



NBS MONOGRAPH **25**—SECTION **19**

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

Standard X-ray Diffraction Powder Patterns

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

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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.

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ERRATA

Circular 539

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

Monograph 25

Section 11, p. 18: Density should be 2.197.
p. 56: Density should be 2.733.

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

p. 32: Z should be 4.
p. 34: Density should be 1.608.

Section 18, p. 3: Figure 2 is upside down.
p. 9: The value c/b should be 0.3548, and the calculated density should be 3.876.
p. 10: Add to the sample description "A final heating was made at 1350°C for 2 days."
p. 35: The value c/b should be 0.5356.
p. 63: In the reference to Bouaziz, delete the volume number 7.
p. 63: In the table, at $d=1.5509$, the intensity should be 14.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 19 --- Data for 51 Substances

by

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

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

INTRODUCTION

The Powder Diffraction File (PDF) is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the JCPDS--International Centre for Diffraction Data¹, the PDF is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the JCPDS, the program at the National Bureau of Standards contributes new or improved data to the PDF. Our work also aids in the development of diffraction techniques. This report presents information for one calculated and 50 experimental patterns, and is the twenty-ninth of the series of Standard X-ray Diffraction Powder Patterns².

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]

¹JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081. This Pennsylvania non-profit corporation functions in co-operation 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.

²See previous page for other published volumes.

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

Optical data. When reported, optical measurements were made by grain immersion methods, in white light, using oils standardized in sodium light, in the refractive index range 1.40 to 2.1 [Hartshorne and Stuart, 1970].

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

Interplanar spacings. All spacing determinations were made using an internal standard mixed with the sample, packed in a shallow holder. Choice of the standard was determined by the need for low angle and unobstructed reflections. The amount of standard was estimated so that the intensity of its strongest peak would be about equal to the intensity of the strongest peak of the sample. The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in Table 1; the 2 θ angles were computed using cell dimensions uncorrected for index of refraction.

Standard Reference Material 640, Si powder ($a=5.43088\text{\AA}$), was used for many patterns. This SRM is now out of stock and has been replaced by SRM 640a ($a=5.430825\text{\AA}$), [1982; Hubbard, 1982a]. The SRM 640a lattice constant for Si was refined from multiple powder data measurements made with tungsten and silver as internal standards. Single crystal cell parameter data were also collected. The lattice parameters from the two methods agreed within three parts in 10⁵. D-spacing results using SRM 640a will be in agreement with patterns recorded in this series of Monographs since 1966.

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

Table 1

| Calculated 2 θ Angles, CuK α_1 λ = 1.540598Å | | | |
|--|----------------------------|-----------------------------|--|
| hk ℓ | W a=3.16524Å ±.00004 | Ag a=4.08651Å ±.00002 | Si a=5.430825Å ±.000011 (SRM 640a)* |
| 110 | 40.262 | | |
| 111 | | 38.112 | 28.443 |
| 200 | 58.251 | 44.295 | |
| 211 | 73.184 | | |
| 220 | 86.996 | 64.437 | 47.304 |
| 310 | 100.632 | | |
| 311 | | 77.390 | 56.124 |
| 222 | 114.923 | 81.533 | |
| 321 | 131.171 | | |
| 400 | 153.535 | 97.875 | 69.132 |
| 331 | | 110.499 | 76.378 |
| 420 | | 114.914 | |
| 422 | | 134.871 | 88.033 |
| 511/333 | | 156.737 | 94.955 |
| 440 | | | 106.712 |
| 531 | | | 114.096 |
| 620 | | | 127.550 |
| 533 | | | 136.900 |
| 444 | | | 158.644 |

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

Table 2

| SRM 675, Fluorophlogopite (FP) | |
|--|------------|
| d ₀₀₁ = 9.98104Å ± 0.00007 | |
| Calculated 2 θ Angles, CuK α_1 λ = 1.540598Å | |
| 00 ℓ | 2 θ |
| 1 | 8.853 |
| 2 | 17.759 |
| 3 | 26.774 |
| 4 | 35.962 |
| 5 | 45.397 |
| 6 | 55.169 |
| 7 | 65.399 |
| 8 | 76.255 |
| 10 | 101.025 |
| 11 | 116.193 |
| 12 | 135.674 |

All data were collected at 25 ± 1 °C on a diffractometer equipped with a focusing graphite crystal monochromator located between the sample

and the scintillation counter. Pulse height discrimination was used as well. The data were collected using copper radiation: λ (CuK α_1 , peak) = 1.540598Å [Deslattes and Henins, 1973].

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

Manual patterns were measured on a diffractometer equipped with a strip chart recorder. The readings of 2 θ were taken at positions about 20% of the way down from the top, and in the center of the peak width. This avoided errors associated with aberrations at the very top of the peaks. The K α_2 peaks were occasionally read to assist in establishing a K α_1 peak position, but K α_2 peaks are not reported.

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

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

All patterns were plotted on paper with the plot program PLOT.PATTERN/HRD on a scale of one degree per inch and were visually inspected. The program POWDER.REFLEC was used to calculate a polynomial correction curve from the expected and observed 2 θ peak positions of the internal standard reflections and to correct the observed 2 θ values of the sample. The program POWDER.EDTPKS was used to flag reflections to be used in the least-squares cell parameter refinement. Reflections due to CuK α_2 radiation were excluded from the refinement.

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

At low angles, K α_1 and K α_2 peaks were unresolved for both the sample and the internal standard. Internal standard corrections were established from the theoretical values for K α_1 and were applied to the unresolved low angle peaks, as well as to the resolved K α_1 peaks in the higher angle regions. For the manual patterns, if the internal standard correction varied along the length of the pattern, linear interpolations were used.

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

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

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

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

The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants published in this series of NBS publications prior to 1973. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

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

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

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

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

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

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

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

N , the number of observed reflections was chosen as 30, or as the maximum number of lines of the pattern if the pattern had fewer than 30 lines. $\overline{|\Delta 2\theta|}$ is the average absolute magnitude of discrepancy between observed and calculated 2θ values for each reported hkl . When multiple indices are reported for an observed reflection, then each possible $\Delta 2\theta$ 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).

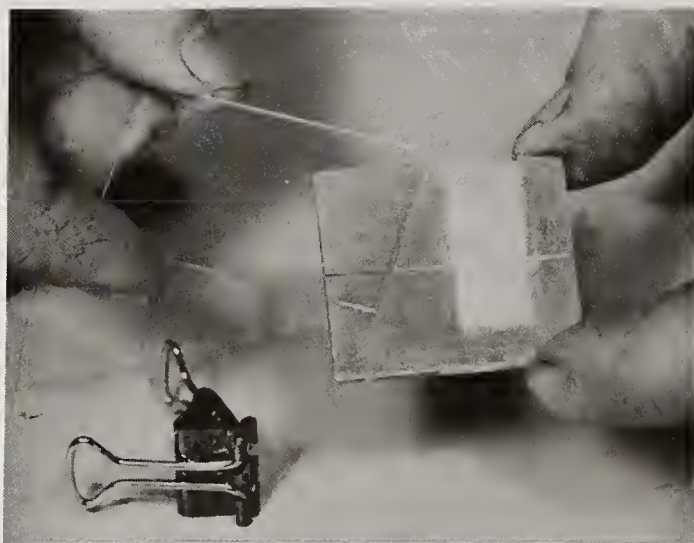


Figure 2.

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:

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

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

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

and

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

where

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

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

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

Reference intensity ratio, $I/I_{corundum}$. The reference intensity ratio, I/I_c , has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the 113 (hexagonal) reflection of corundum ($\alpha-Al_2O_3$) [Visser and de Wolff, 1964]. In this publication the ratios I/I_c are tabulated for copper $K\alpha_1$ radiation, for a 1:1 mixture by weight of the sample and corundum. I/I_c was determined only for very common phases.

A procedure has been adopted to achieve greater statistical accuracy [Hubbard and Smith, 1977]. For any weight fractions of sample and corundum, X_s and X_c ($X_s = 1 - X_c$), the intensities for reflection h_1 of the sample and h_2 of corundum were measured for several combinations of h_1 and h_2 usually within the same region of 2θ , to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{I(h_o)}{I_c(113)} = \frac{X_c}{X_s} \cdot \frac{I_c^{rel}(h_2)}{I^{rel}(h_1)} \cdot \frac{I(h_1)}{I_c(h_2)}$$

where (h_o) indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection (h_o) will be the one with $I = 100$ since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio, I/I_c . These values yielded the tabulated average $\langle I/I_c \rangle$. From these data, the standard deviation, σ , was obtained from

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

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

Format of tables. The printing of the data has been computerized. Superimposed reflections are treated in one of two ways. If a d-spacing has only two possible indices, an \underline{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 ($1\text{Å} = 100\text{ pm}$) 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 Å³ ($1\text{Å}^3 = 1 \times 10^{-30} \text{ m}^3$). Densities are reported in g/cm³ ($1 \text{ gm/cm}^3 = 10^3 \text{ kg/m}^3$).

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Aluminum Yttrium Oxide, AlYO_3

Synonym

Yttrium aluminate

CAS registry no.

12003-86-0

Sample

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

Color

Yellowish white

Structure

Orthorhombic, Pnma (62), $Z = 4$, isostructural with GdFeO_3 and YFeO_3 (Geller and Wood, 1956). The structure of GdFeO_3 was determined by Geller (1956). Coppens and Eibschütz (1965) refined the centric structure of GdFeO_3 and YFeO_3 . The latter was refined also in the alternative non-centrosymmetric space group $\text{Pn}2_1\text{a}$ (33), and that refinement showed small, possibly real, deviations from a centric structure.

Lattice constants of this sample

$a = 5.3286(4)\text{Å}$
 $b = 7.3706(5)$
 $c = 5.1796(3)$

$a/b = 0.7230$
 $c/b = 0.7027$

Volume

203.43 Å^3

Density

(calculated) 5.351 g/cm^3

Polymorphism

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

Figure of merit

$F_{30} = 92.6(0.010, 33)$

Additional patterns

PDF card 11-662 (Roth, 1957)

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

Geller and Wood (1956)

Keith and Roy (1954). The pattern in table 4 labeled $3\text{Y}_2\text{O}_3 \cdot 5\text{Al}_2\text{O}_3$, YCrO_3 type, seems to be the phase reported here.

