3 0 1 | 34.049 |
| 2.520 | 18 | 2 1 2 | 35.595 |
| 2.415 | 2 | 0 1 3 | 37.201 |
| 2.375 | 10 | 3 1 1 | 37.856 |
| 2.363 | 8 | -1 1 3 | 38.052 |
| 2.349 | 5 | -2 0 3 | 38.280 |
| 2.285 | 5 | 1 1 3 | 39.398 |
| 2.2790 | 6 | 0 2 2 | 39.510 |
| 2.2545 | 17 | -2 2 1 | 39.957 |
| 2.2241 | 15 | -1 2 2 | 40.528 |
| 2.2095M | 10 | -3 1 2 | 40.808 |
| 2.2095M | | 2 2 1 | 40.808 |
| 2.1629 | 20 | -2 1 3 | 41.726 |
| 2.1388 | 20 | 4 0 0 | 42.219 |
| 2.0463M | 44 | 2 1 3 | 44.227 |
| 2.0463M | | -2 2 2 | 44.227 |
| 2.0123 | 13 | 0 0 4 | 45.015 |
| 1.9903 | 6 | -1 0 4 | 45.538 |
| 1.9779 | 15 | 2 2 2 | 45.841 |
| 1.9669 | 10 | -4 1 1 | 46.111 |
| 1.9256 | 9 | 0 2 3 | 47.161 |
| 1.9067 | 9 | 4 1 1 | 47.655 |
| 1.8916 | 22 | 0 1 4 | 48.062 |
| 1.8731M | 5 | -1 1 4 | 48.565 |
| 1.8731M | | -2 0 4 | 48.565 |
| 1.8585 | 3 | 1 2 3 | 48.973 |
| 1.8360 | 21 | -4 1 2 | 49.614 |
| 1.8164 | 3 | -3 2 2 | 50.184 |
| 1.7955 | 3 | 0 3 1 | 50.809 |
| 1.7741 | 17 | -2 1 4 | 51.466 |

## Sodium Barium Niobium Oxide, $NaBa_2(NbO_3)_5$

Synonym
B-S-N

Sample
The sample was obtained from Johnson Matthey Chemicals Limited, Royston, Hertfordshire, UK.

Chemical analysis
Analysis given by the manufacturer: parts per million Mg-10, Ca-2, Al, Fe, Si, and Ag - less than 1.

Structure
Tetragonal. Bobb et al. (1969) reported this phase as orthorhombic (Ccc2), with a and b very nearly equal. Our sample showed no definitive departure from tetragonal. It is a distorted tungsten bronze structure with the c axis doubled. Barns (1968) reported the phase as orthorhombic, with a and b equal.

Crystallographic constants of this sample
a = 17.609(2) Å
c = 7.987(2)

c/a = 0.4536

Z = 8
V = 2476.58 $Å^3$
Density (calc) = 5.376 $g/cm^3$

Figure of merit
$F_{30}$ = 20.0(0.0094,160)

Polymorphism
Above ~290 °C this composition is truly tetragonal (Abell et al., 1973).

Additional patterns
PDF card 27-1408 (Abell et al., 1973)
PDF card 27-1409 (Cook, W., Priv. Com.)
PDF card 23-654 (Barns, 1968)

References
Abell, J. S., Harris, I. R., and Cockayne, B. (1973). J. Mater. Sci. 8, 667.

Barns, R. L. (1968). J. Appl. Crystallogr. 1, 290.

Bobb, L. C., Lefkowitz, I., and Muldauer, L. (1969). J. Appl. Crystallogr. 2, 189.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.8 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 8.81 | 1L | 2 | 0 | 0 | 10.034 |
| 6.229 | 2 | 2 | 2 | 0 | 14.208 |
| 5.573 | 6 | 3 | 1 | 0 | 15.891 |
| 3.994 | 19 | 0 | 0 | 2 | 22.241 |
| 3.939 | 11 | 4 | 2 | 0 | 22.555 |
| 3.454 | 32 | 5 | 1 | 0 | 25.775 |
| 3.361 | 15 | 2 | 2 | 2 | 26.498 |
| 3.245 | 89 | 3 | 1 | 2 | 27.466 |
| 3.113 | 4 | 4 | 4 | 0 | 28.653 |
| 3.020 | 100 | 5 | 3 | 0 | 29.556 |
| 2.957 | 23 | 4 | 0 | 2 | 30.195 |
| 2.933 | 26 | 6 | 0 | 0 | 30.452 |
| 2.897 | 3 | 6 | 1 | 0 | 30.839 |
| 2.804 | 87 | 4 | 2 | 2 | 31.894 |
| 2.612 | 23 | 5 | 1 | 2 | 34.305 |
| 2.455 | 9 | 4 | 4 | 2 | 36.566 |
| 2.410 | 2 | 5 | 3 | 2 | 37.288 |
| 2.363 | 4 | 6 | 0 | 2 | 38.052 |
| 2.313 | 8 | 7 | 3 | 0 | 38.908 |
| 2.1363 | 13 | 8 | 2 | 0 | 42.272 |
| 2.0752 | 4 | 6 | 6 | 0 | 43.579 |
| 2.0471 | 1L | 7 | 5 | 0 | 44.208 |
| 1.9955 | 2 | 8 | 3 | 1 | 45.414 |
| 1.9687 | 27 | 8 | 4 | 0 | 46.068 |
| 1.9451 | 1L | 9 | 1 | 0 | 46.660 |
| 1.8806 | 3 | 3 | 1 | 4 | 48.360 |
| 1.8554 | 11 | 9 | 3 | 0 | 49.059 |
| 1.8417 | 11 | 6 | 6 | 2 | 49.450 |
| 1.7802 | 1 | 4 | 2 | 4 | 51.279 |
| 1.7606 | 32 | 8 | 6 | 0 | 51.892 |
| 1.7464 | 18 | 7 | 3 | 3 | 52.346 |
| 1.7259 | 5 | 10 | 2 | 0 | 53.016 |
| 1.7093 | 2 | 9 | 5 | 0 | 53.570 |
| 1.6811 | 10 | 4 | 4 | 4 | 54.543 |
| 1.6654M | 21 | 8 | 2 | 3 | 55.100 |
| 1.6654M | | 5 | 3 | 4 | 55.100 |
| 1.6515 | 6 | 6 | 0 | 4 | 55.606 |
| 1.6228M | 7 | 7 | 5 | 3 | 56.675 |
| 1.6228M | | 6 | 2 | 4 | 56.675 |
| 1.6108 | 18 | 8 | 6 | 2 | 57.138 |
| 1.5952 | 1L | 9 | 6 | 1 | 57.746 |
| 1.5833 | 1 | 8 | 4 | 3 | 58.224 |
| 1.5724M | 4 | 9 | 5 | 2 | 58.666 |
| 1.5724M | | 2 | 0 | 5 | 58.666 |
| 1.5565 | 2 | 8 | 8 | 0 | 59.324 |

# Sodium Germanium Phosphate, $NaGe_2(PO_4)_3$

Synonym
Sodium germanium orthophosphate

CAS registry no.
22239-25-4

Sample
The sample was made by heating a 1:4:6 molar mixture of $Na_2CO_3$, $GeO_2$, and $(NH_4)_2HPO_4$ up to 500 °C. Then it was reground and heated at 1050 °C overnight.

Color
Colorless

Structure
Rhombohedral, R**. This phase was reported to be isostructural with $NaZr_2(PO_4)_3$ in space group $R\bar{3}c$ (Hagman and Kierkegaard, 1968). However several lines could not be indexed on that space group.

Crystallographic constants of this sample (Hexagonal axes)
a = 8.0894(6) Å
c = 21.522(3)

c/a = 2.6605

Z = 6
V = 1219.68 Å$^3$
Density (calc) = 3.701 g/cm$^3$

Figure of merit
$F_{30}$ = 62.9(0.010,46)

Additional pattern
PDF card 22-1219 (Hagman and Kierkegaard, 1968)

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

$CuK\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.869 | 25 | 0 1 2 | 15.083 |
| 4.265 | 68 | 1 0 4 | 20.809 |
| 4.044 | 83 | 1 1 0 | 21.960 |
| 3.524 | 100 | 1 1 3 | 25.255 |
| 3.326 | 1 | 2 0 2 | 26.784 |
| 2.936 | 57 | 0 2 4 | 30.418 |
| 2.717 | 1L | 2 0 5 | 32.946 |
| 2.684 | 88 | 1 1 6 | 33.357 |
| 2.629 | 15 | 2 1 1 | 34.082 |
| 2.570 | 2 | 1 2 2 | 34.882 |
| 2.511 | 4 | 0 1 8 | 35.732 |
| 2.375 | 11 | 2 1 4 | 37.844 |
| 2.336 | 29 | 3 0 0 | 38.508 |
| 2.311 | 1 | 0 2 7 | 38.938 |
| 2.221 | 7 | 3 0 3 | 40.590 |
| 2.1331 | 5 | 2 0 8 | 42.337 |
| 2.0587M | 8 | 1 1 9 | 43.946 |
| 2.0587M | | 1 0 10 | 43.946 |
| 2.0215 | 4 | 2 2 0 | 44.797 |
| 2.0073 | 3 | 2 1 7 | 45.133 |
| 1.9573 | 10 | 3 0 6 | 46.352 |
| 1.9133 | 3 | 3 1 2 | 47.483 |
| 1.8868 | 16 | 1 2 8 | 48.190 |
| 1.8335 | 9 | 0 2 10 | 49.685 |
| 1.8273 | 11 | 1 3 4 | 49.864 |
| 1.7941 | 3 | 0 0 12 | 50.854 |
| 1.7617 | 26 | 2 2 6 | 51.858 |
| 1.7286 | 3 | 0 4 2 | 52.925 |
| 1.6698 | 17 | 2 1 10 | 54.943 |
| 1.6424 | 4 | 1 3 7 | 55.941 |
| 1.6027 | 1 | 3 2 1 | 57.452 |
| 1.5749 | 10 | 3 1 8 | 58.562 |
| 1.5399 | 10 | 3 2 4 | 60.030 |
| 1.5287 | 16 | 4 1 0 | 60.515 |
| 1.5062 | 5 | 2 3 5 | 61.515 |
| 1.5018 | 4 | 0 1 14 | 61.716 |
| 1.4953 | 1 | 4 1 3 | 62.017 |
| 1.4674 | 5 | 0 4 8 | 63.327 |
| 1.4421 | 12 | 1 3 10 | 64.572 |
| 1.4240 | 4 | 3 2 7 | 65.496 |
| 1.4219 | 1 | 3 0 12 | 65.602 |
| 1.4063 | 15 | 4 1 6 | 66.427 |
| 1.3797 | 2 | 2 3 8 | 67.875 |
| 1.3586 | 6 | 4 0 10 | 69.081 |
| 1.3554 | 5 | 0 5 4 | 69.266 |

| d(Å) | $I^{rel}$ $\sigma = \pm 1$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.3525 | 5 | 1 1 15 | 69.436 |
| 1.3480 | 8 | 3 3 0 | 69.699 |
| 1.3293 | 6 | 1 2 14 | 70.826 |
| 1.3213 | 1L | 2 4 1 | 71.319 |
| 1.2880 | 4 | 4 1 9 | 73.463 |
| 1.2657 | 1L | 4 2 5 | 74.975 |

# Sodium Iron Silicate (Acmite), $NaFe(SiO_3)_2$

Synonyms
Sodium iron metasilicate
Aegirine
Aegirite

CAS registry no.
14483-20-6

Sample
The sample was made by heating $Na_2CO_3$, $Fe_2O_3$, and $SiO_2$ for about 10 days at temperatures up to 950 °C. The sample contained a small amount of $Fe_2O_3$.

Color
Deep brown

Structure
Monoclinic, I2/a (15). Clinopyroxene type (Nolan and Edgar, 1963) (Frondel and Klein, 1965). The structure of acmite was determined by Clark et al. (1969).

Crystallographic constants of this sample
a = 9.5277(14) Å
b = 8.8067(14)
c = 5.287(1)
β = 104.686(13)°

a/b = 1.0819
c/b = 0.6003

Z = 4
V = 429.13 $Å^3$
Density (calc) = 3.576 $g/cm^3$

Figure of merit
$F_{30}$ = 53.3(0.011,51)

Additional patterns
PDF card 18-1222 (Frondel and Klein, 1965) Nat. Min.
PDF card 31-1309 (Nickel and Mark, 1965) Nat. Min.
Borg and Smith (1969)
Brown (1982)

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.7 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.37 | 21 | 1 1 0 | 13.887 |
| 4.609 | 1 | 2 0 0 | 19.242 |
| 4.423 | 29 | 0 1 1 | 20.058 |
| 3.613 | 9 | -2 1 1 | 24.620 |
| 3.185 | 6 | 2 2 0 | 27.994 |
| 2.985 | 100 | 1 2 1 | 29.914 |
| 2.901 | 50 | 3 1 0 | 30.799 |
| 2.798 | 1 | 1 3 0 | 31.965 |
| 2.546 | 28 | 0 3 1 | 35.228 |
| 2.523 | 45 | -2 0 2 | 35.550 |
| 2.473 | 37 | -3 2 1 | 36.303 |
| 2.256 | 3 | -4 1 1 | 39.926 |
| 2.212 | 8 | 0 2 2 | 40.767 |
| 2.196 | 20 | -3 1 2 | 41.061 |
| 2.190 | 7 | -2 2 2 | 41.185 |
| 2.118 | 20 | 2 3 1 | 42.650 |
| 2.094 | 12 | 3 2 1 | 43.160 |
| 2.0294 | 10 | 2 0 2 | 44.613 |
| 2.0186 | 10 | -1 4 1 | 44.865 |
| 1.9796 | 7 | -4 0 2 | 45.800 |
| 1.9341 | 5 | 1 4 1 | 46.940 |
| 1.8807 | 2 | 4 1 1 | 48.357 |
| 1.8262 | 2 | -4 3 1 | 49.897 |
| 1.8045M | 1 | -4 2 2 | 50.538 |
| 1.8045M | | 5 1 0 | 50.538 |
| 1.7732 | 1 | -3 4 1 | 51.497 |
| 1.7403 | 2 | -5 2 1 | 52.542 |
| 1.7303 | 9 | 1 5 0 | 52.870 |
| 1.7244 | 7 | 3 1 2 | 53.066 |
| 1.6829 | 2 | -5 1 2 | 54.481 |
| 1.6588 | 4 | -2 4 2 | 55.339 |
| 1.6327 | 11 | -1 2 3 | 56.301 |
| 1.6104 | 12 | 4 3 1 | 57.151 |
| 1.5915 | 6 | 4 4 0 | 57.893 |
| 1.5362 | 7 | 6 0 0 | 60.191 |
| 1.5295 | 9 | 4 0 2 | 60.479 |

References

Borg, I. Y. and Smith, D. K. (1969). Geological Society of America Inc., Memoir 122, Boulder, CO.

Brown, I. W. (1982). J. Non Cryst. Solids 50, 233.

Clark, J., Appleman, D. E., and Papike, J. J. (1969). Contrib. Mineral. Petrol., 20, 81.

Frondel, C. and Klein, C. (1965). Science (Washington, D.C.), 149, 742.

Nickel, E. H. and Mark, E. (1965). Can. Mineral. 8, 185.

Nolan, J. and Edgar, A. D. (1963). Mineral. Mag. J. Mineral. Soc. 33, 634.

# Sodium Molybdenum Oxide Hydrate, $Na_2MoO_4 \cdot 2H_2O$

Synonym
Sodium molybdate hydrate

CAS registry no.
10102-40-6

Sample
The sample was obtained from the General Chemical Division of Allied Chemical, Morristown, NJ.

Color
Colorless

Structure
Orthorhombic, Pcab (61) (Pistorius, 1960). The structure of $Na_2MoO_4 \cdot 2H_2O$ was determined by Matsumato et al. (1975).

Crystallographic constants of this sample
a = 10.566(2) Å
b = 13.842(2)
c = 8.4823(15)

a/b = 0.7633
c/b = 0.6128

Z = 8
V = 1240.65 Å$^3$
Density (calc) 2.591 g/cm$^3$

Figure of merit
$F_{30}$ = 44.4(0.012,59)

Additional pattern
PDF card 13-236 (Pistorius, 1960)

References
Matsumato, K., Kobayashi, A., and Sasaki, Y. (1975). Bull. Chem. Soc. Jpn. 48, 1009.

Pistorius, C. W. F. T. (1960). Z. Kristallogr. 114, 154.