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| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | |
|---|------------------|-------|-------|--|
| Internal standard Ag, a = 4.08651 Å | | | | |
| d(Å) | I ^{rel} | hkl | 2θ(°) | |
| σ = ±2 | | | | |
| 4.233 | 1 | 0 1 1 | 20.97 | |
| 3.711 | 29 | 1 0 1 | 23.96 | |
| 3.685 | 16 | 0 2 0 | 24.13 | |
| 3.317 | 19 | 1 1 1 | 26.86 | |
| 2.664 | 22 | 2 0 0 | 33.62 | |
| 2.617 | 100 | 1 2 1 | 34.24 | |
| 2.589 | 24 | 0 0 2 | 34.62 | |
| 2.505 | 11 | 2 1 0 | 35.82 | |
| 2.368 | 1L | 2 0 1 | 37.97 | |
| 2.329 | 1 | 1 0 2 | 38.63 | |
| 2.255 | 1 | 2 1 1 | 39.94 | |
| 2.220M | 9, | 1 1 2 | 40.60 | |
| 2.220M | | 0 3 1 | 40.60 | |
| 2.1588 | 23 | 2 2 0 | 41.81 | |
| 2.1192 | 25 | 0 2 2 | 42.63 | |
| 2.0483 | 8 | 1 3 1 | 44.18 | |
| 1.9923 | 2 | 2 2 1 | 45.49 | |
| 1.9686 | 2 | 1 2 2 | 46.07 | |
| 1.8565 | 31 | 2 0 2 | 49.03 | |
| 1.8424 | 18 | 0 4 0 | 49.43 | |
| 1.8051 | 9 | 2 3 0 | 50.52 | |
| 1.8005 | 15 | 2 1 2 | 50.66 | |
| 1.7055 | 1L | 2 3 1 | 53.70 | |
| 1.6904 | 1 | 1 3 2 | 54.22 | |
| 1.6579 | 3 | 2 2 2 | 55.37 | |
| 1.6505 | 6 | 1 4 1 | 55.64 | |
| 1.6424 | 6 | 1 0 3 | 55.94 | |
| 1.6381 | 17 | 3 1 1 | 56.10 | |
| 1.6030 | 3 | 1 1 3 | 57.44 | |
| 1.5286 | 10 | 3 2 1 | 60.52 | |

Aluminum Yttrium Oxide, AlYO_3 - (continued)

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

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 1.0335M | 4 | 5 1 1 | 96.37 |
| 1.0335M | | 2 5 3 | 96.37 |
| 1.0278 | 1L | 3 4 3 | 97.09 |
| 1.0247 | 1 | 2 6 2 | 97.48 |
| 1.0170 | 1 | 1 0 5 | 98.48 |
| 1.0141 | 1 | 4 2 3 | 98.86 |
| 1.0129 | 1 | 1 7 1 | 99.02 |
| 1.0067 | 1L | 3 2 4 | 99.84 |
| .9966 | 1 | 4 4 2 | 101.24 |
| .9918 | 2 | 3 6 1 | 101.91 |
| .9885 | 3 | 4 5 0 | 102.38 |
| .9842 | 6 | 2 4 4 | 103.01 |

Aluminum Yttrium Oxide, Al₂Y₄O₉

Synonym

Yttrium Aluminate

Sample

The sample was made from stoichiometric amounts of Y₂O₃ and Al₂O₃. The mixture was heated at 1600 °C for 2 days, ground and reheated at 1675 °C for 3-½ days. After adjusting the composition, the material was ground and heated periodically, 11 days at 1600 °C and finally in two stages at 1675 °C.

Color

Very pale yellowish white

Structure

Monoclinic, P2₁/a (14), Z = 4 (Reed and Chase, 1962).

Comment

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

Lattice constants of this sample

a = 11.1156(16) Å
b = 10.4689(16)
c = 7.3791(9)
β = 108.61(1)°

a/b = 1.0618

c/b = 0.7049

Volume

813.79 Å³

Density

(calculated) 4.518 g/cm³

Figure of merit

F₃₀ = 22.9(0.015,86)

Additional patterns

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

Warshaw and Roy (1959)

Abell et al. (1974)

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| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å | | | | |
|--|----------------------------|--------|-------|--|
| d(Å) | I ^{rel} σ = ±1 | hkl | 2θ(°) | |
| 7.41 | 17 | 1 1 0 | 11.93 | |
| 6.99 | 1 | 0 0 1 | 12.66 | |
| 5.264 | 3 | 2 0 0 | 16.83 | |
| 5.046 | 1 | -2 0 1 | 17.56 | |
| 4.701 | 23 | 2 1 0 | 18.86 | |
| 4.551 | 4 | -2 1 1 | 19.49 | |
| 4.188 | 2 | 0 2 1 | 21.20 | |
| 3.713 | 6 | 2 2 0 | 23.95 | |
| 3.682 | 4 | 2 0 1 | 24.15 | |
| 3.494 | 2 | 0 0 2 | 25.47 | |
| 3.470M | 2 | 2 1 1 | 25.65 | |
| 3.470M | | -2 0 2 | 25.65 | |
| 3.330 | 24 | 3 1 0 | 26.75 | |
| 3.017 | 100 | -1 2 2 | 29.59 | |
| 2.919M | 78 | 1 1 2 | 30.60 | |
| 2.919M | | 3 2 0 | 30.60 | |
| 2.892 | 9 | -2 2 2 | 30.90 | |
| 2.615 | 18 | 0 4 0 | 34.26 | |
| 2.561 | 13 | 2 0 2 | 35.01 | |
| 2.538M | 8 | 1 4 0 | 35.34 | |
| 2.538M | | -1 3 2 | 35.34 | |
| 2.527 | 12 | -4 0 2 | 35.49 | |
| 2.487 | 5 | 2 1 2 | 36.09 | |
| 2.470M | 7 | 0 3 2 | 36.34 | |
| 2.470M | | 3 2 1 | 36.34 | |
| 2.458M | 6 | -2 3 2 | 36.53 | |
| 2.458M | | -4 1 2 | 36.53 | |
| 2.352 | 1L | 4 2 0 | 38.23 | |
| 2.325 | 2 | -2 4 1 | 38.69 | |
| 2.292 | 7 | 1 3 2 | 39.27 | |
| 2.276+ | 6 | -4 2 2 | 39.57 | |
| 2.276+ | | 0 1 3 | 39.57 | |
| 2.256 | 2 | -3 1 3 | 39.93 | |
| 2.210 | 2 | -2 2 3 | 40.79 | |
| 2.174 | 2 | -5 1 1 | 41.51 | |
| 2.133M | 1 | -1 4 2 | 42.33 | |
| 2.133M | | 2 4 1 | 42.33 | |
| 2.129 | 2 | 0 2 3 | 42.43 | |
| 2.095M | 2 | 0 4 2 | 43.15 | |
| 2.095M | | 1 1 3 | 43.15 | |
| 2.088M | 2 | -2 4 2 | 43.29 | |
| 2.088M | | -5 1 2 | 43.29 | |
| 2.066 | 18 | 5 1 0 | 43.78 | |
| 2.053 | 5 | 1 5 0 | 44.07 | |
| 2.047M | 9 | -4 3 2 | 44.22 | |
| 2.047M | | -5 2 1 | 44.22 | |
| 1.984 | 3 | 1 4 2 | 45.69 | |
| 1.973M | 2 | -3 4 2 | 45.97 | |
| 1.973M | | -5 2 2 | 45.97 | |
| 1.955 | 1 | 5 2 0 | 46.41 | |

Aluminum Yttrium Oxide, $\text{Al}_2\text{Y}_4\text{O}_9$ - (continued)

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

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

Aluminum Yttrium Oxide, Al₅Y₃O₁₂

Synonyms

Yttrium aluminate
Yttrogarnet

CAS registry no.

12005-21-9

Sample

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

Color

Colorless

Structure

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

Lattice constant of this sample

$a = 12.0089(3)\text{\AA}$

Volume

1731.85\AA^3

Density

(calculated) 4.552 g/cm³

Polymorphism

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

Figure of merit

$F_{30} = 91.8(0.011, 30)$

Additional patterns

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

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

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

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

| CuK α_1 $\lambda = 1.540598\text{\AA}$; temp. 25±1 °C Internal standard Si, $a = 5.43088\text{\AA}$ | | | |
|--|--------------------------------------|--------|----------------|
| d(\AA) | I^{rel} $\sigma = \pm 2$ | hkl | 2 θ (°) |
| 4.905 | 27 | 2 1 1 | 18.07 |
| 4.247 | 7 | 2 2 0 | 20.90 |
| 3.210 | 19 | 3 2 1 | 27.77 |
| 3.002 | 27 | 4 0 0 | 29.74 |
| 2.687 | 100 | 4 2 0 | 33.32 |
| 2.561 | 1L | 3 3 2 | 35.01 |
| 2.452 | 20 | 4 2 2 | 36.62 |
| 2.355 | 6 | 4 3 1 | 38.18 |
| 2.192 | 23 | 5 2 1 | 41.15 |
| 2.122 | 5 | 4 4 0 | 42.56 |
| 1.9474 | 26 | 5 3 2 | 46.60 |
| 1.8994 | 1L | 6 2 0 | 47.85 |
| 1.8536 | 1L | 5 4 1 | 49.11 |
| 1.7705 | 2 | 6 3 1 | 51.58 |
| 1.7330 | 17 | 4 4 4 | 52.78 |
| 1.6988 | 1L | 5 4 3 | 53.93 |
| 1.6652 | 31 | 6 4 0 | 55.11 |
| 1.6338 | 9 | 7 2 1 | 56.26 |
| 1.6046 | 28 | 6 4 2 | 57.38 |
| 1.5247 | 4 | 6 5 1 | 60.69 |
| 1.5006 | 10 | 8 0 0 | 61.77 |
| 1.4780 | 1L | 7 4 1 | 62.82 |
| 1.4561 | 1L | 8 2 0 | 63.88 |
| 1.4352 | 1 | 6 5 3 | 64.92 |
| 1.4157 | 1 | 6 6 0 | 65.93 |
| 1.3962 | 1L | 7 4 3 | 66.97 |
| 1.3598 | 1L | 7 5 2 | 69.01 |
| 1.3423 | 7 | 8 4 0 | 70.04 |
| 1.3102 | 17 | 8 4 2 | 72.02 |
| 1.2949 | 2 | 7 6 1 | 73.01 |
| 1.2800 | 6 | 6 6 4 | 74.00 |
| 1.2656 | 1 | 8 5 1 | 74.98 |
| 1.2388 | 2 | 9 3 2 | 76.90 |
| 1.2257 | 1L | 8 4 4 | 77.87 |
| 1.2128 | 1L | 9 4 1 | 78.86 |
| 1.2011 | 1L | 8 6 0 | 79.78 |
| 1.1889 | 1L | 10 1 1 | 80.77 |
| 1.1776 | 2 | 10 2 0 | 81.71 |
| 1.1665 | 1L | 9 4 3 | 82.65 |
| 1.1451 | 3 | 10 3 1 | 84.55 |
| 1.1249 | 1L | 8 7 1 | 86.44 |
| 1.1151 | 14 | 10 4 0 | 87.39 |
| 1.1056 | 2 | 9 6 1 | 88.33 |
| 1.0964 | 6 | 10 4 2 | 89.27 |
| 1.0874 | 1L | 9 5 4 | 90.21 |

Aluminum Yttrium Oxide, $\text{Al}_5\text{Y}_3\text{O}_{12}$ - (continued)

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

Ammonium Cadmium Phosphate Hydrate, $\text{NH}_4\text{CdPO}_4 \cdot \text{H}_2\text{O}$

Sample

The sample was prepared at NBS. Water solutions of CdCl_2 and $(\text{NH}_4)_2\text{HPO}_4$ were mixed. NH_4OH was added to the mixture dropwise, until the pH reached 9.

Color

Colorless

Structure

Orthorhombic, $\text{Pmn}2_1$ (31), $Z = 2$. (Tranqui et al., 1968).

Lattice constants of this sample

$a = 5.8173(10)\text{\AA}$
 $b = 8.8797(8)$
 $c = 5.0134(8)$

$a/b = 0.6551$
 $c/b = 0.5646$

Volume

258.97\AA^3

Density

(calculated) 3.122 g/cm^3

Figure of merit

$F_{30} = 98.2(0.009, 34)$

Additional patterns

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

Ropp and Mooney (1960)

References

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

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{\AA}; \text{ temp. } 25 \pm 1^\circ \text{C}$ Internal standard Si, $a = 5.430825 \text{\AA}$ | | | |
|---|------------------|-------|---------------------|
| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
| $\sigma = \pm 3$ | | | |
| 8.87 | 100 | 0 1 0 | 9.96 |
| 4.868 | 4 | 1 1 0 | 18.21 |
| 4.436 | 11 | 0 2 0 | 20.00 |
| 4.367 | 13 | 0 1 1 | 20.32 |
| 3.799 | 13 | 1 0 1 | 23.40 |
| 3.528 | 7 | 1 2 0 | 25.22 |
| 3.493 | 38 | 1 1 1 | 25.48 |
| 3.324 | 3 | 0 2 1 | 26.80 |
| 2.957 | 1L | 0 3 0 | 30.20 |
| 2.908 | 36 | 2 0 0 | 30.72 |

| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
|------------------|------------------|-------|---------------------|
| $\sigma = \pm 3$ | | | |
| 2.885 | 63 | 1 2 1 | 30.97 |
| 2.764 | 10 | 2 1 0 | 32.37 |
| 2.637 | 3 | 1 3 0 | 33.97 |
| 2.549 | 5 | 0 3 1 | 35.18 |
| 2.506 | 6 | 0 0 2 | 35.80 |
| 2.433 | 7 | 2 2 0 | 36.92 |
| 2.420 | 8 | 2 1 1 | 37.12 |
| 2.413 | 7 | 0 1 2 | 37.24 |
| 2.334 | 18 | 1 3 1 | 38.54 |
| 2.2187 | 2 | 0 4 0 | 40.63 |
| 2.1883 | 9 | 2 2 1 | 41.22 |
| 2.1822 | 10 | 0 2 2 | 41.34 |
| 2.0738M | 8 | 2 3 0 | 43.61 |
| 2.0738M | | 1 4 0 | 43.61 |
| 2.0435 | 2 | 1 2 2 | 44.29 |
| 2.0300 | 1 | 0 4 1 | 44.60 |
| 1.9164M | 13 | 2 3 1 | 47.40 |
| 1.9164M | | 1 4 1 | 47.40 |
| 1.9122 | 10 | 0 3 2 | 47.51 |
| 1.8991 | 7 | 2 0 2 | 47.86 |
| 1.8568 | 8 | 2 1 2 | 49.02 |
| 1.8169 | 3 | 1 3 2 | 50.17 |
| 1.7753 | 7 | 0 5 0 | 51.43 |
| 1.7456 | 5 | 2 2 2 | 52.37 |
| 1.6982 | 3 | 1 5 0 | 53.95 |
| 1.6744M | 8 | 3 2 1 | 54.78 |
| 1.6744M | | 0 5 1 | 54.78 |
| 1.6624 | 3 | 0 4 2 | 55.21 |
| 1.6224 | 2 | 3 3 0 | 56.69 |
| 1.5984M | 5 | 2 3 2 | 57.62 |
| 1.5984M | | 1 4 2 | 57.62 |
| 1.5809 | 3 | 1 1 3 | 58.32 |
| 1.5434 | 3 | 3 3 1 | 59.88 |
| 1.5161 | 3 | 2 5 0 | 61.07 |
| 1.4802 | 1L | 0 6 0 | 62.72 |
| 1.4599 | 1 | 3 4 0 | 63.69 |
| 1.4508 | 4 | 2 5 1 | 64.14 |
| 1.4344 | 2 | 1 6 0 | 64.96 |
| 1.4193 | 2 | 0 6 1 | 65.74 |
| 1.4070 | 1 | 1 5 2 | 66.39 |
| 1.4019 | 2 | 3 4 1 | 66.66 |
| 1.3789 | 3 | 1 6 1 | 67.92 |
| 1.3196 | 1L | 2 6 0 | 71.43 |
| 1.3097 | 1L | 3 5 0 | 72.05 |
| 1.2978 | 2 | 2 5 2 | 72.82 |
| 1.2760 | 2 | 2 6 1 | 74.27 |

Barium Aluminum Titanium Oxide, BaAl₆TiO₁₂

Synonym

Barium aluminum titanate

CAS registry no.

58834-02-9

Sample

The sample was synthesized by melting, then very slowly cooling, stoichiometric amounts of BaTiO₃, Al₂O₃, and TiO₂. After heating at 1275 °C for 16.5 days, the sample was reheated at 1350 °C for 23 days. The material was ground every 24 hours.

Color

Colorless

Structure

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

Lattice constants of this sample

$a = 7.1375(3) \text{ \AA}$
 $b = 13.5978(8)$
 $c = 4.8651(2)$

 $a/b = 0.5249$ $c/b = 0.3578$

Volume

 472.18 \AA^3

Density

(calculated) 3.792 g/cm³

Figure of merit

 $F_{30} = 152.7(0.006, 36)$

Additional pattern

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

References

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

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

| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
|------------------|------------------|-------|---------------------|
| $\sigma = \pm 2$ | | | |
| 2.8152 | 50 | 2 1 1 | 31.76 |
| 2.6506 | 2 | 2 2 1 | 33.79 |
| 2.5954 | 80 | 1 4 1 | 34.53 |
| 2.5412 | 17 | 1 5 0 | 35.29 |
| 2.4610 | 3 | 2 4 0 | 36.48 |
| 2.4333 | 24 | 0 0 2 | 36.91 |
| 2.3738 | 2 | 0 5 1 | 37.87 |
| 2.3440 | 11 | 3 1 0 | 38.37 |
| 2.3025 | 8 | 1 0 2 | 39.09 |
| 2.2901 | 6 | 0 2 2 | 39.31 |
| 2.2702 | 22 | 1 1 2 | 39.67 |
| 2.2663 | 22 | 0 6 0 | 39.74 |
| 2.2527 | 17 | 1 5 1 | 39.99 |
| 2.1965 | 10 | 2 4 1 | 41.06 |
| 2.1373 | 11 | 3 0 1 | 42.25 |
| 2.1064 | 8 | 3 3 0 | 42.90 |
| 2.0532 | 5 | 1 3 2 | 44.07 |
| 2.0391 | 6 | 3 2 1 | 44.39 |
| 2.0103 | 12 | 2 0 2 | 45.06 |
| 1.9886 | 6 | 2 1 2 | 45.58 |
| 1.9763 | 24 | 2 5 1 | 45.88 |
| 1.9743 | 24 | 1 6 1 | 45.93 |
| 1.9275 | 33 | 2 2 2 | 47.11 |
| 1.8748 | 5 | 1 7 0 | 48.52 |
| 1.8095 | 39 | 3 4 1 | 50.39 |
| 1.7906 | 6 | 3 5 0 | 50.96 |
| 1.7844 | 9 | 4 0 0 | 51.15 |
| 1.7798 | 7 | 2 6 1 | 51.29 |
| 1.7569 | 11 | 1 5 2 | 52.01 |
| 1.7300 | 4 | 2 4 2 | 52.88 |
| 1.7258 | 4 | 4 2 0 | 53.02 |
| 1.6996 | 2 | 0 8 0 | 53.90 |
| 1.6875 | 1 | 3 1 2 | 54.32 |
| 1.6627 | 5 | 4 1 1 | 55.20 |
| 1.6579 | 11 | 0 6 2 | 55.37 |
| 1.6267 | 1 | 4 2 1 | 56.53 |
| 1.6154 | 1 | 1 6 2 | 56.96 |
| 1.6100M | 3 | 0 1 3 | 57.17 |
| 1.6100M | | 2 7 1 | 57.17 |
| 1.5924 | 11 | 3 3 2 | 57.86 |
| 1.5799 | 2 | 4 4 0 | 58.36 |
| 1.5716M | 6 | 1 1 3 | 58.70 |
| 1.5716M | | 4 3 1 | 58.70 |
| 1.5655 | 6 | 1 8 1 | 58.95 |
| 1.5550 | 24 | 3 6 1 | 59.39 |
| 1.5404 | 7 | 1 2 3 | 60.01 |
| 1.5346 | 16 | 2 8 0 | 60.26 |
| 1.5268 | 6 | 0 3 3 | 60.60 |
| 1.5046M | 2 | 3 7 0 | 61.59 |
| 1.5046M | | 2 6 2 | 61.59 |

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^{\circ}\text{C}$ Internal standard Ag, $a = 4.08651 \text{ \AA}$ | | | |
|--|------------------|-------|---------------------|
| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
| $\sigma = \pm 2$ | | | |
| 6.799 | 22 | 0 2 0 | 13.01 |
| 6.316 | 2 | 1 1 0 | 14.01 |
| 4.581 | 15 | 0 1 1 | 19.36 |
| 4.021 | 2 | 1 0 1 | 22.09 |
| 3.828 | 15 | 1 3 0 | 23.22 |
| 3.570 | 9 | 2 0 0 | 24.92 |
| 3.462 | 82 | 1 2 1 | 25.71 |
| 3.401 | 4 | 0 4 0 | 26.18 |
| 3.318 | 51 | 0 3 1 | 26.85 |
| 3.161 | 100 | 2 2 0 | 28.21 |

Barium Aluminum Titanium Oxide, BaAl₆TiO₁₂ - (continued)

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

Barium Aluminum Titanium Oxide, Ba₃Al₁₀TiO₂₀

Synonym

Barium aluminum titanate

CAS registry no.

58834-01-8

Sample

The sample was synthesized by melting together, then very slowly cooling stoichiometric amounts of BaTiO₃, Al₂O₃, and TiO₂. The sample was heated at 1000 °C for 20 hours, then at 1275 °C for 14 days and finally at 1350 °C for 23 days. The material was ground after each 24 hour period.