$CuK\alpha_1$ $\lambda$ = 1.540598 Å; mean T = 23.3 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.92 | 100 | 0 2 0 | 12.775 |
| 5.973 | 10 | 1 1 1 | 14.820 |
| 5.285 | 10 | 2 0 0 | 16.761 |
| 4.785 | 8 | 1 2 1 | 18.528 |
| 4.262 | 17 | 2 1 1 | 20.824 |
| 4.244 | 32 | 0 0 2 | 20.917 |
| 4.202 | 34 | 2 2 0 | 21.125 |
| 3.783M | 11 | 1 1 2 | 23.497 |
| 3.783M | | 1 3 1 | 23.497 |
| 3.615 | 45 | 0 2 2 | 24.607 |
| 3.462 | 7 | 0 4 0 | 25.712 |
| 3.421 | 6 | 1 2 2 | 26.022 |
| 3.309 | 41 | 2 0 2 | 26.920 |
| 3.215M | 14 | 2 1 2 | 27.726 |
| 3.215M | | 2 3 1 | 27.726 |
| 3.168 | 63 | 3 1 1 | 28.149 |
| 3.064 | 31 | 1 4 1 | 29.125 |
| 2.994 | 18 | 1 3 2 | 29.820 |
| 2.983 | 42 | 2 2 2 | 29.927 |
| 2.895 | 15 | 2 4 0 | 30.866 |
| 2.740 | 7 | 2 4 1 | 32.656 |
| 2.679M | 25 | 0 4 2 | 33.418 |
| 2.679M | | 1 1 3 | 33.418 |
| 2.660M | 14 | 3 1 2 | 33.669 |
| 2.660M | | 3 3 1 | 33.669 |
| 2.598 | 7 | 1 4 2 | 34.495 |
| 2.553 | 1 | 1 5 1 | 35.120 |
| 2.453 | 5 | 2 1 3 | 36.611 |
| 2.390 | 4 | 2 4 2 | 37.607 |
| 2.356 | 7 | 2 5 1 | 38.165 |
| 2.349 | 7 | 1 3 3 | 38.284 |
| 2.308 | 1 | 0 6 0 | 38.991 |
| 2.265 | 1 | 1 5 2 | 39.772 |
| 2.214M | 1 | 4 1 2 | 40.730 |
| 2.214M | | 4 3 1 | 40.730 |
| 2.177M | 16 | 1 6 1 | 41.445 |
| 2.177M | | 3 1 3 | 41.445 |
| 2.144 | 2 | 1 4 3 | 42.119 |
| 2.121 | 4 | 0 0 4 | 42.591 |
| 2.114 | 6 | 2 6 0 | 42.738 |
| 2.108 | 2 | 3 5 1 | 42.867 |
| 2.102M | 1 | 3 2 3 | 43.003 |
| 2.102M | | 4 4 0 | 43.003 |
| 2.0514 | 1 | 2 6 1 | 44.110 |
| 2.0382 | 7 | 4 4 1 | 44.412 |

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 2.0294 | 17 | 5 1 1 | 44.613 |
| 1.9908M | 11 | 1 2 4 | 45.528 |
| 1.9908M | | 1 6 2 | 45.528 |
| 1.9687 | 3 | 2 0 4 | 46.067 |
| 1.8927M | 12 | 2 2 4 | 48.032 |
| 1.8927M | | 2 6 2 | 48.032 |
| 1.8810M | 7 | 3 6 1 | 48.348 |
| 1.8810M | | 4 4 2 | 48.348 |
| 1.8747M | 9 | 5 1 2 | 48.523 |
| 1.8747M | | 5 3 1 | 48.523 |
| 1.8597M | 1 | 3 4 3 | 48.940 |
| 1.8597M | | 4 2 3 | 48.940 |
| 1.8525 | 1 | 2 5 3 | 49.140 |
| 1.8081 | 4 | 0 4 4 | 50.431 |
| 1.8033 | 2 | 5 4 0 | 50.574 |
| 1.7809 | 5 | 4 3 3 | 51.257 |
| 1.7619M | 6 | 1 6 3 | 51.851 |
| 1.7619M | | 6 0 0 | 51.851 |
| 1.7426 | 5 | 4 5 2 | 52.470 |
| 1.7240M | 3 | 3 5 3 | 53.077 |
| 1.7240M | | 6 0 1 | 53.077 |
| 1.7104M | 3 | 6 1 1 | 53.533 |
| 1.7104M | | 2 4 4 | 53.533 |
| 1.6942 | 2 | 2 6 3 | 54.088 |
| 1.6798 | 13 | 5 1 3 | 54.588 |
| 1.6728 | 12 | 6 2 1 | 54.835 |
| 1.6634M | 1 | 1 1 5 | 55.172 |
| 1.6634M | | 1 5 4 | 55.172 |
| 1.6479 | 2 | 5 5 1 | 55.738 |
| 1.6436M | 1 | 2 8 0 | 55.896 |
| 1.6436M | | 5 2 3 | 55.896 |

## Sodium Strontium Niobium Oxide, $NaSr_2(NbO_3)_5$

Synonym
Sodium strontium niobate

Sample
The sample was made by heating $NaNbO_3$, $SrCO_3$, and $Nb_2O_5$ up to 1300 °C for about 48 hours, with intermediate grindings.

Color
Colorless

Structure
Tetragonal. Tungsten bronze structure (Morin, 1973). This phase has been reported as orthorhombic (Giess et al., 1969) but this work found no evidence for symmetry lower than tetragonal. This phase occurs in the region of the $NaNbO_3$-$SrNb_2O_6$ system from 65 to 79% $SrNb_2O_6$ and changes cell size little over the region (Morin, 1973).

Crystallographic constants of this sample
$a = 12.3562(9)$ Å
$c = 3.8979(6)$

$c/a = 0.3155$

$Z = 2$
$V = 595.11$ Å$^3$
Density (calc) = 5.038 g/cm$^3$

Figure of merit
$F_{30} = 57.3(0.011,50)$

Polymorphism
Van Uitert (1968) reports that $NaSr_2Nb_5O_{15}$ is stable as tetragonal only above 184 °C.

Additional pattern
PDF card 27-787 (Morin, Priv. Comm., 1974). The composition given was $Na_{0.18}Sr_{0.41}NbO_3$.

References
Giess, E. A., Scott, B. A., Burns, G., O'Kane, D. F., and Segmüller, A. (1969). J. Am. Ceram. Soc. 52, 276.

Morin, D., Colin, J.-P., LeRoux, G., Pateau, L., and Toledano, J.-C. (1973). Mater. Res. Bull. 8, 1189.

Van Uitert, L. G., Levinstein, H. J., Rubin, J. J., Capio, C. D., Dearborn, E. F., and Bonner, W. A. (1968). Mater. Res. Bull. 3, 47.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 26.1 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.184 | 1 | 2 0 0 | 14.312 |
| 5.526 | 1 | 2 1 0 | 16.025 |
| 4.369 | 1 | 2 2 0 | 20.312 |
| 3.899 | 45 | 0 0 1 | 22.789 |
| 3.556 | 2 | 1 1 1 | 25.022 |
| 3.426 | 32 | 3 2 0 | 25.989 |
| 3.297 | 2 | 2 0 1 | 27.025 |
| 3.185 | 47 | 2 1 1 | 27.992 |
| 3.088 | 8 | 4 0 0 | 28.887 |
| 2.996 | 62 | 4 1 0 | 29.795 |
| 2.909 | 23 | 2 2 1 | 30.711 |
| 2.760 | 100 | 3 1 1 | 32.414 |
| 2.574 | 25 | 3 2 1 | 34.831 |
| 2.421 | 5 | 4 0 1 | 37.101 |
| 2.376 | 2 | 4 1 1 | 37.841 |
| 2.295 | 4 | 5 2 0 | 39.232 |
| 2.255 | 2 | 4 2 1 | 39.952 |
| 2.185 | 1L | 4 4 0 | 41.287 |
| 2.1186 | 7 | 5 3 0 | 42.641 |
| 2.0591M | 1 | 6 0 0 | 43.936 |
| 2.0591M | | 5 1 1 | 43.936 |
| 2.0312 | 2 | 6 1 0 | 44.572 |
| 1.9774 | 1 | 5 2 1 | 45.854 |
| 1.9546 | 9 | 6 2 0 | 46.419 |
| 1.9491 | 23 | 0 0 2 | 46.558 |
| 1.9314 | 1 | 5 4 0 | 47.011 |
| 1.9064 | 1 | 4 4 1 | 47.664 |
| 1.8608 | 2 | 5 3 1 | 48.908 |
| 1.8421 | 12 | 6 3 0 | 49.437 |
| 1.8206 | 9 | 6 0 1 | 50.060 |
| 1.7606 | 4 | 3 0 2 | 51.890 |
| 1.7470M | 33 | 5 5 0 | 52.326 |
| 1.7470M | | 6 2 1 | 52.326 |
| 1.7295 | 12 | 5 4 1 | 52.896 |
| 1.6943 | 8 | 3 2 2 | 54.085 |
| 1.6656 | 9 | 6 3 1 | 55.095 |
| 1.6479 | 2 | 4 0 2 | 55.736 |
| 1.6336 | 17 | 4 1 2 | 56.268 |
| 1.6197 | 3 | 3 3 2 | 56.794 |
| 1.6080 | 4 | 7 0 1 | 57.246 |

| d(Å) | $I^{rel}$ $\sigma = \pm 4$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.5943 | 37 | 5 5 1 | 57.783 |
| 1.5560 | 2 | 7 2 1 | 59.345 |
| 1.5450 | 1 | 8 0 0 | 59.810 |
| 1.5324 | 1 | 7 4 0 | 60.355 |
| 1.4983M | 5 | 8 2 0 | 61.875 |
| 1.4983M | | 7 3 1 | 61.875 |
| 1.4856 | 1 | 5 2 2 | 62.464 |
| 1.4657 | 1L | 6 5 1 | 63.410 |
| 1.4558 | 1 | 6 6 0 | 63.892 |
| 1.4548 | 1 | 4 4 2 | 63.942 |
| 1.4464 | 2 | 8 3 0 | 64.355 |
| 1.4344 | 3 | 5 3 2 | 64.961 |
| 1.3983 | 1 | 8 2 1 | 66.854 |
| 1.3796 | 4 | 6 2 2 | 67.884 |
| 1.3714 | 1 | 5 4 2 | 68.346 |
| 1.3638 | 1L | 6 6 1 | 68.777 |
| 1.3554 | 3 | 8 3 1 | 69.266 |
| 1.3482 | 1L | 7 5 1 | 69.688 |
| 1.3387 | 4 | 6 3 2 | 70.256 |

# Strontium Aluminum Oxide, $SrAl_2O_4$

Synonym
Strontium aluminate

CAS registry no.
12004-37-4

Sample
One mole of $SrCO_3$ was reacted with two moles of $Al(OH)_3$ by heating from 500° to 1000 °C where it was held for 3 hours, then at 1500 °C for 40 hours. The sample was ground and heated at 550 °C for 7 hours.

Color
Colorless

Structure
Monoclinic, P*/*. The cell was found by use of the Visser program. A unit cell given by Ito et al. (1977) was that of a supercell with four times the volume of the Visser cell.

Crystallographic constants of this sample
a = 8.4424(8) Å
b = 8.8221(10)
c = 5.1607(6)
β = 93.415(6)°

a/b = 0.9570
c/b = 0.5850

Z = 4
V = 383.68 Å$^3$
Density (calc) = 3.559 g/cm$^3$

Figures of merit
$F_{30}$ = 83.1(0.0071,51)
$M_{20}$ = 47.6

Polymorphism
There is a hexagonal phase formed above 650 °C (Ito et al., 1977)

Additional pattern
PDF card 9-39 (Carlson, 1955)

References
Carlson, E. (1955). J. Res. Natl. Bur. Stand. 54, 332.

Ito, S., Banno, S., Suzuki, K., and Inagaki, M. (1977). Z. Phys. Chem. Wiesbaden 105, 173.

CuK$\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C
Internal standard Ag, a = 4.08651 Å

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.094 | 9 | 1 1 0 | 14.523 |
| 5.153 | 5 | 0 0 1 | 17.195 |
| 4.447 | 52 | 0 1 1 | 19.952 |
| 4.413 | 27 | 0 2 0 | 20.104 |
| 4.019 | 13 | -1 1 1 | 22.102 |
| 3.907 | 19 | 1 2 0 | 22.741 |
| 3.852 | 12 | 1 1 1 | 23.069 |
| 3.802 | 4 | 2 1 0 | 23.377 |
| 3.351 | 3 | 0 2 1 | 26.580 |
| 3.142 | 100 | -2 1 1 | 28.387 |
| 3.048 | 91 | 2 2 0 | 29.276 |
| 2.984 | 76 | 2 1 1 | 29.923 |
| 2.675 | 3 | 3 1 0 | 33.466 |
| 2.575 | 33 | 0 0 2 | 34.807 |
| 2.5536 | 69 | 0 3 1 | 35.114 |
| 2.5057 | 2 | -1 0 2 | 35.807 |
| 2.4633 | 13 | -1 3 1 | 36.445 |
| 2.4324 | 12 | -3 1 1 | 36.925 |
| 2.4246 | 16 | 1 3 1 | 37.048 |
| 2.4094 | 11 | -1 1 2 | 37.291 |
| 2.3685 | 4 | 3 2 0 | 37.959 |
| 2.3366 | 4 | 1 1 2 | 38.497 |
| 2.3214 | 4 | 3 1 1 | 38.759 |
| 2.2577 | 4 | -2 0 2 | 39.898 |
| 2.2241 | 15 | 0 2 2 | 40.527 |
| 2.2130 | 16 | -2 3 1 | 40.739 |
| 2.2062 | 14 | 0 4 0 | 40.871 |
| 2.1957 | 13 | -3 2 1 | 41.076 |
| 2.1563 | 14 | 2 3 1 | 41.861 |
| 2.1415 | 7 | 2 0 2 | 42.164 |
| 2.1068 | 21 | 4 0 0 | 42.893 |
| 2.0818 | 1L | 2 1 2 | 43.432 |
| 2.0500 | 1L | 4 1 0 | 44.142 |
| 2.0307 | 5 | 3 3 0 | 44.584 |
| 2.0102 | 9 | -2 2 2 | 45.063 |
| 1.9922 | 2 | -4 0 1 | 45.494 |
| 1.9811 | 2 | -1 4 1 | 45.763 |
| 1.9541 | 17 | 2 4 0 | 46.432 |
| 1.9439 | 6 | -4 1 1 | 46.689 |
| 1.9380 | 5 | 0 3 2 | 46.840 |
| 1.9261 | 23 | 2 2 2 | 47.146 |
| 1.9111 | 6 | -3 1 2 | 47.539 |
| 1.9014 | 7 | 4 2 0 | 47.798 |
| 1.8676 | 12 | 4 1 1 | 48.718 |
| 1.8450 | 2 | 3 0 2 | 49.356 |

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.8155 | 3 | -4 2 1 | 50.211 |
| 1.7891 | 3 | -3 2 2 | 51.004 |
| 1.7344 | 4 | 3 4 0 | 52.736 |
| 1.7013 | 3 | 3 2 2 | 53.845 |
| 1.6804 | 5 | -4 0 2 | 54.567 |
| 1.6757 | 5 | 0 4 2 | 54.734 |
| 1.6688 | 6 | 0 5 1 | 54.978 |
| 1.6557 | 7 | 5 1 0 | 55.450 |
| 1.6505 | 6 | -4 1 2 | 55.640 |
| 1.6293 | 8 | -3 3 2 | 56.428 |
| 1.6021 | 11 | 4 3 1 | 57.477 |
| 1.5975 | 10 | -2 1 3 | 57.657 |
| 1.5884 | 4 | -1 2 3 | 58.018 |
| 1.5851 | 6 | 4 0 2 | 58.152 |
| 1.5780 | 6 | -2 4 2 | 58.439 |
| 1.5741 | 6 | 5 0 1 | 58.595 |
| 1.5704 | 6 | -4 2 2 | 58.747 |
| 1.5623 | 8 | -2 5 1 | 59.082 |
| 1.5496 | 2 | 5 1 1 | 59.615 |
| 1.5417 | 7 | 2 5 1 | 59.954 |
| 1.5343 | 12 | 2 1 3 | 60.270 |
| 1.5234 | 5 | 4 4 0 | 60.750 |
| 1.5055 | 2 | -3 0 3 | 61.550 |
| 1.4913 | 4 | 4 2 2 | 62.197 |
| 1.4825 | 13 | 5 2 1 | 62.610 |
| 1.4791 | 8 | -4 4 1 | 62.772 |
| 1.4706 | 9 | 0 6 0 | 63.177 |
| 1.4589 | 3 | -4 3 2 | 63.742 |
| 1.4315 | 3 | -5 1 2 | 65.110 |
| 1.4143 | 3 | 0 6 1 | 66.000 |
| 1.4100 | 3 | 3 1 3 | 66.230 |
| 1.4044 | 5 | 6 0 0 | 66.525 |

# Strontium Silicate, α-$SrSiO_3$

Synonym
Strontium metasilicate

CAS registry no.
12712-63-9

Sample
The sample was made by heating a mixture of $SrCO_3$ and amorphous $SiO_2$ for 21 hours at 1400 °C, followed by grinding and heating about 5 days at 1300 °C.

Color
Colorless

Structure
Monoclinic, C2 (5). The structure of α-$SrSiO_3$ was determined by Machida et al. (1982). This phase was earlier indexed as hexagonal.

Crystallographic constants of this sample
a = 12.340(3) Å
b = 7.136(2)
c = 10.880(3)
β = 111.51(3)°

a/b = 1.7293
c/b = 1.5247

Z = 12
V = 891.35 $Å^3$
Density (calc) = 3.660 $g/cm^3$

Figure of merit
$F_{30}$ = 16.7(0.015,117)

Polymorphism
There are 2 high pressure forms reported by Shimizu et al. (1970).

Additional patterns
PDF card 30-1302 (Shimizu et al., 1970)
PDF card 32-1258 (Moir et al., 1975).

References
Machida, K., Adachi, G., Shiokawa, J., Shimada, M., and Koizumi, M. (1982). Acta Crystallogr. B38, 386.

Moir, G. K., Gand, J. A., and Glasser, F. P. (1975). Z. Kristallogr., 141, 437.

Shimizu, Y., Syono, Y., and Akimoto, S. (1970). High Temp. High Pressures 2, 113.