Color

Colorless

Structure

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

Lattice constants of this sample

a = 14.8884(12) Å

b = 11.3676(13)

c = 4.9781(5)

β = 90.84(1)°

a/b = 1.3097

c/b = 0.4379

Volume

842.43 Å³

Density

(calculated) 4.138 g/cm³

Figure of merit

F₃₀ = 53.24(0.010,55)

Additional pattern

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

References

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

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

| CuK α_1 λ = 1.540598 Å; temp. 25 \pm 1 °C Internal standard Ag, a = 4.08651 Å | | | | | |
|---|------------------|-----|---|---|----------------|
| d(Å) | I ^{rel} | hkl | | | 2 θ (°) |
| $\sigma \approx \pm 3$ | | | | | |
| 5.683 | 23 | 0 | 2 | 0 | 15.58 |
| 4.741 | 2 | -1 | 0 | 1 | 18.70 |
| 4.560 | 34 | 0 | 1 | 1 | 19.45 |
| 3.912 | 1 | -2 | 1 | 1 | 22.71 |
| 3.869 | 1 | 2 | 1 | 1 | 22.97 |

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

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

Barium Boride, BaB₆

Synonym

Barium hexaboride

Sample

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

Color

Very dark gray

Structure

Cubic, Pm3m (221), Z = 1, isostructural with CaB₆. The structure was determined by Stackelberg and Neumann (1932). Keissling (1950) and Bertaut and Blum (1954) studied the hexaborides.

Lattice constant of this sample

a = 4.2624(1) Å

Volume

77.44 Å³

Density

(calculated) 4.336 g/cm³

Figure of merit

F₂₄ = 106.1(0.009,24)

Additional pattern

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

References

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

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.430825 Å W, a = 3.16524 Å | | | |
|---|----------------------------|-------|--------|
| d(Å) | I ^{rel} σ = ±3 | hkl | 2θ(°) |
| 4.261 | 54 | 1 0 0 | 20.83 |
| 3.014 | 100 | 1 1 0 | 29.62 |
| 2.462 | 45 | 1 1 1 | 36.47 |
| 2.1311 | 21 | 2 0 0 | 42.38 |
| 1.9069 | 48 | 2 1 0 | 47.65 |
| 1.7404 | 24 | 2 1 1 | 52.54 |
| 1.5072 | 9 | 2 2 0 | 61.47 |
| 1.4206 | 25 | 3 0 0 | 65.67 |
| 1.3480 | 20 | 3 1 0 | 69.70 |
| 1.2850 | 11 | 3 1 1 | 73.66 |
| 1.2304 | 2 | 2 2 2 | 77.52 |
| 1.1822 | 7 | 3 2 0 | 81.32 |
| 1.1393 | 13 | 3 2 1 | 85.08 |
| 1.0657 | 2 | 4 0 0 | 92.57 |
| 1.0338 | 10 | 4 1 0 | 96.34 |
| 1.0047 | 9 | 3 3 0 | 100.12 |
| .9780 | 3 | 3 3 1 | 103.93 |
| .9532 | 5 | 4 2 0 | 107.82 |
| .9301 | 12 | 4 2 1 | 111.83 |
| .9088 | 4 | 3 3 2 | 115.91 |
| .8701 | 2 | 4 2 2 | 124.58 |
| .8524 | 3 | 5 0 0 | 129.28 |
| .8359 | 13 | 5 1 0 | 134.31 |
| .8203 | 6 | 5 1 1 | 139.79 |

Barium Neodymium Titanium Oxide, BaNd₂Ti₅O₁₄

Synonym

Barium neodymium titanate

Sample

The sample was prepared at NBS from a mixture of BaO, Nd₂O₃, and TiO₂ (rutile). The mixture was heated at 1250 °C for 1 day. After being ground, the sample was heated further at 1350 °C for 4 days, ground, and heated at 1365 °C for 6 days.

Two known phases, rutile and Ba₂Ti₉O₂₀, were present as impurities. Corrections were made for the overlap of intensities.

Color

Colorless

Structure

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

Lattice constants of this sample

a = 12.1983(13) Å
b = 22.347(3)
c = 3.8403(6)

a/b = 0.5459
c/b = 0.1718

Volume

1046.8 Å³

Density

(calculated) 5.643 g/cm³
(measured) 5.44 g/cm³ (Kolar et al., 1981)

Figure of merit

F₃₀ = 50.1(0.012,50)

Additional pattern

Kolar et al. (1981)

Reference

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Ag, a = 4.08651 Å | | | |
|--|----------------------------|-------|-------|
| d(Å) | I ^{rel} σ = ±4 | hkl | 2θ(°) |
| 11.20 | 12 | 0 2 0 | 7.89 |
| 10.73 | 5 | 1 1 0 | 8.23 |
| 8.25 | 1L | 1 2 0 | 10.71 |
| 6.36 | 3 | 1 3 0 | 13.91 |
| 6.10 | 1 | 2 0 0 | 14.51 |

Barium Neodymium Titanium Oxide, BaNd₂Ti₅O₁₄ - (continued)

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

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

Barium Tungsten Oxide, Ba₃WO₆

Synonyms

Barium tungstate
Tribarium tungstate

Sample

The sample was prepared at NBS by T. Negas from spectrographic grade BaCO₃ and WO₃ (73:27 mol ratio). It was heated in a Au crucible in air at 950 °C for 48 hours. This sample is approximately 2 mol % richer in WO₃ than the true 3:1 oxide.

Color

Colorless

Structure

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

Lattice constants of this sample

$a = 17.1765(5)\text{\AA}$

Comment

There are 4 lines with $I_{\text{rel}} \approx 1$ that do not index satisfactorily on this unit cell. Several unit cells have been reported in the literature for Ba₃WO₆; Kreidler (1972), Kovba et al. (1971), and Steward and Rooksby (1951). None of the unit cell values reported by these authors will adequately index their data. Some of these patterns appear to be mixed with the off stoichiometric phase reported here. Structural data for the true 3:1 oxide have not been published.

Volume

5067.6\AA^3

Density

(calculated) 7.254 g/cm³ (based on 3:1 ratio)

Figure of merit

$F_{30} = 68.2(0.012, 38)$

Additional patterns

PDF card 25-82 (Kreidler, 1972)

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

Chang et al., (1966)

References

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

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

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

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

| CuK α_1 $\lambda = 1.540598 \overset{\circ}{\text{\AA}}$; temp. $25 \pm 1 \overset{\circ}{\text{C}}$ Internal standard Si, $a = 5.40388 \overset{\circ}{\text{\AA}}$ | | | | | |
|---|------------------|-----------|---|---|-------------------------|
| d($\overset{\circ}{\text{\AA}}$) | I^{rel} | hk ℓ | | | 2 θ ($^\circ$) |
| $\sigma = \pm 2$ | | | | | |
| 9.89 | 2 | 1 | 1 | 1 | 8.93 |
| 6.075 | 2 | 2 | 2 | 0 | 14.57 |
| 4.962 | 9 | 2 | 2 | 2 | 17.86 |
| 4.296 | 5 | 4 | 0 | 0 | 20.66 |
| 3.942 | 3 | 3 | 3 | 1 | 22.54 |
| 3.509 | 5 | 4 | 2 | 2 | 25.36 |
| 3.307 | 25 | 5 | 1 | 1 | 26.94 |
| 3.036 | 100 | 4 | 4 | 0 | 29.40 |
| 2.905 | 1 | 5 | 3 | 1 | 30.75 |
| 2.863 | 3 | 6 | 0 | 0 | 31.22 |
| 2.716 | 1 | 6 | 2 | 0 | 32.95 |
| 2.620 | 2 | 5 | 3 | 3 | 34.20 |
| 2.590 | 8 | 6 | 2 | 2 | 34.60 |
| 2.405 | 3 | 5 | 5 | 1 | 37.36 |
| 2.236 | 14 | 7 | 3 | 1 | 40.30 |
| 2.146 | 17 | 8 | 0 | 0 | 42.07 |
| 2.084 | 1L | 6 | 4 | 4 | 43.39 |
| 2.024 | 3 | 6 | 6 | 0 | 44.73 |
| 1.9841 ^o | 5 | 7 | 5 | 1 | 45.69 |
| 1.9694 | 5 | 6 | 6 | 2 | 46.05 |
| 1.9206 | 4 | 8 | 4 | 0 | 47.29 |
| 1.8850 | 1 | 7 | 5 | 3 | 48.24 |
| 1.8737 | 2 | 8 | 4 | 2 | 48.55 |
| 1.8306 | 1L | 6 | 6 | 4 | 49.77 |
| 1.8005 | 4 | 9 | 3 | 1 | 50.66 |
| 1.7522 | 21 | 8 | 4 | 4 | 52.16 |
| 1.7261 | 1 | 7 | 7 | 1 | 53.01 |
| 1.6840 | 2 | 10 | 2 | 0 | 54.44 |
| 1.6602 | 9 | 9 | 5 | 1 | 55.29 |
| 1.6522 | 6 | 10 | 2 | 2 | 55.58 |
| 1.6018 | 1 | 9 | 5 | 3 | 57.49 |
| 1.5949 | 1L | 10 | 4 | 0 | 57.76 |
| 1.5486 | 1L | 7 | 7 | 5 | 59.66 |
| 1.5179 | 7 | 8 | 8 | 0 | 60.99 |
| 1.5009 | 1 | 9 | 5 | 5 | 61.76 |
| 1.4952 | 1L | 10 | 4 | 4 | 62.02 |
| 1.4567 | 3 | 9 | 7 | 3 | 63.85 |
| 1.4516 | 7 | 10 | 6 | 2 | 64.10 |
| 1.4313 | 2 | 12 | 0 | 0 | 65.12 |
| 1.4166 | 1 | 11 | 5 | 1 | 65.88 |
| 1.3934 | 3 | 10 | 6 | 4 | 67.12 |
| 1.3797 | 1L | 11 | 5 | 3 | 67.88 |
| 1.3457 | 7 | 9 | 9 | 1 | 69.84 |
| 1.3415 | 1L | 10 | 8 | 0 | 70.09 |
| 1.3134 | 2 | 13 | 1 | 1 | 71.82 |

Barium Tungsten Oxide, Ba₃WO₆ - (continued)

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

Beryllium Carbide, Be₂C

CAS registry no.

506-66-1

Sample

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

Color

Grayish yellow brown

Structure

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

Lattice constant of this sample

a = 4.3422(1) Å

Volume

81.872 Å³

Density

(calculated) 2.437 g/cm³

Figure of merit

F₁₀ = 152.3(0.007,10)

Additional pattern

PDF card 9-196 (Staritzky, 1956)

References

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | |
|---|----------------------------|-------|--------|
| d(Å) | I ^{rel} σ = ±2 | hkl | 2θ(°) |
| 2.5069 | 100 | 1 1 1 | 35.79 |
| 2.1712 | 1L | 2 0 0 | 41.56 |
| 1.5355 | 75 | 2 2 0 | 60.22 |
| 1.3092 | 12 | 3 1 1 | 72.08 |
| 1.2537 | 1L | 2 2 2 | 75.82 |
| 1.0856 | 10 | 4 0 0 | 90.40 |
| .9961 | 6 | 3 3 1 | 101.30 |
| .9709 | 1L | 4 2 0 | 105.00 |
| .8864 | 31 | 4 2 2 | 120.69 |
| .8356 | 7 | 5 1 1 | 134.39 |

Cadmium Iodide, α -CdI₂

CAS registry no.