CuKα$_1$ λ = 1.540598 Å; mean T = 25.2 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.05 | 1L | 1 1 0 | 14.624 |
| 5.73 | 1L | 2 0 0 | 15.457 |
| 5.056 | 17 | 0 0 2 | 17.527 |
| 4.803 | 1L | 1 1 1 | 18.456 |
| 4.755 | 1 | -2 0 2 | 18.647 |
| 4.320 | 1 | -1 1 2 | 20.541 |
| 3.566M | 66 | 0 2 0 | 24.951 |
| 3.566M | | -3 1 1 | 24.951 |
| 3.365 | 30 | 0 2 1 | 26.466 |
| 3.254 | 1 | 2 0 2 | 27.389 |
| 3.225 | 1L | -1 1 3 | 27.639 |
| 2.928 | 50 | 3 1 1 | 30.510 |
| 2.917 | 100 | 0 2 2 | 30.627 |
| 2.760 | 1 | 2 2 1 | 32.409 |
| 2.531+ | 21 | 2 0 3 | 35.437 |
| 2.531+ | | 0 0 4 | 35.437 |
| 2.514 | 9 | -1 1 4 | 35.692 |
| 2.462 | 1 | 3 1 2 | 36.463 |
| 2.452 | 1 | 0 2 3 | 36.621 |
| 2.324 | 1 | -5 1 2 | 38.715 |
| 2.185 | 1L | 5 1 0 | 41.287 |
| 2.073 | 27 | 3 1 3 | 43.629 |
| 2.060 | 75 | -3 3 1 | 43.906 |
| 1.914 | 18 | 6 0 0 | 47.453 |
| 1.909 | 22 | 3 3 1 | 47.593 |
| 1.897 | 3 | -6 0 4 | 47.913 |
| 1.854 | 1L | 1 3 3 | 49.092 |
| 1.808 | 1L | -2 0 6 | 50.430 |
| 1.7837 | 10 | 0 4 0 | 51.169 |
| 1.7579 | 2 | -6 2 1 | 51.976 |
| 1.7525+ | 2 | -3 3 4 | 52.151 |
| 1.7525+ | | -3 1 6 | 52.151 |
| 1.6858M | 9 | 0 0 6 | 54.378 |
| 1.6858M | | 6 2 0 | 54.378 |
| 1.6821 | 11 | 0 4 2 | 54.507 |
| 1.6767 | 7 | -6 2 4 | 54.699 |
| 1.6724 | 2 | -7 1 1 | 54.851 |
| 1.6023 | 4 | 3 3 3 | 57.470 |
| 1.5983 | 5 | 7 1 0 | 57.626 |
| 1.5967 | 4 | 5 1 3 | 57.689 |

# Strontium Zirconium Phosphate, $SrZr_4(PO_4)_6$

Synonym
Strontium zirconium orthophosphate

CAS registry no.
67972-88-7

Sample
The sample was made by heating a 1:4:6 molar mixture of $SrCO_3$, $ZrO_2$, and $(NH_4)_2HPO_4$ up to 500 °C. After regrinding it was heated to 1300 °C for 70 hours.

Color
Colorless

Structure
Rhombohedral, R**. The structure is similar to that of $NaZr_2(PO_4)_3$ (Chernorukov et al., 1978.)

Crystallographic constants of this sample (Hexagonal axes)

a = 8.6935(4) Å
c = 23.389(2)

c/a = 2.6904

Z = 3
V = 1530.85 Å$^3$
Density (calc) = 3.327 g/cm$^3$

Figure of merit
$F_{30}$ = 119.9(0.0068,37)

Reference
Chernorukov, N. G., Korshunov, I. A., and Prokof'eva, T. V. (1978). Sov. Phys. Crystallogr. Engl. Transl. 23, 475.

CuK$\alpha_1$ $\lambda$ = 1.540598 Å; temp. 26±1 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.796 | 4 | 0 0 3 | 11.341 |
| 7.170 | 9 | 1 0 1 | 12.334 |
| 6.333 | 10 | 0 1 2 | 13.972 |
| 4.619 | 35 | 1 0 4 | 19.198 |
| 4.348 | 75 | 1 1 0 | 20.407 |
| 3.972 | 5 | 0 1 5 | 22.366 |
| 3.795 | 74 | 1 1 3 | 23.420 |
| 3.716 | 2 | 0 2 1 | 23.926 |
| 3.583 | 2 | 2 0 2 | 24.829 |
| 3.165 | 36 | 0 2 4 | 28.172 |
| 3.053 | 1 | 1 0 7 | 29.232 |
| 2.933 | 6 | 2 0 5 | 30.451 |
| 2.900 | 100 | 1 1 6 | 30.804 |
| 2.825 | 12 | 2 1 1 | 31.646 |
| 2.766 | 1 | 1 2 2 | 32.341 |
| 2.726 | 5 | 0 1 8 | 32.830 |
| 2.5579 | 10 | 2 1 4 | 35.053 |
| 2.5084 | 34 | 3 0 0 | 35.768 |
| 2.4307 | 4 | 1 2 5 | 36.951 |
| 2.3884 | 3 | 3 0 3 | 37.630 |
| 2.3089 | 5 | 2 0 8 | 38.977 |
| 2.2305 | 5 | 1 1 9 | 40.406 |
| 2.1736 | 8 | 2 2 0 | 41.512 |
| 2.1665 | 8 | 2 1 7 | 41.655 |
| 2.1098 | 13 | 3 0 6 | 42.827 |
| 2.0933 | 4 | 2 2 3 | 43.182 |
| 2.0395 | 16 | 1 2 8 | 44.381 |
| 1.9862 | 7 | 0 2 10 | 45.639 |
| 1.9664 | 7 | 1 3 4 | 46.125 |
| 1.9486 | 2 | 0 0 12 | 46.570 |
| 1.9067 | 4 | 3 1 5 | 47.655 |
| 1.8980 | 29 | 2 2 6 | 47.888 |
| 1.8762 | 1 | 4 0 1 | 48.480 |
| 1.8582 | 2 | 0 4 2 | 48.981 |
| 1.8526 | 1 | 2 0 11 | 49.138 |
| 1.8064M | 16 | 2 1 10 | 50.482 |
| 1.8064M | | 3 0 9 | 50.482 |
| 1.7702 | 3 | 1 3 7 | 51.588 |
| 1.7495 | 1 | 1 0 13 | 52.245 |
| 1.7456 | 1 | 0 4 5 | 52.372 |
| 1.6989 | 8 | 3 1 8 | 53.926 |
| 1.6665 | 1 | 2 2 9 | 55.061 |
| 1.6561 | 6 | 3 2 4 | 55.438 |
| 1.6426 | 20 | 4 1 0 | 55.931 |
| 1.6308 | 5 | 0 1 14 | 56.374 |

Strontium Zirconium Phosphate, $SrZr_4(PO_4)_6$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.6200 | 2 | 2 3 5 | 56.781 |
| 1.6075 | 2 | 4 1 3 | 57.263 |
| 1.5824 | 4 | 0 4 8 | 58.262 |
| 1.5573 | 10 | 1 3 10 | 59.290 |
| 1.5391 | 5 | 3 0 12 | 60.063 |
| 1.5350 | 4 | 3 2 7 | 60.242 |
| 1.5268 | 7 | 2 0 14 | 60.600 |
| 1.5139 | 15 | 4 1 6 | 61.172 |
| 1.4898 | 2 | 3 1 11 | 62.270 |
| 1.4868 | 2 | 2 3 8 | 62.411 |
| 1.4667 | 5 | 4 0 10 | 63.360 |
| 1.4582 | 2 | 0 5 4 | 63.776 |
| 1.4489 | 4 | 3 3 0 | 64.232 |
| 1.4406 | 8 | 1 2 14 | 64.649 |
| 1.4244 | 1 | 3 3 3 | 65.472 |
| 1.3893M | 3 | 3 2 10 | 67.346 |
| 1.3893M | | 4 1 9 | 67.346 |
| 1.3824 | 2 | 2 4 4 | 67.728 |
| 1.3625M | 1 | 1 3 13 | 68.854 |
| 1.3625M | | 0 2 16 | 68.854 |
| 1.3582 | 3 | 3 3 6 | 69.102 |
| 1.3499 | 1 | 5 1 1 | 69.588 |
| 1.3175 | 2 | 5 1 4 | 71.558 |
| 1.3088 | 2 | 2 4 7 | 72.112 |
| 1.3044 | 2 | 3 1 14 | 72.394 |
| 1.2991M | 1 | 0 0 18 | 72.736 |
| 1.2991M | | 1 5 5 | 72.736 |
| 1.2791 | 1 | 4 2 8 | 74.056 |
| 1.2548 | 2 | 6 0 0 | 75.739 |
| 1.2465 | 1L | 3 2 13 | 76.339 |
| 1.2385M | 1L | 6 0 3 | 76.917 |
| 1.2385M | | 1 2 17 | 76.917 |
| 1.2309 | 1L | 3 4 2 | 77.480 |
| 1.2156 | 1 | 2 4 10 | 78.645 |
| 1.2057 | 2 | 5 2 0 | 79.419 |
| 1.2008 | 2 | 2 3 14 | 79.804 |
| 1.1944 | 1L | 6 0 6 | 80.323 |
| 1.1913 | 1L | 5 2 3 | 80.571 |
| 1.1707 | 1L | 5 1 10 | 82.289 |
| 1.1629 | 1L | 3 3 12 | 82.968 |
| 1.1557 | 1 | 0 1 20 | 83.599 |
| 1.1518 | 2 | 5 2 6 | 83.945 |
| 1.1411 | 1 | 1 5 11 | 84.912 |
| 1.1399 | 1L | 3 4 8 | 85.027 |
| 1.1299M | 1L | 2 1 19 | 85.960 |
| 1.1299M | | 6 0 9 | 85.960 |
| 1.1269 | 1L | 1 6 4 | 86.244 |
| 1.1187 | 1L | 5 0 14 | 87.036 |
| 1.1160M | 1 | 2 4 13 | 87.293 |
| 1.1160M | | 3 2 16 | 87.293 |
| 1.0942 | 2 | 4 3 10 | 89.492 |

# Tantalum Tungsten Oxide, $Ta_2WO_8$

Synonym
Tantalum tungstate

Sample
The single phase composition was prepared by heating 52.4 mole % of $Ta_2O_5$ with 47.6 mole % of $WO_3$ for 30 hours at 1350 °C. (A mixture of 50 mole % each yielded 2 phases.) The composition reported here may be regarded either as oxygen deficient $(Ta,W)_3\ O_{7.986}$ or as containing excess metal $(Ta,\ W)_{3.012}\ O_8$ (Santoro et al., 1979).

Color
Pale yellow gray

Structure
Orthorhombic, Pmab (57). The structure was determined by Santoro et al. (1979).

Crystallographic constants of this sample
a = 16.6997(15) Å
b = 17.7296(15)
c = 3.8798(4)

a/b = 0.9419
c/b = 0.2188

Z = 8
V = 1148.7 $Å^3$
Density (calc) = 7.791 $g/cm^3$

Figure of merit
$F_{30}$ = 73.6(0.0074,55)

Additional patterns
PDF card 19-1375 (Kovba and Trunov, 1965)
PDF card 29-1322 (Holcombe, 1976)

References
Holcombe, C., Jr., Oak Ridge Nat. Lab. Rep. No. Y2031 (1976).

Kovba, L. M. and Trunov, V. K. (1965). J. Struct. Chem. Engl. Transl., 6, 224.

Santoro, A., Roth, R. S., and Minor, D. (1979). Acta Crystallogr., B35, 1202.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C
Internal standard Ag, a = 4.08651 Å

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.86 | 20 | 0 2 0 | 9.975 |
| 8.35 | 8 | 2 0 0 | 10.589 |
| 7.827 | 5 | 1 2 0 | 11.296 |
| 4.715 | 2 | 3 2 0 | 18.807 |
| 4.434 | 4 | 0 4 0 | 20.009 |
| 4.287 | 4 | 1 4 0 | 20.704 |
| 3.918 | 35 | 2 4 0 | 22.679 |
| 3.881 | 100 | 0 0 1 | 22.896 |
| 3.778 | 35 | 4 2 0 | 23.528 |
| 3.555 | 2 | 0 2 1 | 25.028 |
| 3.519 | 9 | 2 0 1 | 25.289 |
| 3.469 | 83 | 3 4 0 | 25.660 |
| 3.125 | 46 | 5 2 0 | 28.538 |
| 3.039 | 1 | 4 4 0 | 29.369 |
| 2.996 | 1L | 3 2 1 | 29.799 |
| 2.910 | 29 | 1 6 0 | 30.694 |
| 2.876 | 2 | 1 4 1 | 31.074 |
| 2.786M | 28 | 2 6 0 | 32.102 |
| 2.786M | | 6 0 0 | 32.102 |
| 2.756 | 5 | 2 4 1 | 32.458 |
| 2.707 | 18 | 4 2 1 | 33.069 |
| 2.668 | 6 | 5 4 0 | 33.558 |
| 2.656 | 5 | 6 2 0 | 33.720 |
| 2.611 | 3 | 3 6 0 | 34.322 |
| 2.586M | 46 | 1 5 1 | 34.661 |
| 2.586M | | 3 4 1 | 34.661 |
| 2.4344 | 28 | 5 2 1 | 36.893 |
| 2.4117 | 2 | 4 6 0 | 37.253 |
| 2.3919 | 1L | 4 4 1 | 37.574 |
| 2.3574 | 2 | 6 4 0 | 38.144 |
| 2.3284M | 17 | 1 6 1 | 38.638 |
| 2.3284M | | 5 3 1 | 38.638 |
| 2.3039 | 1 | 7 2 0 | 39.065 |
| 2.2631M | 19 | 2 6 1 | 39.800 |
| 2.2631M | | 6 0 1 | 39.800 |
| 2.2165M | 3 | 0 8 0 | 40.672 |
| 2.2165M | | 4 5 1 | 40.672 |
| 2.1986M | 4 | 5 4 1 | 41.019 |
| 2.1986M | | 1 8 0 | 41.019 |
| 2.1922 | 3 | 6 2 1 | 41.144 |
| 2.1674 | 1L | 3 6 1 | 41.637 |
| 2.1005 | 3 | 7 4 0 | 43.026 |
| 2.0874 | 3 | 8 0 0 | 43.310 |
| 2.0587M | 2 | 3 8 0 | 43.946 |
| 2.0587M | | 5 5 1 | 43.946 |

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 2.0488 | 2 | 4 6 1 | 44.169 |
| 2.0316 | 6 | 8 2 0 | 44.564 |
| 2.0142 | 1 | 6 4 1 | 44.969 |
| 1.9812M | 1 | 7 2 1 | 45.760 |
| 1.9812M | | 3 7 1 | 45.760 |
| 1.9574 | 6 | 4 8 0 | 46.350 |
| 1.9398 | 21 | 0 0 2 | 46.794 |
| 1.9240 | 3 | 0 8 1 | 47.202 |
| 1.8883M | 6 | 8 4 0 | 48.149 |
| 1.8883M | | 2 0 2 | 48.149 |
| 1.8561 | 6 | 7 6 0 | 49.039 |
| 1.8466+ | 13 | 5 8 0 | 49.310 |
| 1.8466+ | | 7 4 1 | 49.310 |
| 1.8381 | 4 | 8 0 1 | 49.553 |
| 1.8185 | 4 | 3 8 1 | 50.123 |
| 1.7999 | 6 | 8 2 1 | 50.677 |
| 1.7768 | 2 | 0 4 2 | 51.384 |
| 1.7727 | 4 | 0 10 0 | 51.513 |
| 1.7628M | 4 | 1 10 0 | 51.822 |
| 1.7628M | | 7 5 1 | 51.822 |
| 1.7474M | 6 | 4 8 1 | 52.313 |
| 1.7474M | | 1 9 1 | 52.313 |
| 1.7381 | 3 | 2 4 2 | 52.615 |
| 1.7341M | 6 | 2 10 0 | 52.746 |
| 1.7341M | | 6 8 0 | 52.746 |
| 1.7255 | 5 | 4 2 2 | 53.029 |
| 1.7047 | 15 | 8 6 0 | 53.727 |
| 1.6983 | 8 | 8 4 1 | 53.946 |
| 1.6930M | 16 | 1 5 2 | 54.128 |
| 1.6930M | | 3 4 2 | 54.128 |
| 1.6744M | 6 | 7 6 1 | 54.779 |
| 1.6744M | | 3 9 1 | 54.779 |
| 1.6701M | 12 | 5 1 2 | 54.933 |
| 1.6701M | | 10 0 0 | 54.933 |
| 1.6670M | 12 | 5 8 1 | 55.045 |
| 1.6670M | | 9 1 1 | 55.045 |
| 1.6482 | 12 | 5 2 2 | 55.727 |
| 1.6317M | 6 | 4 10 0 | 56.340 |
| 1.6317M | | 8 5 1 | 56.340 |
| 1.6235 | 2 | 7 8 0 | 56.650 |
| 1.6138M | 9 | 5 3 2 | 57.019 |
| 1.6138M | | 1 6 2 | 57.019 |
| 1.6050 | 3 | 1 10 1 | 57.364 |
| 1.5917 | 7 | 2 6 2 | 57.885 |
| 1.5917M | | 6 0 2 | 57.885 |
| 1.5831M | 5 | 2 10 1 | 58.230 |
| 1.5831M | | 6 8 1 | 58.230 |
| 1.5713 | 5 | 9 6 0 | 58.711 |
| 1.5663+ | 7 | 6 2 2 | 58.919 |
| 1.5663+ | | 5 10 0 | 58.919 |

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.5608 | 15 | 8 6 1 | 59.146 |
| 1.5490 | 1L | 3 10 1 | 59.640 |
| 1.5336M | 7 | 1 7 2 | 60.300 |
| 1.5336M | | 10 0 1 | 60.300 |
| 1.5195 | 1L | 8 8 0 | 60.921 |
| 1.5112M | 1 | 10 2 1 | 61.291 |
| 1.5112M | | 4 6 2 | 61.291 |
| 1.5041 | 7 | 4 10 1 | 61.611 |
| 1.4974M | 5 | 7 8 1 | 61.918 |
| 1.4974M | | 6 4 2 | 61.918 |
| 1.4840+ | 1L | 7 2 2 | 62.542 |
| 1.4840+ | | 3 7 2 | 62.542 |
| 1.4717 | 2 | 1 12 0 | 63.122 |
| 1.4587M | 4 | 5 6 2 | 63.752 |
| 1.4587M | | 7 3 2 | 63.752 |
| 1.4563 | 5 | 9 6 1 | 63.867 |
| 1.4525M | 6 | 5 10 1 | 64.056 |
| 1.4525M | | 6 5 2 | 64.056 |

# Thorium Molybdenum Oxide, $\alpha$-$Th(MoO_4)_2$

Synonym
Thorium molybdate

Sample
$ThO_2$ and $MoO_3$ in a molar ratio of 1 to 2 were ground together and heated to 700 °C for 70 hours in a Pt crucible.

Color
Colorless

Structure
Orthorhombic, Pcab (61) (Thoret, 1974).

Crystallographic constants of this sample
a = 10.3174(7) Å
b = 14.4835(10)
c = 9.7491(7)

a/b = 0.7124
c/b = 0.6731

Z = 8
V = 1456.8 Å$^3$
Density (calc) = 5.032 g/cm$^3$

Figure of merit
$F_{30}$ = 105.5(0.0071,40)

Polymorphism
There is a hexagonal $\beta$-form existing above 950 °C (Thoret, 1974).