7790-80-9

Sample

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

Color

Colorless

Structure

Hexagonal, P6₃mc (186), Z = 2. The structure was qualitatively done by Mitchell (1965). This is the 4H polytype encountered most frequently.

Lattice constants of this sample

a = 4.2481(3) Å

c = 13.7265(8)

c/a = 3.2312

Volume

214.53 Å³

Density

(calculated) 5.669 g/cm³

Polymorphism

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

Figure of merit

F₃₀ = 26.2(0.012,92)

Additional patterns

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

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

Reference

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

| CuK α_1 λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | |
|--|--------------------------------------|--------|----------------|
| d(Å) | I ^{rel} $\sigma = \pm 3$ | hkl | 2 θ (°) |
| 6.87 | 100 | 0 0 2 | 12.88 |
| 3.433 | 40 | 0 0 4 | 25.93 |
| 3.245 | 38 | 1 0 2 | 27.46 |
| 2.868 | 16 | 1 0 3 | 31.16 |
| 2.287 | 7 | 0 0 6 | 39.36 |
| 2.201 | 7 | 1 0 5 | 40.97 |
| 2.124 | 91 | 1 1 0 | 42.52 |
| 2.030 | 16 | 1 1 2 | 44.61 |
| 1.9435 | 3 | 1 0 6 | 46.70 |
| 1.8061 | 15 | 1 1 4 | 50.49 |
| 1.7779 | 8 | 2 0 2 | 51.35 |
| 1.7159 | 19 | 0 0 8 | 53.35 |
| 1.5564 | 3 | 1 1 6 | 59.33 |
| 1.3725 | 2 | 0 0 10 | 68.28 |
| 1.3622 | 5 | 2 1 2 | 68.87 |
| 1.3347 | 20 | 1 1 8 | 70.50 |
| 1.2859 | 1L | 1 0 10 | 73.60 |
| 1.2263 | 6 | 3 0 0 | 77.83 |
| 1.1820 | 2 | 1 0 11 | 81.34 |
| 1.1530 | 2 | 1 1 10 | 83.84 |
| 1.1441 | 1L | 0 0 12 | 84.64 |
| 1.0621 | 3 | 2 2 0 | 92.98 |
| 1.0146 | 1 | 2 2 4 | 98.79 |
| 1.0070 | 3 | 1 1 12 | 99.80 |
| .9977 | 4 | 3 0 8 | 101.08 |
| .9806 | 1L | 0 0 14 | 103.54 |
| .9780 | 1L | 3 1 4 | 103.93 |
| .9474 | 1L | 1 0 14 | 108.79 |
| .9030 | 2 | 2 2 8 | 117.09 |
| .8578 | 1L | 0 0 16 | 127.79 |

Calcium Aluminum Oxide Hydrate, $\text{Ca}_4\text{Al}_6\text{O}_{13} \cdot 3\text{H}_2\text{O}$

Synonym

Tetracalcium trialuminate trihydrate

CAS registry no.

12355-68-9

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

a = 12.422(3) Å

b = 12.803(3)

c = 8.862(2)

a/b = 0.9702

c/b = 0.6922

Volume

1409.45 Å³

Density

(calculated) 2.753 g/cm³

Figure of merit

F₃₀ = 52.8(0.014,41)

Additional patterns

PDF card 14-464 (Pistorius, 1962)

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

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

Johnson and Thorvaldson, (1943)

References

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

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

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å | | | | |
|--|----------------------------|-------|-------|--|
| d(Å) | I ^{rel} σ = ±4 | hkl | 2θ(°) | |
| 4.432 | 5 | 0 0 2 | 20.02 | |
| 3.639 | 38 | 0 2 2 | 24.44 | |
| 3.602M | 100 | 2 0 2 | 24.70 | |
| 3.602M | | 3 1 1 | 24.70 | |
| 3.493 | 17 | 1 2 2 | 25.48 | |
| 3.270 | 86 | 2 3 1 | 27.25 | |
| 3.199 | 2 | 0 4 0 | 27.87 | |
| 3.141 | 14 | 2 2 2 | 28.39 | |
| 3.103 | 1 | 4 0 0 | 28.75 | |
| 3.028 | 44 | 3 0 2 | 29.48 | |
| 2.846 | 46 | 2 4 0 | 31.41 | |
| 2.820 | 72 | 3 3 1 | 31.70 | |
| 2.805 | 83 | 1 1 3 | 31.88 | |
| 2.797 | 81 | 4 2 0 | 31.97 | |
| 2.734 | 4 | 3 2 2 | 32.73 | |
| 2.612 | 21 | 2 1 3 | 34.31 | |
| 2.594 | 13 | 0 4 2 | 34.55 | |
| 2.541M | 31 | 4 0 2 | 35.29 | |
| 2.541M | | 1 4 2 | 35.29 | |
| 2.416 | 15 | 4 3 1 | 37.18 | |
| 2.392 | 11 | 2 4 2 | 37.57 | |
| 2.383 | 11 | 1 3 3 | 37.72 | |
| 2.364 | 8 | 4 2 2 | 38.04 | |
| 2.351 | 8 | 5 1 1 | 38.25 | |
| 2.287 | 38 | 2 5 1 | 39.36 | |
| 2.261 | 2 | 2 3 3 | 39.83 | |
| 2.229 | 33 | 4 4 0 | 40.44 | |
| 2.216 | 9 | 0 0 4 | 40.69 | |
| 2.199 | 1 | 3 4 2 | 41.02 | |
| 2.181 | 7 | 1 0 4 | 41.36 | |
| 2.167 | 14 | 5 0 2 | 41.64 | |
| 2.133 | 5 | 0 6 0 | 42.33 | |
| 2.115 | 2 | 3 5 1 | 42.72 | |
| 2.094M | 38 | 3 3 3 | 43.17 | |
| 2.094M | | 0 2 4 | 43.17 | |
| 2.087M | 44 | 5 3 1 | 43.32 | |
| 2.087M | | 2 0 4 | 43.32 | |
| 2.069 | 16 | 6 0 0 | 43.71 | |
| 2.065 | 17 | 1 2 4 | 43.80 | |
| 2.019 | 1L | 2 6 0 | 44.85 | |
| 1.985 | 4 | 2 2 4 | 45.67 | |
| 1.970 | 3 | 6 2 0 | 46.03 | |
| 1.928 | 6 | 4 5 1 | 47.11 | |
| 1.913M | 11 | 4 3 3 | 47.49 | |
| 1.913M | | 1 5 3 | 47.49 | |

Calcium Aluminum Oxide Hydrate, $\text{Ca}_4\text{Al}_6\text{O}_{13}\cdot 3\text{H}_2\text{O}$ - (continued)

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

Calcium Aluminum Silicate Hydrate, Chabazite, $\text{Ca}_2\text{Al}_4\text{Si}_8\text{O}_{24}\cdot 12\text{H}_2\text{O}$

Synonym

Calcium aluminosilicate hexahydrate

CAS registry no.

12251-32-0

Sample

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

Chemical Analysis (wt. %)

Ca 6.12%, Al 9.67%, Si 22.17%, Na 0.55%, K 0.86%, Sr 0.10%, Fe 0.043%, H_2O 22.48%

Color

Colorless to salmon pink

Structure

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

Lattice constants of this sample

Hexagonal axes

$a = 13.784(2)\text{\AA}$
 $c = 14.993(3)$

$c/a = 1.0877$

$Z = 3$

Volume

2467.0 \AA^3

Density

(calculated) 2.045 g/cm^3

(observed) $2.05(2)$ (Himes and Mighell, 1981)

Figure of merit

$F_{30} = 65.0(0.012, 38)$

Additional pattern

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

References

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

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

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

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
|---|--------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
| 9.34 | 54 | 1 0 1 | 9.46 |
| 6.89 | 13 | 1 1 0 | 12.83 |
| 6.36 | 7 | 0 1 2 | 13.92 |
| 5.552 | 26 | 0 2 1 | 15.95 |
| 5.001 | 29 | 0 0 3 | 17.72 |
| 4.667 | 6 | 2 0 2 | 19.00 |
| 4.323 | 100 | 2 1 1 | 20.53 |
| 4.053 | 2 | 1 1 3 | 21.91 |
| 3.978 | 4 | 3 0 0 | 22.33 |
| 3.865 | 21 | 1 2 2 | 22.99 |
| 3.576 | 42 | 1 0 4 | 24.88 |
| 3.446 | 19 | 2 2 0 | 25.83 |
| 3.236 | 5 | 1 3 1 | 27.54 |
| 3.176 | 11 | 0 2 4 | 28.07 |
| 2.927 | 93 | 4 0 1 | 30.52 |
| 2.908 | 21 | 0 1 5 | 30.72 |
| 2.882 | 45 | 2 1 4 | 31.01 |
| 2.838 | 6 | 2 2 3 | 31.50 |
| 2.775 | 4 | 0 4 2 | 32.23 |
| 2.693 | 4 | 3 2 1 | 33.24 |
| 2.678 | 9 | 2 0 5 | 33.43 |
| 2.606 | 20 | 4 1 0 | 34.39 |
| 2.572 | 4 | 2 3 2 | 34.85 |
| 2.497M | 21 | 0 0 6 | 35.94 |
| 2.497M | | 1 2 5 | 35.94 |
| 2.351 | 3 | 1 1 6 | 38.26 |
| 2.310 | 4 | 4 1 3 | 38.96 |
| 2.298 | 5 | 3 3 0 | 39.17 |
| 2.275 | 3 | 5 0 2 | 39.58 |
| 2.231 | 1L | 2 4 1 | 40.40 |
| 2.159 | 2 | 4 2 2 | 41.80 |
| 2.122 | 1 | 5 1 1 | 42.57 |
| 2.087 | 9 | 3 3 3 | 43.33 |
| 2.060 | 1 | 1 5 2 | 43.91 |
| 2.013 | 1 | 0 5 4 | 44.99 |
| 1.9455 | 1L | 4 3 1 | 46.65 |
| 1.9126 | 2 | 5 2 0 | 47.50 |
| 1.8664 | 9 | 5 0 5 | 48.75 |
| 1.8515 | 4 | 0 1 8 | 49.17 |
| 1.8035M | 18 | 4 1 6 | 50.57 |
| 1.8035M | | 4 2 5 | 50.57 |
| 1.7857 | 2 | 5 2 3 | 51.11 |
| 1.7689 | 3 | 6 1 2 | 51.63 |
| 1.7306 | 6 | 1 2 8 | 52.86 |
| 1.7236 | 10 | 4 4 0 | 53.09 |

Calcium Aluminum Silicate Hydrate, Chabazite, $\text{Ca}_2\text{Al}_4\text{Si}_8\text{O}_{24} \cdot 12\text{H}_2\text{O}$ - (continued)

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

Calcium Silicate (Larnite), β - Ca_2SiO_4

Synonyms

Beta dicalcium silicate
Belite

CAS registry no.
10034-77-2

Sample

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

Chemical analysis

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

Color

Colorless

Structure

Monoclinic, $\text{P2}_1/\text{n}$ (14), $Z = 4$. The structure of β - Ca_2SiO_4 was determined by Midgley (1952).