Additional pattern
PDF card 27-1468 (Thoret, 1974)

Reference
Thoret, J. (1974). Rev. Chim. Minér. 11, 237.

$CuK\alpha_1$ $\lambda$ = 1.540598 Å; mean T = 25.9 °C
Internal standard Ag, a = 4.08651 Å

| d(Å) | $I^{rel}$ $\sigma$ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.241 | 15 | 0 2 0 | 12.213 |
| 6.371 | 8 | 1 1 1 | 13.890 |
| 5.929 | 5 | 1 2 0 | 14.929 |
| 5.156 | 29 | 2 0 0 | 17.185 |
| 5.065 | 77 | 1 2 1 | 17.496 |
| 4.874 | 27 | 0 0 2 | 18.185 |
| 4.348 | 16 | 2 1 1 | 20.408 |
| 4.202 | 6 | 2 2 0 | 21.125 |
| 4.045 | 10 | 0 2 2 | 21.955 |
| 3.991 | 15 | 1 3 1 | 22.256 |
| 3.859 | 10 | 2 2 1 | 23.031 |
| 3.766 | 63 | 1 2 2 | 23.604 |
| 3.621 | 47 | 0 4 0 | 24.563 |
| 3.544 | 100 | 2 0 2 | 25.105 |
| 3.417 | 21 | 1 4 0 | 26.059 |
| 3.315 | 7 | 2 3 1 | 26.877 |
| 3.257 | 11 | 1 3 2 | 27.364 |
| 3.225 | 33 | 1 4 1 | 27.635 |
| 3.184 | 23 | 2 2 2 | 28.003 |
| 3.163 | 7 | 3 1 1 | 28.194 |
| 3.107 | 62 | 3 2 0 | 28.713 |
| 3.032 | 25 | 1 1 3 | 29.437 |
| 2.961M | 71 | 2 4 0 | 30.154 |
| 2.961M | | 3 2 1 | 30.154 |
| 2.908 | 31 | 0 4 2 | 30.722 |
| 2.850 | 22 | 1 2 3 | 31.361 |
| 2.799 | 11 | 1 4 2 | 31.947 |
| 2.750 | 2 | 2 0 3 | 32.531 |
| 2.701 | 7 | 2 1 3 | 33.135 |
| 2.682 | 2 | 1 5 1 | 33.382 |
| 2.620 | 17 | 3 2 2 | 34.197 |
| 2.609 | 11 | 1 3 3 | 34.347 |
| 2.579 | 4 | 4 0 0 | 34.755 |
| 2.574 | 3 | 2 2 3 | 34.833 |
| 2.5326 | 25 | 2 4 2 | 35.414 |
| 2.4936M | 10 | 3 4 0 | 35.987 |
| 2.4936M | | 4 0 1 | 35.987 |
| 2.4582 | 6 | 4 1 1 | 36.524 |
| 2.4374 | 15 | 0 0 4 | 36.846 |
| 2.4297M | 9 | 4 2 0 | 36.968 |
| 2.4297M | | 3 3 2 | 36.968 |
| 2.4151M | 5 | 3 4 1 | 37.199 |
| 2.4151M | | 0 6 0 | 37.199 |
| 2.3538 | 8 | 1 4 3 | 38.205 |
| 2.2849 | 24 | 1 6 1 | 39.404 |

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 2.2786 | 15 | 4 0 2 | 39.517 |
| 2.2460 | 26 | 3 2 3 | 40.115 |
| 2.2195 | 3 | 3 4 2 | 40.616 |
| 2.2039 | 5 | 2 0 4 | 40.916 |
| 2.1901 | 12 | 2 4 3 | 41.185 |
| 2.1747M | 6 | 0 3 4 | 41.491 |
| 2.1747M | | 4 2 2 | 41.491 |
| 2.1599 | 2 | 3 5 1 | 41.787 |
| 2.1334 | 11 | 2 6 1 | 42.331 |
| 2.1279 | 8 | 1 3 4 | 42.447 |
| 2.1161M | 7 | 1 6 2 | 42.694 |
| 2.1161M | | 1 5 3 | 42.694 |
| 2.0617 | 5 | 4 3 2 | 43.878 |
| 2.0535 | 12 | 4 4 1 | 44.062 |
| 2.0212M | 10 | 0 4 4 | 44.805 |
| 2.0212M | | 4 0 3 | 44.805 |
| 2.0164 | 8 | 3 5 2 | 44.918 |
| 1.9995 | 21 | 5 1 1 | 45.319 |
| 1.9950M | 31 | 2 6 2 | 45.427 |
| 1.9950M | | 2 5 3 | 45.427 |
| 1.9844+ | 15 | 5 2 0 | 45.683 |
| 1.9844+ | | 1 4 4 | 45.683 |
| 1.9793 | 11 | 3 4 3 | 45.806 |
| 1.9446 | 18 | 5 2 1 | 46.672 |
| 1.9362 | 19 | 3 6 1 | 46.886 |
| 1.9179 | 12 | 3 2 4 | 47.361 |
| 1.9046M | 18 | 0 7 2 | 47.712 |
| 1.9046M | | 1 6 3 | 47.712 |
| 1.8994 | 15 | 1 1 5 | 47.850 |
| 1.8897 | 7 | 4 5 1 | 48.113 |
| 1.8834+ | 10 | 2 7 1 | 48.284 |
| 1.8834+ | | 5 1 2 | 48.284 |
| 1.8639 | 11 | 4 3 3 | 48.822 |
| 1.8519 | 10 | 1 2 5 | 49.158 |
| 1.8380M | 24 | 3 3 4 | 49.554 |
| 1.8380M | | 5 2 2 | 49.554 |
| 1.8312M | 25 | 3 6 2 | 49.752 |
| 1.8312M | | 3 5 3 | 49.752 |
| 1.8139 | 6 | 2 6 3 | 50.258 |
| 1.8097M | 7 | 0 8 0 | 50.384 |
| 1.8097M | | 2 1 5 | 50.384 |
| 1.7917 | 4 | 4 5 2 | 50.925 |
| 1.7870 | 5 | 2 7 2 | 51.071 |
| 1.7804 | 7 | 1 3 5 | 51.271 |
| 1.7717 | 11 | 4 0 4 | 51.544 |
| 1.7627M | 14 | 5 4 1 | 51.824 |
| 1.7627M | | 4 6 0 | 51.824 |
| 1.7585 | 14 | 4 1 4 | 51.957 |
| 1.7541M | 20 | 1 8 1 | 52.098 |
| 1.7541M | | 2 5 4 | 52.098 |

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.7434M | 8 | 3 7 1 | 52.442 |
| 1.7434M | | 3 4 4 | 52.442 |
| 1.7344 | 7 | 4 6 1 | 52.735 |
| 1.7299 | 6 | 5 1 3 | 52.883 |
| 1.7211M | 4 | 1 7 3 | 53.174 |
| 1.7211M | | 4 2 4 | 53.174 |
| 1.7156 | 7 | 0 6 4 | 53.360 |
| 1.7083 | 14 | 2 8 0 | 53.605 |
| 1.6975 | 16 | 0 8 2 | 53.975 |
| 1.6934+ | 24 | 1 4 5 | 54.115 |
| 1.6934+ | | 6 0 1 | 54.115 |
| 1.6888 | 19 | 3 6 3 | 54.274 |
| 1.6830+ | 16 | 2 8 1 | 54.476 |
| 1.6830+ | | 5 4 2 | 54.476 |
| 1.6658 | 3 | 3 7 2 | 55.085 |
| 1.6625 | 2 | 4 3 4 | 55.205 |
| 1.6573+ | 2 | 4 6 2 | 55.395 |
| 1.6573+ | | 4 5 3 | 55.395 |
| 1.6531 | 2 | 2 7 3 | 55.545 |
| 1.6509 | 2 | 3 2 5 | 55.625 |
| 1.6386 | 3 | 5 3 3 | 56.082 |
| 1.6289 | 3 | 2 4 5 | 56.444 |
| 1.6117M | 3 | 2 8 2 | 57.104 |
| 1.6117M | | 6 1 2 | 57.104 |
| 1.5976M | 5 | 1 5 5 | 57.654 |
| 1.5976M | | 6 3 1 | 57.654 |
| 1.5920M | 4 | 4 7 1 | 57.876 |
| 1.5920M | | 4 4 4 | 57.876 |
| 1.5827 | 3 | 6 2 2 | 58.246 |
| 1.5807 | 4 | 3 8 1 | 58.327 |
| 1.5770 | 4 | 0 7 4 | 58.479 |
| 1.5681 | 7 | 5 6 0 | 58.842 |
| 1.5636 | 10 | 1 8 3 | 59.030 |
| 1.5592 | 8 | 1 7 4 | 59.213 |
| 1.5485M | 6 | 4 6 3 | 59.662 |
| 1.5485M | | 5 6 1 | 59.662 |
| 1.5393M | 6 | 0 3 6 | 60.055 |
| 1.5393M | | 5 2 4 | 60.055 |
| 1.5339 | 12 | 6 4 1 | 60.289 |

# Thorium Molybdenum Oxide, $\beta$-$Th(MoO_4)_2$

Synonym
Thorium molybdate

Sample
The sample was prepared by heating $ThO_2$ and $MoO_3$ in a 1 to 2 molar ratio in a Pt crucible at 700 °C for 20 3/4 hours, then reheated at 1000 °C for 2 1/4 hours.

Color
Colorless

Structure
Hexagonal, $P\bar{6}$ (174). The structure was determined by Thoret et al. (1968).

Crystallographic constants of this sample
$a = 17.5764(6)$ Å
$c = 6.2265(2)$

$c/a = 0.3543$

$Z = 9$
$V = 1665.84$ Å$^3$
Density (calc) = 4.951 g/cm$^3$

Figure of merit
$F_{30} = 42.7(0.011,64)$

Polymorphism
There is an orthorhombic $\alpha$-form existing below 950 °C (Thoret, 1974).

Additional pattern
PDF card 27-1469 (Thoret, 1974)

References
Thoret, J. (1974). Rev. Chim. Minér. 11, 237.

Thoret, J., Rimsky, A., and Freundlich, W. (1968). C. R. Séances Acad. Sci., Ser. C 267, 1682.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 25.6 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 8.79 | 2 | 1 1 0 | 10.051 |
| 5.764M | 8 | 1 0 1 | 15.360 |
| 5.764M | | 2 1 0 | 15.360 |
| 5.075M | 48 | 1 1 1 | 17.461 |
| 5.075M | | 3 0 0 | 17.461 |
| 4.821 | 7 | 2 0 1 | 18.389 |
| 4.227M | 17 | 2 1 1 | 21.002 |
| 4.227M | | 3 1 0 | 21.002 |
| 3.935 | 51 | 3 0 1 | 22.580 |
| 3.592 | 79 | 2 2 1 | 24.768 |
| 3.495M | 10 | 3 1 1 | 25.465 |
| 3.495M | | 3 2 0 | 25.465 |
| 3.321 | 34 | 4 1 0 | 26.820 |
| 3.247 | 5 | 4 0 1 | 27.443 |
| 3.115 | 14 | 0 0 2 | 28.635 |
| 3.047M | 6 | 3 2 1 | 29.283 |
| 3.047M | | 5 0 0 | 29.283 |
| 2.932M | 100 | 1 4 1 | 30.461 |
| 2.932M | | 3 3 0 | 30.461 |
| 2.735M | 2 | 5 0 1 | 32.714 |
| 2.735M | | 5 1 0 | 32.714 |
| 2.650 | 3 | 3 3 1 | 33.793 |
| 2.612 | 4 | 4 2 1 | 34.309 |
| 2.541 | 23 | 2 2 2 | 35.298 |
| 2.503M | 3 | 5 1 1 | 35.852 |
| 2.503M | | 4 3 0 | 35.852 |
| 2.439 | 5 | 5 2 0 | 36.826 |
| 2.348 | 1 | 6 0 1 | 38.299 |
| 2.322M | 7 | 4 3 1 | 38.755 |
| 2.322M | | 6 1 0 | 38.755 |
| 2.271 | 46 | 4 1 2 | 39.646 |
| 2.198 | 1 | 4 4 0 | 41.027 |
| 2.175M | 4 | 6 1 1 | 41.481 |
| 2.175M | | 5 3 0 | 41.481 |
| 2.133 | 10 | 3 3 2 | 42.337 |
| 2.0715 | 1 | 4 4 1 | 43.660 |
| 2.0528 | 7 | 5 3 1 | 44.079 |
| 2.0196 | 4 | 1 1 3 | 44.843 |
| 1.9985 | 4 | 6 2 1 | 45.341 |
| 1.9671 | 2 | 6 0 2 | 46.108 |
| 1.9523 | 2 | 2 1 3 | 46.478 |
| 1.9181M | 94 | 7 1 1 | 47.357 |
| 1.9181M | | 6 3 0 | 47.357 |
| 1.8769 | 16 | 2 2 3 | 48.461 |
| 1.8628 | 3 | 3 1 3 | 48.853 |
| 1.8592M | 2 | 5 4 1 | 48.954 |
| 1.8592M | | 7 2 0 | 48.954 |
| 1.8326 | 3 | 6 3 1 | 49.711 |
| 1.8196 | 2 | 8 0 1 | 50.089 |
| 1.7954 | 21 | 4 4 2 | 50.815 |
| 1.7842 | 3 | 3 2 3 | 51.154 |
| 1.7807M | 2 | 7 2 1 | 51.263 |
| 1.7807M | | 8 1 0 | 51.263 |
| 1.7602 | 14 | 4 1 3 | 51.906 |
| 1.7129M | 2 | 8 1 1 | 53.450 |
| 1.7129M | | 7 3 0 | 53.450 |
| 1.6920M | 32 | 7 1 2 | 54.164 |
| 1.6920M | | 5 5 1 | 54.164 |
| 1.6811 | 4 | 6 4 1 | 54.545 |
| 1.6608 | 3 | 8 2 0 | 55.266 |

| d(Å) | $I^{rel}$ σ = ±3 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.6510M | 3 | 5 4 2 | 55.623 |
| 1.6510M | | 7 3 1 | 55.623 |
| 1.6328M | 11 | 6 3 2 | 56.297 |
| 1.6328M | | 9 0 1 | 56.297 |
| 1.6048 | 8 | 8 2 1 | 57.371 |
| 1.5972 | 2 | 4 3 3 | 57.667 |
| 1.5787 | 5 | 7 4 0 | 58.408 |
| 1.5569 | 5 | 0 0 4 | 59.308 |
| 1.5458M | 3 | 6 5 1 | 59.776 |
| 1.5458M | | 8 3 0 | 59.776 |
| 1.5303M | 19 | 5 5 2 | 60.444 |
| 1.5303M | | 7 4 1 | 60.444 |
| 1.4995M | 2 | 8 3 1 | 61.822 |
| 1.4995M | | 9 2 0 | 61.822 |
| 1.4881 | 4 | 3 0 4 | 62.347 |
| 1.4797 | 2 | 6 2 3 | 62.744 |
| 1.4650M | 3 | 8 2 2 | 63.444 |
| 1.4650M | | 6 6 0 | 63.444 |
| 1.4580M | 2 | 9 2 1 | 63.786 |
| 1.4580M | | 7 5 0 | 63.786 |
| 1.4461 | 16 | 7 1 3 | 64.371 |
| 1.4259 | 4 | 6 6 1 | 65.398 |
| 1.4196M | 2 | 6 5 2 | 65.724 |
| 1.4196M | | 7 5 1 | 65.724 |
| 1.4096 | 10 | 4 1 4 | 66.248 |
| 1.4075M | 21 | 7 4 2 | 66.362 |
| 1.4075M | | 10 1 1 | 66.362 |
| 1.4011 | 2 | 8 4 1 | 66.703 |
| 1.3847M | 2 | 7 2 3 | 67.597 |
| 1.3847M | | 8 3 2 | 67.597 |
| 1.3750 | 8 | 3 3 4 | 68.139 |
| 1.3723 | 5 | 9 3 1 | 68.295 |
| 1.3533 | 1 | 5 1 4 | 69.389 |
| 1.3513M | 2 | 9 2 2 | 69.508 |
| 1.3513M | | 11 0 1 | 69.508 |
| 1.3412 | 3 | 5 5 3 | 70.106 |
| 1.3353 | 1 | 10 2 1 | 70.464 |
| 1.3268 | 5 | 6 0 4 | 70.981 |
| 1.3206M | 2 | 7 3 3 | 71.362 |
| 1.3206M | | 7 5 2 | 71.362 |
| 1.3102M | 20 | 10 1 2 | 72.018 |
| 1.3102M | | 8 5 1 | 72.018 |
| 1.2967 | 4 | 8 2 3 | 72.891 |
| 1.2824 | 4 | 9 3 2 | 73.838 |
| 1.2685 | 5 | 12 0 0 | 74.785 |
| 1.2652 | 4 | 6 5 3 | 75.010 |
| 1.2563 | 6 | 7 4 3 | 75.635 |
| 1.2412 | 1 | 1 0 5 | 76.718 |
| 1.2396 | 1 | 8 3 3 | 76.838 |
| 1.2308M | 10 | 8 5 2 | 77.486 |
| 1.2308M | | 7 7 1 | 77.486 |
| 1.2169 | 2 | 2 1 5 | 78.542 |
| 1.2145M | 1 | 9 5 1 | 78.726 |
| 1.2145M | | 12 1 0 | 78.726 |
| 1.2085 | 12 | 6 3 4 | 79.199 |
| 1.1982 | 5 | 2 2 5 | 80.015 |
| 1.1962 | 6 | 10 4 1 | 80.173 |
| 1.1858 | 4 | 10 1 3 | 81.019 |
| 1.1745 | 3 | 12 0 2 | 81.968 |
| 1.1660 | 7 | 4 1 5 | 82.699 |
| 1.1641M | 17 | 7 7 2 | 82.860 |
| 1.1641M | | 9 6 0 | 82.860 |
| 1.1508M | 1 | 8 7 1 | 84.039 |
| 1.1508M | | 10 5 0 | 84.039 |
| 1.1453 | 3 | 9 0 4 | 84.531 |
| 1.1441 | 1 | 9 6 1 | 84.646 |
| 1.1426 | 2 | 4 2 5 | 84.780 |
| 1.1411 | 1 | 12 2 1 | 84.913 |
| 1.1348 | 7 | 10 4 2 | 85.495 |
| 1.1258 | 7 | 8 5 3 | 86.348 |
| 1.1134M | 1 | 11 3 2 | 87.557 |
| 1.1134M | | 11 4 1 | 87.557 |
| 1.1089 | 2 | 5 2 5 | 88.002 |
| 1.1072M | 6 | 13 1 1 | 88.167 |
| 1.1072M | | 12 3 0 | 88.167 |
| 1.0902M | 6 | 9 6 2 | 89.913 |
| 1.0902M | | 12 3 1 | 89.913 |
| 1.0818 | 1 | 8 8 1 | 90.808 |
| 1.0806 | 1L | 5 3 5 | 90.934 |
| 1.0792M | 1 | 10 5 2 | 91.085 |
| 1.0792M | | 9 7 1 | 91.085 |
| 1.0742 | 3 | 7 7 3 | 91.624 |
| 1.0715 | 2 | 8 6 3 | 91.932 |
| 1.0668 | 2 | 6 6 4 | 92.447 |
| 1.0631M | 1 | 11 4 2 | 92.864 |
| 1.0631M | | 13 2 1 | 92.864 |
| 1.0596 | 3 | 7 1 5 | 93.269 |
| 1.0581M | 4 | 13 1 2 | 93.443 |
| 1.0581M | | 11 5 1 | 93.443 |
| 1.0509 | 2 | 10 4 3 | 94.272 |
| 1.0484 | 2 | 12 1 3 | 94.567 |
| 1.0440 | 4 | 9 3 4 | 95.099 |
| 1.0379 | 3 | 0 0 6 | 95.839 |
| 1.0360 | 1 | 8 8 2 | 96.072 |
| 1.0334M | 1 | 14 1 1 | 96.385 |
| 1.0334M | | 9 8 0 | 96.385 |
| 1.0307 | 1 | 1 1 6 | 96.724 |
| 1.0281 | 1 | 2 0 6 | 97.056 |
| 1.0196M | 1 | 13 2 2 | 98.141 |
| 1.0196M | | 9 8 1 | 98.141 |

# Thorium Silicate (Huttonite), β-$ThSiO_4$

Sample
The sample was prepared by heating an equimolar mixture of $ThO_2$ and $SiO_2$ for a total of 60 hours at 1550 °C, with periodic grinding. The sample contains a small amount of $ThO_2$ as a second phase.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14). Isostructural with monazite (Pabst and Hutton, 1951). The structure of monazite, $CePO_4$, was determined by Mooney (1948).