Lattice constants of this sample

$a = 9.310(2)\text{\AA}$
 $b = 6.7565(10)$
 $c = 5.5059(11)$
 $\beta = 94.46(2)^\circ$

$a/b = 1.3779$
 $c/b = 0.8149$

Volume

345.29\AA^3

Density

(calculated) 3.313 g/cm^3

Polymorphism

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

Figure of merit

$F_{30} = 54.5(0.013, 43)$

Additional patterns

PDF card 9-351 (Yannaquis, 1955)

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

Brownmiller and Bogue, (1930)

References

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

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

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

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

| CuK α_1 $\lambda = 1.540598\text{\AA}$; temp. $25 \pm 1\text{ }^\circ\text{C}$ Internal standard Si, $a = 5.43088\text{\AA}$ | | | |
|---|------------------|--------|-------------------|
| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^\circ)$ |
| $\sigma = \pm 1$ | | | |
| 4.892 | 3 | -1 0 1 | 18.12 |
| 4.641 | 9 | 2 0 0 | 19.11 |
| 3.824 | 5 | 2 1 0 | 23.24 |
| 3.786 | 5 | 1 1 1 | 23.48 |
| 3.378 | 7 | 0 2 0 | 26.36 |
| 3.241 | 6 | -2 1 1 | 27.50 |
| 3.176 | 5 | 1 2 0 | 28.07 |
| 3.049 | 9 | 2 1 1 | 29.27 |
| 2.877 | 21 | 0 2 1 | 31.06 |
| 2.814 | 22 | 3 1 0 | 31.77 |
| 2.790 | 97 | -3 0 1 | 32.05 |
| 2.783 | 100 | -1 2 1 | 32.14 |
| 2.745 | 83 | 0 0 2 | 32.59 |
| 2.718 | 30 | 1 2 1 | 32.93 |
| 2.610 | 42 | 3 0 1 | 34.33 |
| 2.545 | 9 | 0 1 2 | 35.24 |
| 2.448 | 12 | -2 0 2 | 36.68 |
| 2.433 | 9 | 3 1 1 | 36.91 |
| 2.410 | 13 | 1 1 2 | 37.28 |
| 2.403 | 18 | 2 2 1 | 37.40 |
| 2.323 | 2 | 4 0 0 | 38.74 |
| 2.301 | 4 | -2 1 2 | 39.12 |
| 2.281 | 22 | 3 2 0 | 39.48 |
| 2.189 | 51 | 1 3 0 | 41.21 |
| 2.165 | 13 | 2 1 2 | 41.69 |
| 2.129 | 7 | 0 2 2 | 42.42 |
| 2.103 | 1 | -1 2 2 | 42.97 |
| 2.091 | 6 | -4 1 1 | 43.24 |
| 2.083 | 6 | 0 3 1 | 43.40 |
| 2.050 | 14 | 1 2 2 | 44.15 |
| 2.037 | 9 | -3 1 2 | 44.43 |
| 2.027 | 15 | 2 3 0 | 44.68 |
| 2.020 | 15 | 1 3 1 | 44.83 |
| 1.987 | 20 | 4 1 1 | 45.61 |
| 1.982 | 24 | -2 2 2 | 45.75 |
| 1.9115 | 6 | 4 2 0 | 47.53 |
| 1.8979 | 9 | 3 1 2 | 47.89 |
| 1.8935 | 11 | 2 2 2 | 48.01 |
| 1.8441 | 4 | -4 0 2 | 49.38 |
| 1.8441M | | -4 2 1 | 49.38 |
| 1.8210 | 3 | 3 3 0 | 50.05 |
| 1.8051 | 9 | -3 2 2 | 50.52 |
| 1.8018 | 9 | -5 0 1 | 50.62 |
| 1.7899 | 7 | 5 1 0 | 50.98 |
| 1.7657 | 1 | 0 1 3 | 51.73 |

Calcium Silicate, (Larnite), β -Ca₂SiO₄ - (continued)

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

Calcium Silicon Fluoride Hydrate, $\text{CaSiF}_6 \cdot 2\text{H}_2\text{O}$

Synonym

Calcium fluorosilicate dihydrate

CAS registry no.

16961-80-1

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$a = 10.477(2)\text{\AA}$
 $b = 9.1771(13)$
 $c = 5.7281(13)$
 $\beta = 98.98(2)^\circ$

$a/b = 1.1416$

$c/b = 0.6242$

Volume

543.99\AA^3

Density

(calculated) 2.664 g/cm^3

Figure of merit

$F_{30} = 47.1(0.013, 49)$

$M_{20} = 29.4$

Additional pattern

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

References

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{temp. } 25 \pm 1 \text{ } ^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | | | |
|--|------------------|-------|---|---|---------------------|
| $d(\text{\AA})$ | I^{rel} | hkl | | | $2\theta(^{\circ})$ |
| $\sigma = \pm 2$ | | | | | |
| 6.85 | 16 | 1 | 1 | 0 | 12.91 |
| 5.323 | 43 | -1 | 0 | 1 | 16.64 |
| 5.166 | 5 | 2 | 0 | 0 | 17.15 |
| 4.810 | 23 | 0 | 1 | 1 | 18.43 |
| 4.598M | 16 | -1 | 1 | 1 | 19.29 |

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

Calcium Silicon Fluoride, Hydrate, $\text{CaSiF}_6 \cdot 2\text{H}_2\text{O}$ - (continued)

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

Cesium Iodide, CsI₃

Synonym

Cesium triiodide

CAS registry no.

12527-22-9

Sample

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

Color

Unground: dark purplish blue.

Ground: dark grayish reddish brown.

Structure

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

Lattice constants of this sample

a = 10.0289(9) Å

b = 11.0869(9)

c = 6.8457(8)

a/b = 0.9062

c/b = 0.6186

Volume

761.17 Å³

Density

(calculated) 4.482 g/cm³

Figure of merit

F₃₀ = 83.5(0.007,50)

Reference

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

| d(Å) | I ^{rel} σ = ±3 | hkP | 2θ(°) |
|---------|----------------------------|-------|-------|
| 2.729 | 30 | 2 3 1 | 32.79 |
| 2.671 | 9 | 1 4 0 | 33.52 |
| 2.5687 | 5 | 0 4 1 | 34.90 |
| 2.5185 | 9 | 2 2 2 | 35.62 |
| 2.4781 | 1 | 3 3 0 | 36.22 |
| 2.4461 | 13 | 4 1 0 | 36.71 |
| 2.4372 | 12 | 1 3 2 | 36.85 |
| 2.4264 | 5 | 2 4 0 | 37.02 |
| 2.3312 | 4 | 3 3 1 | 38.59 |
| 2.3036 | 2 | 4 1 1 | 39.07 |
| 2.2846M | 2 | 2 4 1 | 39.41 |
| 2.2846M | | 4 2 0 | 39.41 |
| 2.1960 | 10 | 3 2 2 | 41.07 |
| 2.1662M | 10 | 4 2 1 | 41.66 |
| 2.1662M | | 1 5 0 | 41.66 |
| 2.1544 | 10 | 0 4 2 | 41.90 |
| 2.1339 | 5 | 3 4 0 | 42.32 |
| 2.1060 | 8 | 1 4 2 | 42.91 |
| 2.0751 | 5 | 4 3 0 | 43.58 |
| 2.0652M | 6 | 1 2 3 | 43.80 |
| 2.0652M | | 1 5 1 | 43.80 |
| 2.0417 | 7 | 2 1 3 | 44.33 |
| 2.0231 | 2 | 4 0 2 | 44.76 |
| 2.0082 | 1 | 3 3 2 | 45.11 |
| 1.9898 | 12 | 4 1 2 | 45.55 |
| 1.9853 | 11 | 4 3 1 | 45.66 |
| 1.9796 | 5 | 2 4 2 | 45.80 |
| 1.9451M | 17 | 2 2 3 | 46.66 |
| 1.9451M | | 2 5 1 | 46.66 |
| 1.9248 | 5 | 5 0 1 | 47.18 |
| 1.9054 | 3 | 1 3 3 | 47.69 |
| 1.9002 | 4 | 4 2 2 | 47.83 |
| 1.8957 | 4 | 5 1 1 | 47.95 |
| 1.8850M | 5 | 5 2 0 | 48.24 |
| 1.8850M | | 3 0 3 | 48.24 |
| 1.8575 | 3 | 3 1 3 | 49.00 |
| 1.8476M | 1 | 3 5 0 | 49.28 |
| 1.8476M | | 0 6 0 | 49.28 |
| 1.8295 | 6 | 1 5 2 | 49.80 |
| 1.8172M | 5 | 5 2 1 | 50.16 |
| 1.8172M | | 1 6 0 | 50.16 |
| 1.8105M | 10 | 3 4 2 | 50.36 |
| 1.8105M | | 2 3 3 | 50.36 |
| 1.7945 | 11 | 4 4 1 | 50.84 |
| 1.7847M | 5 | 3 2 3 | 51.14 |
| 1.7847M | | 3 5 1 | 51.14 |
| 1.7737 | 3 | 4 3 2 | 51.48 |
| 1.7566 | 7 | 1 6 1 | 52.02 |
| 1.7336 | 2 | 2 6 0 | 52.76 |
| 1.7111 | 8 | 0 0 4 | 53.51 |

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | |
|---|----------------------------|-------|-------|
| d(Å) | I ^{rel} σ = ±3 | hkl | 2θ(°) |
| 5.658 | 5 | 1 0 1 | 15.65 |
| 5.542 | 4 | 0 2 0 | 15.98 |
| 5.035 | 7 | 1 1 1 | 17.60 |
| 3.959 | 36 | 1 2 1 | 22.44 |
| 3.800 | 43 | 2 1 1 | 23.39 |
| 3.720 | 15 | 2 2 0 | 23.90 |
| 3.468 | 20 | 1 3 0 | 25.67 |
| 3.423 | 79 | 0 0 2 | 26.01 |
| 3.268 | 100 | 2 2 1 | 27.27 |
| 3.093 | 10 | 1 3 1 | 28.84 |
| 3.004 | 10 | 3 0 1 | 29.72 |
| 2.899 | 11 | 3 1 1 | 30.82 |
| 2.863 | 14 | 3 2 0 | 31.22 |
| 2.826 | 4 | 2 0 2 | 31.63 |
| 2.772 | 12 | 0 4 0 | 32.27 |

Cesium Iodide, CsI₃ - (continued)

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

Cesium Molybdenum Oxide, Cs₂Mo₃O₁₀

Synonyms

Cesium molybdate
Dicesium trimolybdate

Sample

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

Color

Colorless

Structure

Monoclinic, C2/c (15), Z = 4, isostructural with K₂Mo₃O₁₀. The structure of K₂Mo₃O₁₀ was determined by Gatehouse and Leverett (1968).

Lattice constants of this sample

a = 14.469(2) Å
b = 8.4022(9)
c = 9.4609(14)
β = 97.73(1)°

a/b = 1.7220
c/b = 1.1260

Volume

1139.7 Å³

Density

(calculated) 4.159 g/cm³

Figure of merit

F₃₀ = 94.2(0.008,42)

Additional pattern

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

References

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å | | | |
|--|----------------------------|--------|-------|
| d(Å) | I ^{rel} σ = ±4 | hkl | 2θ(°) |
| 7.237 | 17 | 1 1 0 | 12.22 |
| 5.933 | 18 | -1 1 1 | 14.92 |
| 5.552 | 19 | 1 1 1 | 15.95 |
| 4.199 | 47 | 0 2 0 | 21.14 |
| 4.155 | 18 | 3 1 0 | 21.37 |
| 4.064 | 8 | -1 1 2 | 21.85 |
| 3.975 | 13 | -3 1 1 | 22.35 |
| 3.823 | 100 | 1 1 2 | 23.25 |
| 3.699 | 34 | 2 0 2 | 24.04 |
| 3.644 | 88 | 3 1 1 | 24.41 |
| 3.625 | 35 | 2 2 0 | 24.54 |
| 3.586 | 15 | 4 0 0 | 24.81 |
| 3.462 | 93 | -2 2 1 | 25.71 |
| 3.306M | 14 | -3 1 2 | 26.95 |
| 3.306M | | 2 2 1 | 26.95 |
| 3.127 | 19 | 0 2 2 | 28.52 |
| 3.052 | 50 | -4 0 2 | 29.24 |
| 2.966 | 45 | -2 2 2 | 30.11 |
| 2.942M | 41 | -1 1 3 | 30.36 |
| 2.942M | | 3 1 2 | 30.36 |
| 2.801 | 2 | 1 1 3 | 31.93 |
| 2.778 | 2 | 2 2 2 | 32.20 |
| 2.749 | 5 | 1 3 0 | 32.55 |
| 2.727 | 18 | 4 2 0 | 32.82 |
| 2.715 | 32 | 5 1 0 | 32.97 |
| 2.694 | 4 | -4 2 1 | 33.23 |
| 2.657 | 3 | -1 3 1 | 33.71 |
| 2.620 | 11 | 1 3 1 | 34.20 |
| 2.548 | 3 | 4 2 1 | 35.20 |
| 2.470 | 7 | -4 2 2 | 36.35 |
| 2.451 | 4 | -2 2 3 | 36.64 |
| 2.416 | 1 | 3 3 0 | 37.18 |
| 2.3903 | 5 | 6 0 0 | 37.60 |
| 2.3031 | 20 | 3 3 1 | 39.08 |
| 2.2762 | 25 | -1 1 4 | 39.56 |
| 2.2565 | 12 | -6 0 2 | 39.92 |
| 2.2287 | 5 | 5 1 2 | 40.44 |
| 2.1909 | 1L | -5 1 3 | 41.17 |
| 2.1868 | 2 | 1 1 4 | 41.25 |
| 2.1677 | 13 | -4 2 3 | 41.63 |
| 2.1514 | 6 | -3 1 4 | 41.96 |
| 2.1456 | 8 | 2 0 4 | 42.08 |
| 2.0902M | 6 | -1 3 3 | 43.25 |
| 2.0902M | | 3 3 2 | 43.25 |
| 2.0801 | 7 | -6 2 1 | 43.47 |

Cesium Molybdenum Oxide, Cs₂Mo₃O₁₀ - (continued)

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

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

Chromium Boride, CrB₂

Synonym

Chromium diboride

CAS registry no.

12007-16-8

Sample

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

Color

Olive gray

Structure

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

Lattice constants of this sample

a = 2.9730(13) Å

c = 3.0709(2)

c/a = 1.0329

Volume

23.506 Å³

Density

(calculated) 5.200 g/cm³

Figure of merit

F₂₀ = 94.4(0.011,20)

Additional pattern

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | | |
|---|------------------|-----|---|---|--------|
| Internal standard W, a = 3.16524 Å | | | | | |
| d(Å) | I ^{rel} | hkl | | | 2θ(°) |
| σ = ±1 | | | | | |
| 3.071 | 20 | 0 | 0 | 1 | 29.05 |
| 2.574 | 57 | 1 | 0 | 0 | 34.82 |
| 1.9730 | 100 | 1 | 0 | 1 | 45.96 |
| 1.5355 | 10 | 0 | 0 | 2 | 60.22 |
| 1.4866 | 25 | 1 | 1 | 0 | 62.42 |
| 1.3380 | 14 | 1 | 1 | 1 | 70.30 |
| 1.3191 | 15 | 1 | 0 | 2 | 71.46 |
| 1.2871 | 7 | 2 | 0 | 0 | 73.52 |
| 1.1874 | 16 | 2 | 0 | 1 | 80.89 |
| 1.0682 | 16 | 1 | 1 | 2 | 92.29 |
| 1.0238 | 1 | 0 | 0 | 3 | 97.60 |
| .9865 | 8 | 2 | 0 | 2 | 102.67 |
| .9732 | 6 | 2 | 1 | 0 | 104.65 |
| .9512 | 9 | 1 | 0 | 3 | 108.15 |
| .9277 | 20 | 2 | 1 | 1 | 112.26 |
| .8582 | 7 | 3 | 0 | 0 | 127.67 |
| .8430 | 4 | 1 | 1 | 3 | 132.05 |
| .8265 | 4 | 3 | 0 | 1 | 137.50 |
| .8220 | 11 | 2 | 1 | 2 | 139.15 |
| .8012 | 8 | 2 | 0 | 3 | 148.09 |

Chromium Niobium Oxide, CrNbO₄

Synonyms

Niobium chromium oxide
Chromium niobate

CAS registry no.

58500-35-9

Sample

Made by heating Cr₂O₃ and Nb₂O₅ at 1000 °C for 24 hours. The sample contained some Cr₂O₃.

Color

Gray olive

Structure

Tetragonal, P₄/mm (136), Z = 1. Rutile structure (Brandt, 1943). The structure of CrNbO₄ is discussed by Khazai et al. (1981).

Lattice constants of this sample

a = 4.6443(2) Å
c = 3.0125(3)

c/a = 0.6486

Volume

64.977 Å³

Density

(calculated) 5.338 g/cm³

Figure of merit

F₂₈ = 60.94(0.013,36)

Additional patterns

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

PDF card 31-927 (Ben-Dor and Shimony, 1978).
The composition of this phase is Cr_{0.4}Nb_{0.6}O₂.

References

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

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

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

| d(Å) | I ^{rel} | hkl | 2θ(°) |
|--------|------------------|-------|--------|
| σ = ±1 | | | |
| 1.7102 | 62 | 2 1 1 | 53.54 |
| 1.6421 | 18 | 2 2 0 | 55.95 |
| 1.5066 | 7 | 0 0 2 | 61.50 |
| 1.4690 | 13 | 3 1 0 | 63.25 |
| 1.4419 | 1L | 2 2 1 | 64.58 |
| 1.3772 | 17 | 3 0 1 | 68.02 |
| 1.3696 | 12 | 1 1 2 | 68.45 |
| 1.3204 | 1 | 3 1 1 | 71.38 |
| 1.2638 | 3 | 2 0 2 | 75.11 |
| 1.2190 | 1 | 2 1 2 | 78.38 |
| 1.1845 | 6 | 3 2 1 | 81.13 |
| 1.1614 | 2 | 4 0 0 | 83.10 |
| 1.1100 | 6 | 2 2 2 | 87.89 |
| 1.0945 | 3 | 3 3 0 | 89.46 |
| 1.0551 | 7 | 4 1 1 | 93.79 |
| 1.0516 | 8 | 3 1 2 | 94.19 |
| 1.0384 | 3 | 4 2 0 | 95.77 |
| .9816M | 2 | 4 2 1 | 103.39 |
| .9816M | | 1 0 3 | 103.39 |
| .9289 | 1 | 4 3 0 | 112.05 |
| .9108 | 1L | 5 1 0 | 115.51 |
| .9039 | 3 | 2 1 3 | 116.90 |
| .8875 | 4 | 4 3 1 | 120.43 |
| .8854 | 4 | 3 3 2 | 120.91 |

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | |
|---|------------------|-------|-------|
| d(Å) | I ^{rel} | hkl | 2θ(°) |
| σ = ±1 | | | |
| 3.283 | 100 | 1 1 0 | 27.14 |
| 2.528 | 65 | 1 0 1 | 35.48 |
| 2.322 | 15 | 2 0 0 | 38.75 |
| 2.220 | 11 | 1 1 1 | 40.60 |
| 2.077 | 4 | 2 1 0 | 43.54 |

Cobalt Arsenate Hydrate (Erythrite), $\text{Co}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$

Synonym

Cobalt orthoarsenate octahydrate

CAS registry no.

54496-59-2

Sample

The sample was made by slowly adding 2 grams of $\text{Na}_2\text{HAsO}_4 \cdot 7\text{H}_2\text{O}$ dissolved in 1 liter of H_2O to 2 grams of CoSO_4 in 3 liters of H_2O . The liquid was kept at about 70 °C for 40 days.

Spectrographic analysis

Major impurities

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

Color

Medium purplish pink

Structure

Monoclinic, $\text{I}2/\text{m}$ (12), $Z = 2$. Vivianite structure (Wolfe, 1940). The structure of vivianite, $\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$, was discussed by Mori and Ito (1950).

Lattice constants of this sample

$a = 10.118(5)\text{\AA}$
 $b = 13.433(4)$
 $c = 4.762(2)$
 $\beta = 101.90(3)^\circ$

$a/b = 0.7532$

$c/b = 0.3545$

Volume

633.32\AA^3

Density

(calculated) 3.140 g/cm^3

Comment

Note the similarity between the data above, and the data for the phase $\text{Zn}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$, also appearing in this Monograph.