Crystallographic constants of this sample
a = 6.7759(4) Å
b = 6.9648(4)
c = 6.4982(4)
β = 104.99(1)°

Z = 4
V = 296.23 $Å^3$
Density (calc) = 7.267 $g/cm^3$

Figure of merit
$F_{30}$ = 142.8(0.0045,47)

Polymorphism
A tetragonal modification, thorite, also exists (Pabst and Hutton, 1951). This tetragonal modification has the zircon structure.

Additional pattern
PDF card 4-613 (Pabst and Hutton, 1951).

References
Mooney, R. C. L. (1948). J. Chem. Phys. 16, 1003.

Pabst, A. and Hutton, C. O. (1951). Am. Mineral. 36, 60.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 27.1 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.260 | 19 | -1 0 1 | 16.842 |
| 4.769 | 8 | 1 1 0 | 18.591 |
| 4.663 | 42 | 0 1 1 | 19.017 |
| 4.198 | 74 | -1 1 1 | 21.145 |
| 4.039 | 31 | 1 0 1 | 21.988 |
| 3.493 | 30 | 1 1 1 | 25.478 |
| 3.2726 | 60 | 2 0 0 | 27.228 |
| 3.1395 | 7 | 0 0 2 | 28.406 |
| 3.0743 | 100 | 1 2 0 | 29.021 |
| 3.0440 | 13 | 0 2 1 | 29.317 |
| 2.9618 | 26 | 2 1 0 | 30.149 |
| 2.8830 | 27 | -1 1 2 | 30.994 |
| 2.8622 | 61 | 0 1 2 | 31.225 |
| 2.6302 | 21 | -2 0 2 | 34.059 |
| 2.4614 | 18 | -2 1 2 | 36.475 |
| 2.4210 | 13 | 1 1 2 | 37.105 |
| 2.3835 | 7 | -2 2 1 | 37.711 |
| 2.3432 | 7 | -1 2 2 | 38.384 |
| 2.2493 | 1 | -3 0 1 | 40.054 |
| 2.1774 | 25 | 0 3 1 | 41.437 |
| 2.1617 | 23 | -1 0 3 | 41.751 |
| 2.1402 | 25 | -3 1 1 | 42.191 |
| 2.1020 | 23 | 2 2 1 | 42.995 |
| 2.0821 | 4 | 3 1 0 | 43.426 |
| 2.0129 | 3 | 1 3 1 | 45.000 |
| 1.9733 | 6 | -3 1 2 | 45.953 |
| 1.9392 | 27 | 2 1 2 | 46.810 |
| 1.9129 | 10 | 3 0 1 | 47.492 |
| 1.8924 | 19 | -2 3 1 | 48.040 |
| 1.8721 | 24 | -1 3 2 | 48.593 |
| 1.8584 | 8 | 1 0 3 | 48.975 |
| 1.8488 | 15 | 3 2 0 | 49.247 |
| 1.7933 | 13 | 0 2 3 | 50.876 |
| 1.7715 | 16 | -3 2 2 | 51.549 |
| 1.7533 | 8 | -3 0 3 | 52.123 |
| 1.7424 | 16 | 2 3 1 | 52.473 |
| 1.7261 | 19 | 1 3 2 | 53.010 |
| 1.7002 | 1 | -3 1 3 | 53.881 |
| 1.6828 | 11 | 1 4 0 | 54.484 |
| 1.6778 | 6 | 0 4 1 | 54.660 |
| 1.6527 | 1 | -1 4 1 | 55.560 |
| 1.6458 | 5 | -4 1 1 | 55.816 |
| 1.6351 | 10 | -4 0 2 | 56.213 |
| 1.6154 | 2 | -3 3 1 | 56.960 |
| 1.5992 | 3 | 1 4 1 | 57.590 |

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.5929 | 8 | 4 1 0 | 57.840 |
| 1.5895 | 8 | 3 3 0 | 57.973 |
| 1.5819M | 4 | -1 3 3 | 58.279 |
| 1.5819M | | -1 1 4 | 58.279 |
| 1.5690 | 5 | 0 0 4 | 58.806 |
| 1.5656 | 7 | 3 1 2 | 58.947 |
| 1.5441 | 8 | -2 1 4 | 59.849 |
| 1.5405 | 9 | -3 3 2 | 60.005 |
| 1.5367 | 8 | -2 4 1 | 60.167 |
| 1.5315 | 4 | 0 1 4 | 60.394 |
| 1.5259 | 3 | -1 4 2 | 60.640 |
| 1.5227 | 3 | 0 4 2 | 60.780 |
| 1.4799 | 2 | -4 2 2 | 62.731 |
| 1.4720 | 4 | -1 2 4 | 63.110 |
| 1.4593 | 2 | 3 2 2 | 63.720 |
| 1.4527 | 5 | 2 4 1 | 64.044 |
| 1.4439M | 3 | 2 2 3 | 64.481 |
| 1.4439M | | 1 4 2 | 64.481 |
| 1.4348 | 2 | -3 1 4 | 64.940 |
| 1.3993 | 2 | -3 3 3 | 66.801 |
| 1.3716 | 5 | 4 2 1 | 68.332 |
| 1.3684 | 9 | -4 3 1 | 68.514 |
| 1.3609 | 2 | 3 4 0 | 68.947 |
| 1.3559 | 3 | -1 4 3 | 69.234 |
| 1.3467 | 5 | -1 5 1 | 69.778 |
| 1.3385 | 3 | 0 4 3 | 70.270 |
| 1.3337 | 7 | 1 2 4 | 70.557 |
| 1.3307 | 8 | -1 3 4 | 70.740 |
| 1.3293 | 7 | -3 4 2 | 70.830 |
| 1.3215M | 7 | 3 1 3 | 71.311 |
| 1.3215M | | 3 3 2 | 71.311 |
| 1.3183M | 6 | 2 4 2 | 71.510 |
| 1.3183M | | 4 0 2 | 71.510 |
| 1.3097 | 3 | 2 3 3 | 72.055 |
| 1.2949 | 3 | 4 1 2 | 73.004 |
| 1.2926 | 7 | -4 1 4 | 73.160 |
| 1.2879 | 7 | 3 4 1 | 73.470 |
| 1.2814 | 4 | -2 5 1 | 73.902 |
| 1.2733 | 8 | 0 5 2 | 74.450 |
| 1.2674 | 3 | -2 1 5 | 74.857 |

# Thorium Tantalum Oxide, $Th_2Ta_2O_9$

Synonym
Thorium tantalate

Sample
The sample was prepared from stoichiometric proportions of $ThO_2$ and $Ta_2O_5$. The following heating schedule, alternating with further grinding, yielded a nearly single phase product: 1400 °C for 4½ days, at 1625 °C for 2 hours, at 1625 °C again for 2 hours, and finally at 1625 °C for 2½ hours. Traces of unreacted $ThO_2$ remained.

Comment
Due to the minor radiation hazard, only one intensity chart was processed. Because of the $ThO_2$ impurity and lack of repetitive measurements, the intensities may be in error by a few percent.

Color
Yellowish white

Structure
Monoclinic. The cell was found by use of the Visser program, followed by calculation of the supercell given below. The data may also be indexed on a C-centered orthorhomic cell with twice the volume of the given monoclinic cell. The phase is apparently not isostructural with $Th_2Nb_2O_9$, for which single crystal work has been done by Cava et al. (1981).

Crystallographic constants of this sample

a = 9.681(2) Å
b = 7.4006(11)
c = 9.6766(15)
β = 106.398(10)°

a/b = 1.3081
c/b = 1.3075

Z = 4 (assumed)
V = 665.08 Å$^3$
Density (calc) = 9.687 g/cm$^3$

Figures of merit
$F_{30}$ = 30.4(0.0092,107)
$M_{20}$ = 24.0

Reference
Cava, R. J., Roth, R. S., and Minor, D. B. (1981). J. Am. Ceram. Soc. 64, #4, C-64.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.8 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 4.722M | 2 | -2 0 1 | 18.777 |
| 4.722M | | -1 0 2 | 18.777 |
| 3.976M | 4 | -2 1 1 | 22.344 |
| 3.976M | | -1 1 2 | 22.344 |
| 3.932M | 3 | 2 1 0 | 22.596 |
| 3.932M | | 0 1 2 | 22.596 |
| 3.749M | 4 | 2 0 1 | 23.711 |
| 3.749M | | 1 0 2 | 23.711 |
| 3.701 | 6 | 0 2 0 | 24.024 |
| 3.437M | 8 | 1 2 0 | 25.900 |
| 3.437M | | 0 2 1 | 25.900 |
| 3.336 | 7 | -1 2 1 | 26.700 |
| 3.223M | 100 | -3 0 1 | 27.659 |
| 3.223M | | -1 0 3 | 27.659 |
| 3.119 | 64 | 1 2 1 | 28.594 |
| 3.094M | 7 | 3 0 0 | 28.837 |
| 3.094M | | 0 0 3 | 28.837 |
| 2.995M | 5 | -3 0 2 | 29.810 |
| 2.995M | | -2 0 3 | 29.810 |
| 2.955M | 3 | -3 1 1 | 30.221 |
| 2.955M | | -1 1 3 | 30.221 |
| 2.912M | 48 | -2 2 1 | 30.679 |
| 2.912M | | -1 2 2 | 30.679 |
| 2.894M | 46 | 2 2 0 | 30.869 |
| 2.894M | | 0 2 2 | 30.869 |
| 2.856M | 1 | 3 1 0 | 31.291 |
| 2.856M | | 0 1 3 | 31.291 |
| 2.676 | 39 | -2 2 2 | 33.462 |
| 2.634M | 11 | 2 2 1 | 34.004 |
| 2.634M | | 1 2 2 | 34.004 |
| 2.430M | 5 | -3 2 1 | 36.959 |
| 2.430M | | -1 2 3 | 36.959 |
| 2.375M | 3 | 3 2 0 | 37.859 |
| 2.375M | | 0 2 3 | 37.859 |
| 2.350 | 1 | -1 3 1 | 38.271 |
| 2.299M | 1 | -4 1 1 | 39.154 |
| 2.299M | | -1 1 4 | 39.154 |
| 2.2821 | 1 | 2 2 2 | 39.454 |
| 2.1895+ | 7 | 3 2 1 | 41.196 |
| 2.1895+ | | 1 2 3 | 41.196 |
| 2.1742M | 1 | -4 0 3 | 41.500 |
| 2.1742M | | -3 0 4 | 41.500 |
| 2.1180 | 1 | -3 2 3 | 42.654 |
| 2.0875M | 2 | -4 1 3 | 43.309 |
| 2.0875M | | -3 1 4 | 43.309 |
| 2.0811 | 2 | -2 3 2 | 43.449 |
| 2.0342M | 1 | 4 1 1 | 44.503 |
| 2.0342M | | 1 1 4 | 44.503 |
| 1.9887M | 2 | -4 2 2 | 45.579 |
| 1.9887M | | -2 2 4 | 45.579 |

| d(Å) | $I^{rel}$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.9660M | 33 | 4 2 0 | 46.135 |
| 1.9660M | | 0 2 4 | 46.135 |
| 1.9374 | 9 | -4 0 4 | 46.855 |
| 1.9211M | 2 | -5 0 2 | 47.278 |
| 1.9211M | | -2 0 5 | 47.278 |
| 1.9036M | 1 | -3 3 2 | 47.739 |
| 1.9036M | | -2 3 3 | 47.739 |
| 1.8751+ | 8 | 2 0 4 | 48.511 |
| 1.8751+ | | -3 2 4 | 48.511 |
| 1.8657M | 4 | -5 1 1 | 48.771 |
| 1.8657M | | -1 1 5 | 48.771 |
| 1.8564M | 7 | 5 0 0 | 49.031 |
| 1.8564M | | 0 0 5 | 49.031 |
| 1.8505 | 15 | 0 4 0 | 49.198 |
| 1.8368+ | 14 | 4 2 1 | 49.590 |
| 1.8368+ | | 1 2 4 | 49.590 |
| 1.8258M | 2 | 3 3 1 | 49.910 |
| 1.8258M | | 1 3 3 | 49.910 |
| 1.7291M | 13 | 5 0 1 | 52.908 |
| 1.7291M | | 1 0 5 | 52.908 |
| 1.7161 | 13 | -4 2 4 | 53.341 |
| 1.7128 | 17 | 3 2 3 | 53.453 |
| 1.7052+ | 15 | -4 3 2 | 53.711 |
| 1.7052+ | | -2 3 4 | 53.711 |
| 1.6903M | 3 | 4 3 0 | 54.221 |
| 1.6903M | | 0 3 4 | 54.221 |
| 1.6798M | 1L | 3 3 2 | 54.588 |
| 1.6798M | | 2 3 3 | 54.588 |
| 1.6725M | 3 | 4 2 2 | 54.848 |
| 1.6725M | | 2 2 4 | 54.848 |
| 1.6596+ | 4 | -4 1 5 | 55.309 |
| 1.6596+ | | 0 2 5 | 55.309 |
| 1.6458M | 10 | -5 2 3 | 55.816 |
| 1.6458M | | -3 2 5 | 55.816 |
| 1.6310M | 1 | -4 3 3 | 56.366 |
| 1.6310M | | -3 3 4 | 56.366 |
| 1.6108M | 13 | -6 0 2 | 57.137 |
| 1.6108M | | -2 0 6 | 57.137 |
| 1.6046M | 29 | -3 4 1 | 57.379 |
| 1.6046M | | -1 4 3 | 57.379 |
| 1.5885M | 2 | 3 4 0 | 58.013 |
| 1.5885M | | 0 4 3 | 58.013 |
| 1.5774M | 4 | 5 0 2 | 58.464 |
| 1.5774M | | 2 0 5 | 58.464 |
| 1.5662+ | 3 | 1 2 5 | 58.923 |
| 1.5662+ | | -6 1 1 | 58.923 |
| 1.5599 | 11 | 2 4 2 | 59.183 |
| 1.5389M | 1 | -6 1 3 | 60.074 |
| 1.5389M | | -3 1 6 | 60.074 |
| 1.5172 | 1L | -5 1 5 | 61.021 |
| 1.5154+ | 1L | -2 3 5 | 61.102 |
| 1.5154+ | | 6 1 0 | 61.102 |
| 1.5049+ | 4 | 4 2 3 | 61.575 |
| 1.5049+ | | 3 2 4 | 61.575 |
| 1.4972M | 1 | -6 0 4 | 61.927 |

| d(Å) | $I^{rel}$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4972M | | -4 0 6 | 61.927 |
| 1.4769M | 3 | -6 2 2 | 62.876 |
| 1.4769M | | -2 2 6 | 62.876 |
| 1.4736M | 1 | -5 3 3 | 63.034 |
| 1.4736M | | -3 3 5 | 63.034 |
| 1.4695+ | 2 | -4 4 1 | 63.228 |
| 1.4695+ | | -1 2 6 | 63.228 |
| 1.4496 | 4 | 4 0 4 | 64.201 |
| 1.4162M | 1L | 5 3 1 | 65.904 |
| 1.4162M | | 1 3 5 | 65.904 |
| 1.4106M | 1L | 2 5 0 | 66.197 |
| 1.4106M | | 0 5 2 | 66.197 |
| 1.4020M | 1 | -5 3 4 | 66.655 |
| 1.4020M | | -4 3 5 | 66.655 |
| 1.3585+ | 1 | -2 1 7 | 69.086 |
| 1.3585+ | | 1 2 6 | 69.086 |
| 1.3381 | 5 | -4 4 4 | 70.293 |
| 1.3295+ | 1L | 5 2 3 | 70.817 |
| 1.3295+ | | 3 2 5 | 70.817 |
| 1.3265+ | 1 | 7 0 0 | 70.998 |
| 1.3265+ | | -6 3 3 | 70.998 |
| 1.3107+ | 4 | 5 4 0 | 71.987 |
| 1.3107+ | | 0 3 6 | 71.987 |
| 1.3081M | 3 | -6 2 5 | 72.154 |
| 1.3081M | | -5 2 6 | 72.154 |
| 1.2833M | 3 | -7 2 1 | 73.773 |
| 1.2833M | | -1 2 7 | 73.773 |
| 1.2746M | 4 | 6 2 2 | 74.364 |
| 1.2746M | | 2 2 6 | 74.364 |
| 1.2636+ | 7 | 5 4 1 | 75.121 |
| 1.2636+ | | 1 4 5 | 75.121 |
| 1.2604M | 7 | -7 0 5 | 75.346 |
| 1.2604M | | -5 0 7 | 75.346 |
| 1.2573M | 1 | 6 3 1 | 75.567 |
| 1.2573M | | 1 3 6 | 75.567 |
| 1.2485M | 4 | 7 2 0 | 76.189 |
| 1.2485M | | 0 2 7 | 76.189 |
| 1.2306M | 1L | 4 4 3 | 77.504 |
| 1.2306M | | 3 4 4 | 77.504 |
| 1.2196 | 2 | -6 2 6 | 78.338 |
| 1.2150M | 5 | -6 4 2 | 78.691 |
| 1.2150M | | -2 4 6 | 78.691 |
| 1.2066M | 3 | 1 6 1 | 79.348 |
| 1.2066M | | -7 3 2 | 79.348 |
| 1.2007 | 1 | 5 4 2 | 79.810 |
| 1.1983M | 2 | -6 4 3 | 80.008 |
| 1.1983M | | -3 4 6 | 80.008 |
| 1.1934+ | 3 | -7 2 5 | 80.398 |
| 1.1934+ | | -2 6 1 | 80.398 |
| 1.1846M | 3 | 6 2 3 | 81.119 |
| 1.1846M | | 3 2 6 | 81.119 |
| 1.1784 | 1L | -1 1 8 | 81.640 |
| 1.1755 | 2 | -2 6 2 | 81.886 |

# Thorium Tungsten Oxide, $\alpha$-$Th(WO_4)_2$

Synonym
Thorium tungstate

Sample
The sample was prepared by grinding together stoichiometric amounts of $ThO_2$ and $WO_3$, heating with daily intermittent grinding for extended periods at temperatures up to 875 °C. The sample contained a small amount of $ThO_2$ as impurity. Hence, the intensity of lines 2θ = 27.370, 31.927, 45.765, and 54.293 may be somewhat in error.

Color
Colorless

Structure
Orthorhombic, Pcab (61). The unit cell and space group were determined by Freundlich and Pagès (1969).

Crystallographic constants of this sample
a = 10.3709(14) Å
b = 14.518(2)
c = 9.7133(13)

a/b = 0.7143
c/b = 0.6601

Z = 8
V = 1462.5 Å$^3$
Density (calc) = 6.610 g/cm$^3$

Figure of merit
$F_{30}$ = 81.5(0.0092,40)

Polymorphism
A hexagonal high temperature form was described by Spitsyn et al. (1969).

Additional pattern
PDF card 28-1373 (Thoret, 1974)

References

Freundlich, W. and Pagès, M. (1969). C. R. Séances Acad. Sci., Ser. C, 269, 392.

Spitsyn, V. I., Pokrovskii, A. N., Afonskii, N. S., and Trunov, V. K. (1969). Dokl. Chem. (Engl. Transl.), 188, 825.

Thoret, J. (1974). Rev. Chim. Minér. 11, 237.


| $CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.6 °C<br>Internal standard Ag, a = 4.08651 Å | | | | | |
|---|---|---|---|---|---|
| d(Å) | $I^{rel}$<br>σ = ±3 | hkℓ | | | 2θ(°) |
| 7.26 | 13 | 0 | 2 | 0 | 12.180 |
| 6.374 | 6 | 1 | 1 | 1 | 13.883 |
| 5.939 | 1 | 1 | 2 | 0 | 14.904 |
| 5.183 | 8 | 2 | 0 | 0 | 17.094 |
| 5.072 | 19 | 1 | 2 | 1 | 17.472 |
| 4.854 | 13 | 0 | 0 | 2 | 18.263 |
| 4.608 | 7 | 0 | 1 | 2 | 19.246 |
| 4.573 | 8 | 2 | 0 | 1 | 19.393 |
| 4.362 | 19 | 2 | 1 | 1 | 20.342 |
| 4.219 | 13 | 2 | 2 | 0 | 21.042 |
| 4.038 | 16 | 0 | 2 | 2 | 21.997 |
| 3.994 | 16 | 1 | 3 | 1 | 22.239 |
| 3.872 | 11 | 2 | 2 | 1 | 22.951 |
| 3.762 | 75 | 1 | 2 | 2 | 23.630 |
| 3.628 | 36 | 0 | 4 | 0 | 24.514 |
| 3.546 | 100 | 2 | 0 | 2 | 25.091 |
| 3.425M | 29 | 0 | 3 | 2 | 25.993 |
| 3.425M | | 1 | 4 | 0 | 25.993 |
| 3.325 | 6 | 2 | 3 | 1 | 26.792 |
| 3.256 | 13 | 1 | 3 | 2 | 27.370 |
| 3.232 | 27 | 1 | 4 | 1 | 27.580 |
| 3.184 | 30 | 2 | 2 | 2 | 28.003 |
| 3.121 | 75 | 3 | 2 | 0 | 28.581 |
| 3.022 | 18 | 1 | 1 | 3 | 29.537 |
| 2.972M | 55 | 2 | 4 | 0 | 30.044 |
| 2.972M | | 3 | 2 | 1 | 30.044 |
| 2.908 | 21 | 0 | 4 | 2 | 30.722 |
| 2.844M | 10 | 1 | 2 | 3 | 31.427 |
| 2.844M | | 2 | 4 | 1 | 31.427 |
| 2.801 | 13 | 1 | 4 | 2 | 31.927 |
| 2.767 | 1 | 3 | 1 | 2 | 32.330 |
| 2.699 | 11 | 2 | 1 | 3 | 33.160 |
| 2.626 | 14 | 3 | 2 | 2 | 34.115 |
| 2.606 | 10 | 1 | 3 | 3 | 34.390 |
| 2.537 | 14 | 2 | 4 | 2 | 35.350 |
| 2.503M | 9 | 4 | 0 | 1 | 35.848 |
| 2.503M | | 3 | 4 | 0 | 35.848 |
| 2.434 | 17 | 3 | 3 | 2 | 36.892 |
| 2.355 | 11 | 1 | 6 | 0 | 38.181 |
| 2.335M | 3 | 1 | 1 | 4 | 38.531 |
| 2.335M | | 3 | 1 | 3 | 38.531 |
| 2.288M | 9 | 1 | 6 | 1 | 39.342 |
| 2.288M | | 4 | 0 | 2 | 39.342 |
| 2.2596 | 15 | 4 | 1 | 2 | 39.863 |
| 2.2467M | 18 | 3 | 2 | 3 | 40.103 |

| d(Å) | $I^{rel}$ $\sigma = \pm 3$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 2.2467M | | 2 5 2 | 40.103 |
| 2.2234M | 10 | 3 4 2 | 40.540 |
| 2.2234M | | 4 3 1 | 40.540 |
| 2.1984 | 4 | 2 0 4 | 41.023 |
| 2.1934 | 4 | 2 6 0 | 41.120 |
| 2.1807 | 6 | 4 2 2 | 41.370 |
| 2.1712 | 4 | 0 3 4 | 41.560 |
| 2.1396 | 12 | 2 6 1 | 42.203 |
| 2.1180 | 6 | 1 5 3 | 42.655 |
| 2.0614 | 6 | 4 4 1 | 43.886 |
| 2.0188 | 7 | 0 4 4 | 44.862 |
| 2.0035 | 29 | 4 1 3 | 45.223 |
| 1.9992 | 30 | 2 6 2 | 45.325 |
| 1.9810+ | 10 | 1 4 4 | 45.765 |
| 1.9810+ | | 3 4 3 | 45.765 |
| 1.9543 | 19 | 5 2 1 | 46.427 |
| 1.9424 | 14 | 3 6 1 | 46.728 |
| 1.9175 | 13 | 3 2 4 | 47.372 |
| 1.9073 | 11 | 0 7 2 | 47.641 |
| 1.8968 | 13 | 4 5 1 | 47.922 |
| 1.8914 | 18 | 5 1 2 | 48.066 |
| 1.8807 | 8 | 2 4 4 | 48.356 |
| 1.8671 | 12 | 4 3 3 | 48.732 |
| 1.8625 | 9 | 0 5 4 | 48.861 |
| 1.8447 | 27 | 5 2 2 | 49.362 |
| 1.8381 | 27 | 3 3 4 | 49.552 |
| 1.8352 | 25 | 3 6 2 | 49.637 |
| 1.8191 | 5 | 2 0 5 | 50.106 |
| 1.8167 | 5 | 2 6 3 | 50.177 |
| 1.8049 | 6 | 2 1 5 | 50.526 |
| 1.7963 | 6 | 4 5 2 | 50.786 |
| 1.7759 | 16 | 1 3 5 | 51.413 |
| 1.7723 | 20 | 4 0 4 | 51.525 |
| 1.7576 | 20 | 1 8 1 | 51.986 |
| 1.7409 | 11 | 4 6 1 | 52.524 |
| 1.7228M | 7 | 1 7 3 | 53.119 |
| 1.7228M | | 4 2 4 | 53.119 |
| 1.7128 | 13 | 2 8 0 | 53.454 |
| 1.6977 | 25 | 5 2 3 | 53.966 |
| 1.6883 | 20 | 5 4 2 | 54.293 |
| 1.6634M | 2 | 4 3 4 | 55.174 |
| 1.6634M | | 5 5 1 | 55.174 |
| 1.6431 | 6 | 5 3 3 | 55.913 |
| 1.6395 | 3 | 3 5 4 | 56.049 |

# Vanadium Oxide (Karelianite), $V_2O_3$

Synonyms
Vanadium sesquioxide
Vanadium trioxide
Vanadic oxide

Sample
The sample was prepared by reducing $V_2O_5$ in a controlled atmosphere with the partial pressure of oxygen less than or equal to $10^{-20}$ atm. It was then heated at 600 °C for 8 hours, at 925 °C for 18 hours, and at 900 °C for 30 hours with intermittent grinding.

Color
Black

Structure
Rhombohedral, $R\bar{3}c$ (167). The structure was solved by Zachariasen (1928).

Crystallographic constants of this sample
(Hexagonal axes)
$a = 4.9540(2)$ Å
$c = 14.0083(10)$

$c/a = 2.8277$

$Z = 6$
$V = 297.7$ Å$^3$
Density (calc) = 5.016 g/cm$^3$

Figure of merit
$F_{30} = 64.6(0.0097,48)$

Additional pattern
PDF card 26-278 (Hanawalt et al., 1938)

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

Zachariasen, F. W. H. (1928). Skr. Nor. Vidensk.-Akad., Kl. 1: Mat.-Naturvidensk. Kl. 4.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 27.4 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 3.658 | 71 | 0 1 2 | 24.314 |
| 2.713 | 100 | 1 0 4 | 32.987 |
| 2.477 | 80 | 1 1 0 | 36.231 |
| 2.336 | 6 | 0 0 6 | 38.514 |
| 2.189 | 36 | 1 1 3 | 41.216 |
| 2.0519 | 7 | 2 0 2 | 44.099 |
| 1.8292 | 34 | 0 2 4 | 49.811 |
| 1.6990 | 85 | 1 1 6 | 53.923 |
| 1.6210 | 1 | 0 1 8 | 56.745 |
| 1.5798 | 7 | 1 2 2 | 58.366 |
| 1.4718 | 24 | 2 1 4 | 63.115 |
| 1.4298 | 31 | 3 0 0 | 65.195 |
| 1.3316 | 14 | 1 0 10 | 70.688 |
| 1.3180 | 3 | 1 1 9 | 71.527 |
| 1.2385 | 6 | 2 2 0 | 76.916 |
| 1.2193 | 4 | 3 0 6 | 78.357 |
| 1.1972 | 1 | 2 2 3 | 80.092 |
| 1.1728M | 9 | 3 1 2 | 82.114 |
| 1.1728M | | 0 2 10 | 82.114 |
| 1.1674 | 2 | 0 0 12 | 82.575 |
| 1.1267 | 4 | 1 3 4 | 86.267 |
| 1.0940 | 12 | 2 2 6 | 89.515 |
| 1.0601M | 9 | 0 4 2 | 93.207 |
| 1.0601M | | 2 1 10 | 93.207 |
| 1.0559 | 3 | 1 1 12 | 93.693 |
| 1.0255 | 1 | 4 0 4 | 97.381 |
| .9745M | 1 | 2 3 2 | 104.456 |
| .9745M | | 0 1 14 | 104.456 |
| .9690 | 1L | 2 2 9 | 105.295 |
| .9476 | 8 | 3 2 4 | 108.760 |
| .9363 | 4 | 4 1 0 | 110.711 |
| .9068M | 4 | 1 3 10 | 116.309 |
| .9068M | | 2 0 14 | 116.309 |
| .9044 | 5 | 3 0 12 | 116.799 |
| .8689 | 5 | 4 1 6 | 124.874 |

# Ytterbium Fluoride, $YbF_3$

CAS registry no.
13760-80-0

Sample
The sample was obtained from Research Chemicals, Nuclear Corp. of America, Phoenix, AR.

Structure
Orthorhombic, Pnma (62); isostructural with $YF_3$. The structure of $YF_3$ was determined by Zalkin and Templeton (1953).

Crystallographic constants of this sample
a = 6.2164(2) Å
b = 6.7857(2)
c = 4.4316(2)

a/b = 0.9161
c/b = 0.6531

Z = 4
V = 186.94 $Å^3$
Density (calc) = 8.173 $g/cm^3$

Figure of merit
$F_{30}$ = 130.2(0.0062,37)

Polymorphism
Thoma and Brunton (1966) report that a hexagonal form exists. The transition temperature is reported to be 985 °C.

Additional patterns
PDF card 5-551 (Zalkin, Thesis, U. Calif., Berkeley, 1951)
PDF card 32-1418 (Greis, Thesis, U. Freiburg i. Br., Germany, 1976)


References
Thoma, R. E. and Brunton, G. D. (1966). Inorg. Chem. 11, 1937.

Zalkin, A. and Templeton, D. H. (1953). J. Am. Chem. Soc. 75, 2453.


$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.8 °C
Internal standards W, a = 3.16524 Å
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±2 | hkℓ | 2θ(°) |
|---|---|---|---|
| 3.712 | 19 | 0 1 1 | 23.956 |
| 3.610 | 60 | 1 0 1 | 24.641 |
| 3.394 | 62 | 0 2 0 | 26.239 |
| 3.187 | 100 | 1 1 1 | 27.973 |
| 3.107 | 1L | 2 0 0 | 28.711 |
| 2.826 | 66 | 2 1 0 | 31.638 |
| 2.5447 | 3 | 2 0 1 | 35.240 |
| 2.4720 | 27 | 1 2 1 | 36.312 |
| 2.3828 | 3 | 2 1 1 | 37.722 |
| 2.2912 | 1L | 2 2 0 | 39.291 |
| 2.2162 | 12 | 0 0 2 | 40.679 |
| 2.0869 | 2 | 1 0 2 | 43.322 |
| 2.0355 | 15 | 2 2 1 | 44.473 |
| 2.0142 | 1L | 0 3 1 | 44.970 |
| 1.9956 | 20 | 1 1 2 | 45.411 |
| 1.9164 | 40 | 1 3 1 | 47.401 |
| 1.8769 | 26 | 3 0 1 | 48.461 |
| 1.8551 | 15 | 0 2 2 | 49.068 |
| 1.8286 | 32 | 2 3 0 | 49.828 |
| 1.8090 | 18 | 3 1 1 | 50.404 |
| 1.7778 | 14 | 1 2 2 | 51.354 |
| 1.7437 | 23 | 2 1 2 | 52.432 |
| 1.6962 | 12 | 0 4 0 | 54.017 |
| 1.6425 | 17 | 3 2 1 | 55.938 |
| 1.5539 | 6 | 4 0 0 | 59.435 |
| 1.5349 | 12 | 1 4 1 | 60.245 |
| 1.5135 | 2 | 3 0 2 | 61.190 |
| 1.4771 | 6 | 3 1 2 | 62.866 |
| 1.4664 | 1L | 4 0 1 | 63.377 |
| 1.4443 | 12 | 3 3 1 | 64.461 |
| 1.4334 | 8 | 4 1 1 | 65.014 |
| 1.4130 | 1 | 4 2 0 | 66.072 |
| 1.4107 | 16 | 2 3 2 | 66.192 |
| 1.4058 | 5 | 1 1 3 | 66.452 |
| 1.3821 | 2 | 3 2 2 | 67.744 |
| 1.3469 | 5 | 0 4 2 | 69.766 |
| 1.3343 | 3 | 2 0 3 | 70.525 |
| 1.3234 | 1 | 1 2 3 | 71.189 |
| 1.3165 | 1 | 1 4 2 | 71.620 |
| 1.3090 | 1L | 2 1 3 | 72.096 |
| 1.2976 | 1L | 0 5 1 | 72.827 |
| 1.2808 | 1L | 4 3 0 | 73.942 |
| 1.2725 | 6 | 4 0 2 | 74.508 |
| 1.2703 | 6 | 1 5 1 | 74.656 |
| 1.2585 | 7 | 3 4 1 | 75.477 |

| d(Å) | $I^{rel}$ $\sigma = \pm 2$ | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 1.2507 | 1L | 4 | 1 | 2 | 76.035 |
| 1.2438 | 9 | 2 | 5 | 0 | 76.535 |
| 1.2418 | 9 | 2 | 2 | 3 | 76.678 |
| 1.2369 | 1L | 0 | 3 | 3 | 77.040 |
| 1.2306 | 1L | 4 | 3 | 1 | 77.508 |
| 1.2130 | 1L | 1 | 3 | 3 | 78.849 |
| 1.2033 | 1L | 3 | 0 | 3 | 79.611 |
| 1.1974M | 1L | 2 | 5 | 1 | 80.078 |
| 1.1974M | | 5 | 0 | 1 | 80.078 |
| 1.1914 | 5 | 4 | 2 | 2 | 80.567 |
| 1.1847 | 1 | 3 | 1 | 3 | 81.117 |
| 1.1790 | 4 | 5 | 1 | 1 | 81.593 |
| 1.1460 | 4 | 4 | 4 | 0 | 84.470 |
| 1.1379 | 3 | 1 | 5 | 2 | 85.211 |
| 1.1337 | 5 | 3 | 2 | 3 | 85.603 |
| 1.1310 | 5 | 0 | 6 | 0 | 85.861 |
| 1.1290 | 5 | 5 | 2 | 1 | 86.047 |
| 1.1087 | 1L | 4 | 3 | 2 | 88.019 |
| 1.0998 | 2 | 3 | 5 | 1 | 88.919 |
| 1.0968 | 2 | 1 | 4 | 3 | 89.231 |
| 1.0906 | 1L | 1 | 0 | 4 | 89.870 |
| 1.0846 | 5 | 2 | 5 | 2 | 90.503 |
| 1.0792 | 3 | 1 | 6 | 1 | 91.080 |
| 1.0767 | 3 | 1 | 1 | 4 | 91.351 |
| 1.0707M | 1L | 4 | 0 | 3 | 92.016 |
| 1.0707M | | 5 | 1 | 2 | 92.016 |
| 1.0620 | 1L | 3 | 3 | 3 | 92.991 |
| 1.0578M | 9 | 5 | 3 | 1 | 93.468 |
| 1.0578M | | 4 | 1 | 3 | 93.468 |
| 1.0488 | 4 | 2 | 4 | 3 | 94.528 |
| 1.0384 | 1L | 1 | 2 | 4 | 95.769 |
| 1.0329 | 3 | 5 | 2 | 2 | 96.454 |
| 1.0243 | 2 | 6 | 1 | 0 | 97.532 |
| 1.0179 | 3 | 4 | 4 | 2 | 98.358 |
| 1.0104 | 4 | 3 | 5 | 2 | 99.349 |
| 1.0074 | 2 | 0 | 6 | 2 | 99.746 |
| .9994 | 1L | 0 | 5 | 3 | 100.850 |
| .9961 | 1L | 4 | 5 | 1 | 101.307 |
| .9944 | 1L | 1 | 6 | 2 | 101.542 |
| .9867 | 1L | 1 | 5 | 3 | 102.652 |
| .9825 | 1 | 1 | 3 | 4 | 103.267 |
| .9812 | 1L | 3 | 4 | 3 | 103.451 |
| .9780 | 1 | 5 | 4 | 1 | 103.925 |
| .9687 | 8 | 3 | 6 | 1 | 105.350 |
| .9677 | 7 | 4 | 3 | 3 | 105.495 |
| .9669M | 6 | 3 | 1 | 4 | 105.620 |
| .9669M | | 6 | 2 | 1 | 105.620 |
| .9513M | 1L | 2 | 5 | 3 | 108.140 |
| .9513M | | 5 | 0 | 3 | 108.140 |
| .9420M | 4 | 5 | 1 | 3 | 109.716 |
| .9420M | | 6 | 3 | 0 | 109.716 |

# Zinc Vanadium Oxide, $Zn_3(VO_4)_2$

Synonym
Zinc vanadate

Sample
The sample was made by heating a 3:1 molar mixture of ZnO and $V_2O_5$ at 780 °C for 3 days, with several regrindings.

Color
Yellowish white

Structure
Orthorhombic, Abam (64) (Brisi, 1960).
Isostructural with $Co_3(VO_4)_2$.

Crystallographic constants of this sample
a = 8.299(1) Å
b = 11.5284(14)
c = 6.1116(7)

a/b = 0.7199
c/b = 0.5301

Z = 4
V = 584.72 Å$^3$
Density (calc) = 4.839 g/cm$^3$

Figure of merit
$F_{30}$ = 66.6(0.010,44)

Polymorphism
Brown and Hummel (1965) report two polymorphic changes in $Zn_3(VO_4)_2$ at 795° and 815 °C. This is disputed by Makarov et al. (1971).

Additional patterns
PDF card 16-830 (Brisi, 1960)
PDF card 19-1469 (Brown and Hummel, 1965)
Makarov et al. (1971)

References
Brisi, C. (1960). Ric. Sci. 30, 1339.

Brown, J. J. and Hummel, F. A. (1965). Trans. Br. Ceram. Soc. 64, 419.

Makarov, V. A., Fotiev, A. A., and Serebryakova, L. N. (1971). Russ. J. Inorg. Chem. Eng. Transl. 16, 1515.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±5 | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.762 | 13 | 0 2 0 | 15.364 |
| 4.731 | 18 | 1 2 0 | 18.742 |
| 4.147 | 7 | 2 0 0 | 21.410 |
| 3.367 | 20 | 2 2 0 | 26.452 |
| 3.290 | 27 | 2 1 1 | 27.080 |
| 3.059 | 1 | 0 0 2 | 29.165 |
| 3.030 | 57 | 1 3 1 | 29.460 |
| 2.882 | 30 | 0 4 0 | 31.004 |
| 2.723 | 4 | 1 4 0 | 32.866 |
| 2.700 | 9 | 0 2 2 | 33.156 |
| 2.568 | 100 | 1 2 2 | 34.907 |
| 2.494 | 47 | 3 2 0 | 35.980 |
| 2.462M | 25 | 3 1 1 | 36.466 |
| 2.462M | | 2 0 2 | 36.466 |
| 2.367 | 3 | 2 4 0 | 37.984 |
| 2.263 | 3 | 2 2 2 | 39.797 |
| 2.0964 | 37 | 0 4 2 | 43.116 |
| 2.0878 | 36 | 1 5 1 | 43.302 |
| 2.0747 | 1 | 4 0 0 | 43.589 |
| 2.0323 | 1 | 1 4 2 | 44.546 |
| 1.9533 | 3 | 4 2 0 | 46.453 |
| 1.9319 | 4 | 3 2 2 | 46.998 |
| 1.9203 | 4 | 0 6 0 | 47.299 |
| 1.9154 | 4 | 2 5 1 | 47.426 |
| 1.8716M | 5 | 1 6 0 | 48.608 |
| 1.8716M | | 2 4 2 | 48.608 |
| 1.8061 | 4 | 2 1 3 | 50.491 |
| 1.7588 | 6 | 1 3 3 | 51.950 |
| 1.7167 | 8 | 4 0 2 | 53.323 |
| 1.6509 | 3 | 2 3 3 | 55.627 |
| 1.6457 | 4 | 4 2 2 | 55.817 |
| 1.6237 | 7 | 3 1 3 | 56.641 |
| 1.5963 | 23 | 1 6 2 | 57.704 |
| 1.5863 | 8 | 5 1 1 | 58.103 |
| 1.5778 | 12 | 3 6 0 | 58.444 |
| 1.5276 | 13 | 0 0 4 | 60.562 |
| 1.5145 | 6 | 2 6 2 | 61.145 |
| 1.5014 | 3 | 1 5 3 | 61.734 |
| 1.4848 | 4 | 2 7 1 | 62.503 |
| 1.4748 | 38 | 4 4 2 | 62.975 |
| 1.4542 | 2 | 1 2 4 | 63.972 |
| 1.4414 | 13 | 0 8 0 | 64.609 |
| 1.4377 | 2 | 5 4 0 | 64.793 |
| 1.4331M | 1 | 2 0 4 | 65.028 |
| 1.4331M | | 2 5 3 | 65.028 |

Zinc Vanadium Oxide, $Zn_3(VO_4)_2$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 5$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4095 | 1 | 4 6 0 | 66.254 |
| 1.3918 | 1 | 2 2 4 | 67.211 |
| 1.3786 | 2 | 3 7 1 | 67.937 |
| 1.3495 | 3 | 0 4 4 | 69.610 |
| 1.3400 | 1L | 6 1 1 | 70.180 |
| 1.3028 | 9 | 3 2 4 | 72.493 |
| 1.2838 | 2 | 2 4 4 | 73.744 |
| 1.2789 | 4 | 5 1 3 | 74.070 |
| 1.2563 | 1 | 5 6 0 | 75.638 |
| 1.2471 | 3 | 6 4 0 | 76.290 |
| 1.2436 | 2 | 2 8 2 | 76.543 |
| 1.2302 | 3 | 4 0 4 | 77.534 |

# Zirconium Boride, $ZrB_2$

Synonym
Zirconium diboride

CAS registry no.
12045-64-6

Sample
The sample was prepared at NBS by S. Lang.

Color
Very dark gray

Structure
Hexagonal, P6/mmm (191). Kiessling (1949) and Norton et al. (1949) studied the structure of $ZrB_2$. This phase is isomorphous with $AlB_2$.

Crystallographic constants of this sample
$a = 3.16870(8)$ Å
$c = 3.53002(10)$

$c/a = 1.1140$

$Z = 1$
$V = 30.70$ Å$^3$
Density (calc) = 6.104 g/cm$^3$

Figure of merit
$F_{23} = 175.3(0.0057,23)$

Additional pattern
PDF card 6-610 (Am. Electro Metal Co.)

References
Kiessling, R. (1949). Acta Chem. Scand. 3, 90.

Norton, J. T., Blumenthal, H., and Sindeband, J. (1949). Metall. Trans. 185, 749.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; mean T = 24.9 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ $\sigma = \pm 1$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 3.530 | 30 | 0 0 1 | 25.205 |
| 2.7445 | 67 | 1 0 0 | 32.601 |
| 2.1663 | 100 | 1 0 1 | 41.658 |
| 1.7652 | 9 | 0 0 2 | 51.746 |
| 1.5843 | 19 | 1 1 0 | 58.184 |
| 1.4845 | 21 | 1 0 2 | 62.515 |
| 1.4455 | 16 | 1 1 1 | 64.404 |
| 1.3722 | 8 | 2 0 0 | 68.298 |
| 1.2789 | 16 | 2 0 1 | 74.071 |
| 1.1790 | 13 | 1 1 2 | 81.585 |
| 1.1769 | 1 | 0 0 3 | 81.770 |
| 1.0832 | 8 | 2 0 2 | 90.654 |
| 1.0813 | 10 | 1 0 3 | 90.853 |
| 1.0372 | 7 | 2 1 0 | 95.918 |
| .9951 | 14 | 2 1 1 | 101.442 |
| .9446 | 4 | 1 1 3 | 109.266 |
| .9147 | 3 | 3 0 0 | 114.733 |
| .8942 | 10 | 2 1 2 | 118.958 |
| .8932 | 6 | 2 0 3 | 119.185 |
| .8855 | 4 | 3 0 1 | 120.899 |
| .8825 | 2 | 0 0 4 | 121.593 |
| .8402 | 4 | 1 0 4 | 132.938 |
| .8122 | 7 | 3 0 2 | 143.047 |

# Zirconium Hydrogen Phosphate Hydrate, $Zr(HPO_4)_2 \cdot H_2O$

Synonym
Zirconium hydrogen orthophosphate hydrate

CAS registry no.
13933-56-7

Sample
The sample was prepared by the method of Alberti and Torracca (1968). $ZrOCl \cdot 8H_2O$ was dissolved in $H_2O$. HF and $H_3PO_4$ were added and the solution allowed to evaporate slowly at room temperature. The crystals formed were very fine needles.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14) (Ahrland and Albertsson, 1969). The structure was determined by Clearfield and Smith (1969).

Crystallographic constants of this sample

a = 15.463(4) Å
b = 5.294(2)
c = 9.0674(15)
β = 101.70(2)°

a/b = 2.9209
c/b = 1.7128

Z = 4
V = 726.83 $Å^3$
Density (calc) = 2.753 $g/cm^3$

Figure of merit
$F_{30}$ = 21.0(0.013,108)

Additional patterns
PDF card 19-1489 (Sedlakova and Pekarks, 1966)
PDF card 21-396 (Michel and Weiss, 1967)
PDF card 21-397 (Priv. Comm., Winkler, 1968)
PDF card 22-1022 (Ahrland and Albertsson, 1969)

References

Ahrland, S. and Albertsson, J. (1969). Acta Chem. Scand. 23, 1446.

Alberti, G. and Torracca, E. (1968). J. Inorg. Nucl. Chem. 30, 317.

Clearfield, A. and Smith, G. D. (1969). Inorg. Chem. 8, 431.

Michel, E. and Weiss, A. (1967). Z. Naturforsch. 22B, 1100.

Sedlakova, L. and Pekarks, V. (1966). J. Less-Common Met. 10, 130.


$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26±2 °C
Internal standards Si, SRM 640a
Fluorophlogopite, SRM 675

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | | | 2θ(°) |
|---|---|---|---|---|---|
| 7.59 | 100 | 2 | 0 | 0 | 11.653 |
| 4.489 | 14 | -1 | 1 | 1 | 19.761 |
| 4.441 | 8 | 0 | 0 | 2 | 19.978 |
| 4.052 | 1L | 3 | 0 | 1 | 21.917 |
| 3.785 | 1 | 4 | 0 | 0 | 23.483 |
| 3.568 | 51 | -3 | 1 | 1 | 24.934 |
| 3.531 | 31 | 2 | 0 | 2 | 25.198 |
| 3.220 | 3 | -4 | 0 | 2 | 27.683 |
| 3.082 | 1 | 4 | 1 | 0 | 28.948 |
| 3.045 | 2 | -3 | 1 | 2 | 29.309 |
| 3.022 | 1L | -1 | 0 | 3 | 29.539 |
| 2.649M | 14 | -5 | 1 | 1 | 33.811 |
| 2.649M | | 0 | 2 | 0 | 33.811 |
| 2.626 | 14 | -1 | 1 | 3 | 34.112 |
| 2.524M | 4 | -1 | 2 | 1 | 35.539 |
| 2.524M | | 6 | 0 | 0 | 35.539 |
| 2.475 | 1L | 1 | 1 | 3 | 36.263 |
| 2.408 | 6 | 5 | 1 | 1 | 37.305 |
| 2.353 | 2 | 3 | 0 | 3 | 38.219 |
| 2.277 | 1L | 6 | 1 | 0 | 39.544 |
| 2.219 | 1L | 0 | 0 | 4 | 40.631 |
| 2.197 | 1 | -6 | 1 | 2 | 41.059 |
| 2.169 | 3 | 4 | 2 | 0 | 41.600 |
| 2.164 | 2 | -5 | 1 | 3 | 41.705 |
| 2.118 | 3 | 2 | 2 | 2 | 42.663 |
| 2.111 | 2 | -4 | 0 | 4 | 42.806 |
| 2.045 | 5 | -4 | 2 | 2 | 44.258 |
| 2.038 | 4 | -7 | 1 | 1 | 44.425 |
| 2.023 | 3 | 2 | 0 | 4 | 44.769 |
| 1.996 | 1 | 3 | 2 | 2 | 45.407 |
| 1.968 | 1L | -7 | 1 | 2 | 46.077 |
| 1.930 | 1L | 5 | 0 | 3 | 47.055 |
| 1.8922M | 5 | 8 | 0 | 0 | 48.044 |
| 1.8922M | | 5 | 2 | 1 | 48.044 |
| 1.8791 | 5 | 7 | 1 | 1 | 48.400 |
| 1.8647M | 5 | 4 | 2 | 2 | 48.800 |
| 1.8647M | | -6 | 0 | 4 | 48.800 |

# Zirconium Titanium Oxide, $ZrTiO_4$

Synonym
Zirconium titanate

CAS registry no.
12036-70-3

Sample
The sample was prepared by heating equimolar amounts of $ZrO_2$ and $TiO_2$ at 1500 °C for 66 hours. It was then heat-treated at 1500 °C for 17 hours and quenched in distilled water.

Color
Pale pink

Structure
Orthorhombic, Pnab (60). The unit cell was determined by Coughanour et al. (1954) and the space group by Newnham (1967).

Crystallographic constants of this sample

a = 5.0358(5) Å
b = 5.4874(6)
c = 4.8018(6)

a/b = 0.9177
c/b = 0.8751

Z = 2
V = 132.69 $Å^3$
Density (calc) = 5.084 $g/cm^3$

Figure of merit
$F_{30}$ = 68.0(0.011,41)

Additional pattern
PDF card 7-290 (Coughanour et al., 1954)

References
Coughanour, L. W., Roth, R. S., and DeProsse, V. A. (1954). J. Res. Natl. Bur. Stand. (U.S.), 52, 37.

Newnham, R. E. (1967). J. Am. Ceram. Soc. 50, 216.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 25.5 °C
Internal standard W, a = 3.16524 Å

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 3.614 | 16 | 0 1 1 | 24.614 |
| 2.934 | 100 | 1 1 1 | 30.443 |
| 2.744 | 13 | 0 2 0 | 32.612 |
| 2.517 | 10 | 2 0 0 | 35.642 |
| 2.408 | 9 | 1 2 0 | 37.312 |
| 2.229 | 3 | 2 0 1 | 40.431 |
| 2.154 | 10 | 1 2 1 | 41.911 |
| 2.0661 | 4 | 2 1 1 | 43.781 |
| 2.0158 | 1L | 1 1 2 | 44.931 |
| 1.8542 | 13 | 2 2 0 | 49.092 |
| 1.8067 | 11 | 0 2 2 | 50.472 |
| 1.7376 | 13 | 2 0 2 | 52.632 |
| 1.7096 | 9 | 0 3 1 | 53.562 |
| 1.7013 | 12 | 1 2 2 | 53.843 |
| 1.6192 | 6 | 1 3 1 | 56.813 |
| 1.5366 | 1L | 0 1 3 | 60.174 |
| 1.5224 | 10 | 3 1 1 | 60.794 |
| 1.4679 | 11 | 2 2 2 | 63.305 |
| 1.4318 | 4 | 3 2 0 | 65.096 |
| 1.4144 | 6 | 2 3 1 | 65.996 |
| 1.3506 | 1L | 2 0 3 | 69.548 |
| 1.3345 | 1L | 3 1 2 | 70.508 |
| 1.3233 | 4 | 1 4 0 | 71.199 |
| 1.3121 | 1L | 2 1 3 | 71.899 |
| 1.2763 | 1 | 1 4 1 | 74.250 |
| 1.2590 | 1 | 4 0 0 | 75.441 |
| 1.2298 | 1L | 3 2 2 | 77.562 |
| 1.2174 | 1L | 4 0 1 | 78.503 |
| 1.2046M | 2 | 2 4 0 | 79.504 |
| 1.2046M | | 0 3 3 | 79.504 |
| 1.2003 | 1 | 0 0 4 | 79.844 |
| 1.1978 | 1 | 3 3 1 | 80.044 |
| 1.1910 | 1 | 0 4 2 | 80.594 |
| 1.1890 | 1 | 4 1 1 | 80.764 |
| 1.1716 | 1L | 1 3 3 | 82.215 |
| 1.1591 | 3 | 1 4 2 | 83.296 |
| 1.1443 | 1 | 4 2 0 | 84.627 |
| 1.1336 | 1 | 3 1 3 | 85.608 |
| 1.1152 | 1 | 4 0 2 | 87.379 |
| 1.0997M | 1L | 0 2 4 | 88.930 |
| 1.0997M | | 3 3 2 | 88.930 |
| 1.0864 | 2 | 2 3 3 | 90.312 |

# Zirconium Titanium Oxide, $Zr_5Ti_7O_{24}$

Synonym
Zirconium titanate

Sample
The sample was prepared by blending $ZrO_2$ and $TiO_2$ in the molar ratio of 5:7, doped with 1/2 mole % of $Y_2O_3$ to promote crystallinity, and calcined at 1000 °C for 24 hours, twice reground and fired at 1500 °C for 20 hours, heat-treated at 1300 °C for several hours and cooled at 1 °C/hour to 650 °C (McHale et al., 1983).

Color
Pale yellowish pink

Structure
Orthorhombic, Pcan (60). The material has the columbite structure (McHale et al., 1983). The structure was confirmed by neutron powder diffraction (Bourdot, 1983).

Crystallographic constants of this sample
a = 5.3255(5) Å
b = 14.374(2)
c = 5.0236(5)

a/b = 0.3705
c/b = 0.3495

Z = 1
V = 384.55 Å$^3$
Density (calc) = 5.075 g/cm$^3$

Figure of merit
$F_{30}$ = 66.8(0.011,43)

References
Bourdot, P. (1983). Private communication.

McHale, A. E., Roth, R. S., Santoro, A., and Simmons, J. (1983). Am. Ceram. Soc. Bull. 62, 387.

$CuK\alpha_1$ λ = 1.540598 Å; mean T = 26.0 °C
Internal standard Si, SRM 640a

| d(Å) | $I^{rel}$ σ = ±1 | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.19 | 4 | 0 2 0 | 12.305 |
| 3.592 | 6 | 0 4 0 | 24.765 |
| 3.561 | 14 | 1 3 0 | 24.986 |
| 3.543 | 11 | 1 1 1 | 25.116 |
| 3.257 | 8 | 1 2 1 | 27.358 |
| 2.904 | 100 | 1 3 1 | 30.760 |
| 2.663 | 15 | 2 0 0 | 33.628 |
| 2.561 | 3 | 1 4 1 | 35.013 |
| 2.513 | 9 | 0 0 2 | 35.704 |
| 2.498 | 4 | 2 2 0 | 35.921 |
| 2.475 | 2 | 0 1 2 | 36.264 |
| 2.396 | 4 | 0 6 0 | 37.506 |
| 2.353 | 4 | 2 0 1 | 38.217 |
| 2.321 | 1L | 2 1 1 | 38.758 |
| 2.260 | 4 | 1 5 1 | 39.863 |
| 2.225 | 1 | 0 3 2 | 40.513 |
| 2.1389 | 4 | 2 4 0 | 42.218 |
| 2.1123 | 10 | 2 3 1 | 42.776 |
| 2.0594 | 5 | 0 4 2 | 43.931 |
| 2.0531 | 4 | 1 3 2 | 44.071 |
| 1.9680 | 1 | 2 4 1 | 46.084 |
| 1.9190 | 2 | 1 4 2 | 47.332 |
| 1.8904 | 2 | 0 5 2 | 48.092 |
| 1.8267 | 14 | 2 0 2 | 49.883 |
| 1.8127 | 2 | 2 1 2 | 50.293 |
| 1.7905 | 3 | 1 7 1 | 50.964 |
| 1.7814 | 15 | 2 6 0 | 51.241 |
| 1.7705 | 6 | 2 2 2 | 51.580 |
| 1.7333 | 10 | 0 6 2 | 52.772 |
| 1.6788 | 7 | 2 6 1 | 54.626 |
| 1.6651 | 11 | 3 3 0 | 55.112 |
| 1.6620 | 8 | 3 1 1 | 55.222 |
| 1.6285 | 2 | 2 4 2 | 56.461 |
| 1.5880 | 5 | 1 1 3 | 58.035 |
| 1.5804 | 11 | 3 3 1 | 58.342 |
| 1.5592 | 3 | 1 2 3 | 59.211 |
| 1.5425 | 1 | 2 5 2 | 59.920 |
| 1.5293 | 1L | 1 9 0 | 60.489 |
| 1.5153 | 5 | 1 3 3 | 61.108 |
| 1.4895 | 1 | 2 8 0 | 62.283 |
| 1.4634 | 6 | 1 9 1 | 63.520 |
| 1.4612 | 5 | 0 8 2 | 63.627 |
| 1.4592 | 4 | 1 4 3 | 63.724 |
| 1.4534 | 4 | 2 6 2 | 64.012 |
| 1.4459 | 2 | 3 5 1 | 64.381 |

Zirconium Titanium Oxide, $Zr_5Ti_7O_{24}$ - (continued)

| d(Å) | $I^{rel}$ $\sigma = \pm 1$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4209 | 1L | 3 2 2 | 65.655 |
| 1.4176 | 1 | 2 0 3 | 65.827 |
| 1.4109 | 3 | 2 1 3 | 66.179 |
| 1.3877 | 2 | 3 3 2 | 67.434 |
| 1.3649 | 1 | 2 7 2 | 68.714 |
| 1.3448 | 1L | 3 4 2 | 69.889 |
| 1.3093 | 2 | 4 2 0 | 72.076 |
| 1.2971 | 1L | 3 7 1 | 72.862 |
| 1.2872 | 2 | 4 0 1 | 73.517 |
| 1.2817 | 1 | 4 1 1 | 73.886 |
| 1.2612 | 1L | 1 7 3 | 75.292 |
| 1.2556 | 1L | 0 0 4 | 75.681 |
| 1.2511 | 1 | 0 1 4 | 76.007 |
| 1.2371 | 1 | 0 2 4 | 77.022 |
| 1.2135 | 1 | 3 1 3 | 78.804 |
| 1.2050 | 1L | 1 2 4 | 79.470 |
| 1.1979 | 1L | 0 12 0 | 80.041 |
| 1.1874 | 1 | 3 9 0 | 80.892 |
| 1.1846M | 1L | 1 3 4 | 81.121 |
| 1.1846M | | 3 7 2 | 81.121 |
| 1.1807 | 1 | 3 3 3 | 81.443 |
| 1.1762 | 1 | 4 0 2 | 81.827 |
| 1.1636 | 2 | 4 6 0 | 82.901 |
| 1.1607 | 2 | 4 2 2 | 83.156 |
| 1.1553 | 2 | 3 9 1 | 83.632 |
| 1.1336 | 2 | 4 6 1 | 85.613 |
| 1.1297M | 1L | 2 10 2 | 85.981 |
| 1.1297M | | 1 9 3 | 85.981 |

# Molybdenum Oxide (Molybdite), $MoO_3$

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

Synonym
Molybdenum trioxide

CAS registry no.
1313-27-5

Structure
Orthorhombic, Pbnm (62). The structure was refined from single crystal data (Kihlborg, 1963).

Atom positions
All atoms were in special positions 4(c).

Intensities
The peak intensities here differ from those on PDF card 5-508 (Swanson et al., 1954), especially at hkℓ's 040 and 060. From a spray-dried sample, recent experimental intensity measurements at NBS support the intensity values given in this calculated pattern.

Crystallographic constants of this sample
a = 3.9630 Å
b = 13.856
c = 3.6966

a/b = 0.2860
c/b = 0.2668

(published values: 3.9628, 13.855, 3.6964 Å; Kihlborg, 1963)

Z = 4
V = 202.99 $Å^3$
Density (calc) = 4.710 $g/cm^3$

Thermal parameters
Isotropic (Kihlborg, 1963)

Scattering factors
$O^{-2}$ (Suzuki, 1960)
$Mo^0$ (Thomas and Umeda, 1957), corrected for the real part of the anomalous dispersion (Cromer and Liberman, 1970).

Scale factors
$\gamma = 0.686 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 4.80, for the scale reflection hkℓ = 021.

Polymorphism
A hexagonal form has been reported (PDF card 21-569, Spangenberg, Westinghouse Electric Corp., Horseheads, NY).

Additional pattern
PDF card 5-508 (Swanson et al., 1954)

References

Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.

Kihlborg, L. (1963). Ark. Kemi 21, 357.

Suzuki, T. (1960). Acta Crystallogr. 13, 279.

Swanson, H. E., Fuyat, R. K., and Ugrinic, G. M. (1954). Natl. Bur. Stand. (U.S.) Circ. 539, 3, 30.

Thomas, L. H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.


Calculated Pattern (Peak heights)
λ=1.540598Å

| d(Å) | $I^{rel}$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.921 | 36 | 0 2 0 | 12.78 |
| 3.808 | 77 | 1 1 0 | 23.34 |
| 3.464 | 38 | 0 4 0 | 25.70 |
| 3.440 | 31 | 1 2 0 | 25.88 |
| 3.259 | 100 | 0 2 1 | 27.34 |
| 3.008 | 7 | 1 3 0 | 29.68 |
| 2.703 | 15 | 1 0 1 | 33.12 |
| 2.653 | 26 | 1 1 1 | 33.76 |
| 2.608 | 3 | 1 4 0 | 34.36 |
| 2.5267 | 7 | 0 4 1 | 35.50 |
| 2.3329 | 8 | 1 3 1 | 38.56 |
| 2.3088 | 21 | 0 6 0 | 38.98 |
| 2.2707 | 13 | 1 5 0 | 39.66 |
| 2.1311 | 7 | 1 4 1 | 42.38 |
| 1.9953 | 2 | 1 6 0 | 45.42 |
| 1.9812 | 8 | 2 0 0 | 45.76 |
| 1.9586+ | 12 | 0 6 1 | 46.32 |
| 1.9349 | 1 | 1 5 1 | 46.92 |
| 1.9051 | 1 | 2 2 0 | 47.70 |
| 1.8483 | 15 | 0 0 2 | 49.26 |
| 1.8206 | 9 | 2 3 0 | 50.06 |
| 1.7860 | 2 | 0 2 2 | 51.10 |
| 1.7705 | 2 | 1 7 0 | 51.58 |
| 1.7559 | 4 | 1 6 1 | 52.04 |
| 1.7324 | 13 | 2 1 1 | 52.80 |
| 1.7203 | 2 | 2 4 0 | 53.20 |
| 1.6933 | 5 | 2 2 1 | 54.12 |
| 1.6627 | 10 | 1 1 2 | 55.20 |
| 1.6301 | 9 | 0 4 2 | 56.40 |
| 1.6285 | 9 | 1 2 2 | 56.46 |
| 1.5969 | 12 | 1 7 1 | 57.68 |
| 1.5869 | 3 | 1 8 0 | 58.08 |
| 1.5745 | 2 | 1 3 2 | 58.58 |
| 1.5682 | 11 | 0 8 1 | 58.84 |
| 1.5079 | 1 | 1 4 2 | 61.44 |
| 1.5039 | 3 | 2 6 0 | 61.62 |
| 1.4776 | 10 | 2 5 1 | 62.84 |
| 1.4585 | 1 | 1 8 1 | 63.76 |
| 1.4431 | 7 | 0 6 2 | 64.52 |
| 1.4337+ | 8 | 1 5 2 | 65.00 |

| d(Å) | $I^{rel}$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4004 | 4 | 2 7 0 | 66.74 |
| 1.3931 | 1 | 2 6 1 | 67.14 |
| 1.3854 | 3 | 0 10 0 | 67.56 |
| 1.3558 | 1 | 1 6 2 | 69.24 |
| 1.3518 | 3 | 2 0 2 | 69.48 |
| 1.3453 | 3 | 2 1 2 | 69.86 |
| 1.3380 | 1 | 1 9 1 | 70.30 |
| 1.3096 | 1 | 2 7 1 | 72.06 |
| 1.2975+ | 8 | 2 3 2 | 72.84 |
| 1.2788 | 1 | 1 7 2 | 74.08 |
| 1.2591 | 1 | 2 4 2 | 75.44 |
| 1.2440 | 4 | 3 0 1 | 76.52 |
| 1.2331+ | 2 | 1 10 1 | 77.32 |
| 1.2299 | 3 | 2 8 1 | 77.56 |
| 1.2157 | 1 | 2 9 0 | 78.64 |
| 1.2131 | 4 | 0 2 3 | 78.84 |
| 1.2041 | 2 | 1 8 2 | 79.54 |
| 1.2011+ | 2 | 3 3 1 | 79.78 |

+ More than one hkℓ possible

Calculated Pattern (Integrated)
λ=1.540598Å

| d(Å) | $I^{rel}$ | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.927 | 31 | 0 2 0 | 12.77 |
| 3.8098 | 73 | 1 1 0 | 23.33 |
| 3.4636 | 34 | 0 4 0 | 25.70 |
| 3.4399 | 25 | 1 2 0 | 25.88 |
| 3.2618 | 100 | 0 2 1 | 27.32 |
| 3.0076 | 7 | 1 3 0 | 29.68 |
| 2.7034 | 15 | 1 0 1 | 33.11 |
| 2.6528 | 27 | 1 1 1 | 33.76 |
| 2.6079 | 3 | 1 4 0 | 34.36 |
| 2.5274 | 7 | 0 4 1 | 35.49 |
| 2.5185 | 1 | 1 2 1 | 35.62 |
| 2.3329 | 8 | 1 3 1 | 38.56 |
| 2.3093 | 22 | 0 6 0 | 38.97 |
| 2.2713 | 14 | 1 5 0 | 39.65 |
| 2.1311 | 8 | 1 4 1 | 42.38 |
| 1.9953 | 2 | 1 6 0 | 45.42 |
| 1.9816 | 8 | 2 0 0 | 45.75 |
| 1.9613 | 8 | 2 1 0 | 46.25 |
| 1.9586 | 8 | 0 6 1 | 46.32 |
| 1.9349 | 1 | 1 5 1 | 46.92 |
| 1.9051 | 1 | 2 2 0 | 47.70 |
| 1.8483 | 17 | 0 0 2 | 49.26 |
| 1.8210 | 11 | 2 3 0 | 50.05 |
| 1.7860 | 2 | 0 2 2 | 51.10 |
| 1.7708 | 2 | 1 7 0 | 51.57 |
| 1.7559 | 4 | 1 6 1 | 52.04 |
| 1.7327 | 15 | 2 1 1 | 52.79 |
| 1.7200 | 2 | 2 4 0 | 53.21 |
| 1.6935 | 6 | 2 2 1 | 54.11 |
| 1.6629 | 12 | 1 1 2 | 55.19 |
| 1.6335 | 2 | 2 3 1 | 56.27 |
| 1.6306 | 7 | 0 4 2 | 56.38 |
| 1.6282 | 5 | 1 2 2 | 56.47 |
| 1.5969 | 14 | 1 7 1 | 57.68 |
| 1.5871 | 2 | 1 8 0 | 58.07 |
| 1.5748 | 2 | 1 3 2 | 58.57 |
| 1.5684 | 13 | 0 8 1 | 58.83 |
| 1.5081 | 1 | 1 4 2 | 61.43 |
| 1.5037 | 3 | 2 6 0 | 61.63 |
| 1.4774 | 12 | 2 5 1 | 62.85 |
| 1.4583 | 1 | 1 8 1 | 63.77 |
| 1.4429 | 8 | 0 6 2 | 64.53 |
| 1.4350 | 4 | 1 9 0 | 64.93 |
| 1.4334 | 7 | 1 5 2 | 65.01 |
| 1.4004 | 5 | 2 7 0 | 66.74 |
| 1.3929 | 1 | 2 6 1 | 67.15 |
| 1.3856 | 3 | 0 10 0 | 67.55 |
| 1.3558 | 1 | 1 6 2 | 69.24 |
| 1.3516 | 4 | 2 0 2 | 69.49 |
| 1.3452 | 4 | 2 1 2 | 69.87 |
| 1.3378 | 1 | 1 9 1 | 70.31 |
| 1.3096 | 1 | 2 7 1 | 72.06 |
| 1.2976 | 4 | 3 2 0 | 72.83 |
| 1.2972 | 7 | 2 3 2 | 72.86 |
| 1.2786 | 1 | 1 7 2 | 74.09 |
| 1.2591 | 1 | 2 4 2 | 75.44 |
| 1.2440 | 4 | 3 0 1 | 76.52 |
| 1.2343 | 1 | 3 4 0 | 77.23 |
| 1.2331 | 2 | 1 10 1 | 77.32 |
| 1.2297 | 3 | 2 8 1 | 77.57 |
| 1.2158 | 1 | 2 9 0 | 78.63 |
| 1.2132 | 4 | 0 2 3 | 78.83 |
| 1.2040 | 2 | 1 8 2 | 79.55 |
| 1.2011 | 1 | 3 3 1 | 79.78 |
| 1.2005 | 1 | 1 11 0 | 79.83 |

## 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.

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| Picric acid | $C_6H_3N_3O_7$ | 16m | 56 |
| Pimelic acid | $(CH_2)_5(CO_2H)_2$ | 7m | 153 |
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| 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 |
| $\Delta^9$-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

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Section 20 - Data for 71 Substances

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Standard x-ray powder diffraction patterns are presented for 71 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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