Figure of merit

$F_{30} = 43.0(0.013, 53)$

Additional pattern

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

References

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | | |
|---|------------------|-----|---|---|-------|
| Internal standard Si, a = 5.43088 Å | | | | | |
| d(Å) | I ^{rel} | hkl | | | 2θ(°) |
| σ = ±1 | | | | | |
| 7.96 | 26 | 1 | 1 | 0 | 11.11 |
| 6.72 | 100 | 0 | 2 | 0 | 13.17 |
| 4.951 | 9 | 2 | 0 | 0 | 17.90 |
| 4.602 | 2 | -1 | 0 | 1 | 19.27 |
| 4.403 | 19 | 0 | 1 | 1 | 20.15 |
| 4.081 | 5 | 1 | 3 | 0 | 21.76 |
| 3.978 | 7 | 2 | 2 | 0 | 22.33 |
| 3.916 | 12 | 1 | 0 | 1 | 22.69 |
| 3.787 | 2 | -1 | 2 | 1 | 23.47 |
| 3.663 | 7 | -2 | 1 | 1 | 24.28 |
| 3.381 | 3 | 1 | 2 | 1 | 26.34 |
| 3.357 | 4 | 0 | 4 | 0 | 26.53 |
| 3.227 | 42 | 0 | 3 | 1 | 27.62 |
| 3.003 | 47 | -3 | 0 | 1 | 29.73 |
| 2.779 | 9 | 2 | 4 | 0 | 32.18 |
| 2.740 | 30 | -3 | 2 | 1 | 32.66 |
| 2.712 | 24 | -1 | 4 | 1 | 33.00 |
| 2.658 | 14 | 3 | 3 | 0 | 33.69 |
| 2.593 | 1 | 1 | 5 | 0 | 34.56 |
| 2.549 | 9 | 1 | 4 | 1 | 35.18 |
| 2.463 | 18 | 3 | 0 | 1 | 36.45 |
| 2.327 | 17 | 0 | 5 | 1 | 38.66 |
| 2.238M | 3 | 0 | 6 | 0 | 40.26 |
| 2.238M | | -3 | 4 | 1 | 40.26 |
| 2.196 | 9 | -2 | 5 | 1 | 41.06 |
| 2.094 | 7 | -3 | 1 | 2 | 43.17 |
| 2.083 | 9 | 3 | 5 | 0 | 43.41 |
| 2.040 | 2 | 2 | 6 | 0 | 44.36 |
| 2.012 | 3 | -1 | 6 | 1 | 45.02 |
| 1.987 | 5 | 3 | 4 | 1 | 45.61 |
| 1.954 | 7 | 1 | 3 | 2 | 46.44 |
| 1.9172 | 8 | -3 | 3 | 2 | 47.38 |

Cobalt Phosphate Hydrate, $\text{Co}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$

Synonym

Cobalt orthophosphate octahydrate

CAS registry no.

10294-50-5

Sample

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

Color

Unground: deep red

Ground: moderate pale red

Structure

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

Lattice constants of this sample

 $a = 9.9265(14)\text{\AA}$ $b = 13.3360(14)$ $c = 4.6786(7)$ $\beta = 102.310(12)^\circ$ $a/b = 0.7443$ $c/b = 0.3508$

Volume

 605.11\AA^3

Density

(calculated) 2.804 g/cm^3

Figure of merit

 $F_{30} = 97.0(0.007,43)$

Additional pattern

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

References

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

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

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

$\text{CuK}\alpha_1$ $\lambda = 1.540598\text{\AA}$; temp. $25 \pm 1^\circ\text{C}$
Internal standard Ag, $a = 4.08651\text{\AA}$

| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
|------------------|------------------|--------|---------------------|
| $\sigma = \pm 3$ | | | |
| 7.852 | 23 | 1 1 0 | 11.26 |
| 6.667 | 100 | 0 2 0 | 13.27 |
| 4.849 | 25 | 2 0 0 | 18.28 |
| 4.521 | 15 | -1 0 1 | 19.62 |
| 4.323 | 6 | 0 1 1 | 20.53 |

Cobalt Phosphate Hydrate, $\text{Co}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$ - (continued)

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

Erbium Iron, ErFe₂

Synonym

Erbium diiron

CAS registry no.

12060-15-4

Sample

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

Color

Dark grayish olive

Structure

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

Lattice constant of this sample

a = 7.2777(2) Å

Volume

385.46 Å³

Density

(calculated) 9.614 g/cm³

Figure of merit

F₂₃ = 63.8(0.014,26)

Additional pattern

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

Reference

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

| CuK α_1 λ = 1.540598 Å; temp. 25 \pm 1 °C Internal standard Ag, a = 4.08651 Å | | | | | |
|---|------------------|-----|---|---|----------------|
| d(Å) | I ^{rel} | hkl | | | 2 θ (°) |
| $\sigma = \pm 3$ | | | | | |
| 4.201 | 9 | 1 | 1 | 1 | 21.13 |
| 2.572 | 54 | 2 | 2 | 0 | 34.85 |
| 2.193 | 100 | 3 | 1 | 1 | 41.13 |
| 2.101 | 18 | 2 | 2 | 2 | 43.01 |
| 1.8193 | 1L | 4 | 0 | 0 | 50.10 |
| | | | | | |
| 1.6699 | 5 | 3 | 3 | 1 | 54.94 |
| 1.4861 | 26 | 4 | 2 | 2 | 62.44 |
| 1.4006 | 32 | 5 | 1 | 1 | 66.73 |
| 1.2862 | 20 | 4 | 4 | 0 | 73.58 |
| 1.2305 | 3 | 5 | 3 | 1 | 77.51 |
| | | | | | |
| 1.1509 | 13 | 6 | 2 | 0 | 84.03 |
| 1.1098 | 12 | 5 | 3 | 3 | 87.91 |
| 1.0971 | 6 | 6 | 2 | 2 | 89.19 |
| 1.0504 | 1L | 4 | 4 | 4 | 94.33 |
| 1.0190 | 2 | 5 | 5 | 1 | 98.21 |
| | | | | | |
| .9726 | 12 | 6 | 4 | 2 | 104.74 |
| .9476 | 20 | 7 | 3 | 1 | 108.76 |
| .9096 | 6 | 8 | 0 | 0 | 115.75 |
| .8892 | 1L | 7 | 3 | 3 | 120.06 |
| .8576 | 8 | 6 | 6 | 0 | 127.85 |
| | | | | | |
| .8403 | 12 | 7 | 5 | 1 | 132.89 |
| .8349 | 4 | 6 | 6 | 2 | 134.63 |
| .7988 | 2 | 9 | 1 | 1 | 149.28 |

Ethylenediamine Hydrochloride, $C_2H_8N_2 \cdot 2HCl$

Synonyms

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

CAS registry no.

20273-40-9

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$a = 9.9683(13) \text{ \AA}$
 $b = 6.8913(12)$
 $c = 4.4293(6)$
 $\beta = 91.311(12)^\circ$

$a/b = 1.4465$

$c/b = 0.6427$

Volume

304.19 \AA^3

Density

(calculated) 1.452 g/cm^3

Figure of merit

$F_{30} = 57.8(0.011, 49)$

Additional patterns

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

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

References

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

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

| | | | | | |
|---|------------------|-------|---|---|---------------------|
| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ } ^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | | | |
| $d(\text{\AA})$ | I^{rel} | hkl | | | $2\theta(^{\circ})$ |
| $\sigma = \pm 3$ | | | | | |
| 5.669 | 1 | 1 | 1 | 0 | 15.62 |
| 4.427 | 5 | 0 | 0 | 1 | 20.04 |
| 3.725 | 15 | 0 | 1 | 1 | 23.87 |
| 3.466 | 100 | 1 | 1 | 1 | 25.68 |
| 3.350 | 89 | -2 | 0 | 1 | 26.59 |

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

Ethylenediamine Hydrochloride, $C_2H_8N_2 \cdot 2HCl$ - (continued)

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

Ethylenediaminetetraacetic Acid, C₁₀H₁₆N₂O₈

Synonyms

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

CAS registry no.
60-00-4

Sample

The sample was prepared at NBS and recrystal-
lized from water.

Color

Colorless

Structure

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

Lattice constants of this sample

a = 16.112(3) Å
b = 5.5774(15)
c = 13.287(3)
β = 96.30(2)°

a/b = 2.8890
c/b = 2.3825

Volume

1186.8 Å³

Density

(calculated) 1.636 g/cm³

Figure of merit

F₃₀ = 47.7(0.013,50)

Additional pattern

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

Reference

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | |
|---|------------------|--------|-------|
| Internal standard Ag, a = 4.08651 Å | | | |
| d(Å) | I ^{rel} | hkl | 2θ(°) |
| σ = ±4 | | | |
| 8.01 | 17 | 2 0 0 | 11.04 |
| 6.59 | 23 | 0 0 2 | 13.42 |
| 5.394 | 13 | -2 0 2 | 16.42 |
| 5.142 | 12 | 0 1 1 | 17.23 |
| 4.960 | 40 | -1 1 1 | 17.87 |
| 4.847M | 4 | 2 0 2 | 18.29 |
| 4.847M | | 1 1 1 | 18.29 |
| 4.412 | 32 | -2 1 1 | 20.11 |
| 4.003 | 100 | 4 0 0 | 22.19 |
| 3.783 | 12 | -3 1 1 | 23.50 |

Hafnium Nitride, HfN

Synonym

Hafnium mononitride

CAS registry no.

25817-87-2

Sample

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

Color

Dark olive brown

Structure

Cubic, $Fm\bar{3}m$ (225), $Z = 4$. Glaser et al. (1953).

Lattice constant of this sample

$$a = 4.5253(4) \text{ \AA}$$

Volume

 92.67 A^3

Density

(calculated) 13.797 g/cm³

Figure of merit

$$F_{10} = 63.3(0.016, 10)$$

Additional pattern

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

Reference

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

| CuKα ₁ $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ } ^\circ\text{C}$ Internal standard Ag, $a = 4.08651 \text{ \AA}$ | | | | | |
|--|------------------|-------|---|---|---------------------|
| $d(\text{\AA})$ | I^{rel} | hkl | | | $2\theta(^{\circ})$ |
| $\sigma = \pm 1$ | | | | | |
| 2.612 | 100 | 1 | 1 | 1 | 34.31 |
| 2.262 | 62 | 2 | 0 | 0 | 39.82 |
| 1.6002 | 37 | 2 | 2 | 0 | 57.55 |
| 1.3641 | 33 | 3 | 1 | 1 | 68.76 |
| 1.3061 | 9 | 2 | 2 | 2 | 72.28 |
| 1.1314 | 4 | 4 | 0 | 0 | 85.82 |
| 1.0379 | 8 | 3 | 3 | 1 | 95.84 |
| 1.0120 | 10 | 4 | 2 | 0 | 99.13 |
| .9237 | 7 | 4 | 2 | 2 | 113.01 |
| .8710 | 7 | 5 | 1 | 1 | 124.36 |

p-Iodobenzoic Acid, C₇H₅IO₂

CAS registry no.
691-58-9

Sample

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

Color

Colorless

Structure

Monoclinic, P2₁/n (14), Z = 4. The structure was determined qualitatively by Toussaint (1950, 1952).

Lattice constants of this sample

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

a/b = 4.9857
c/b = 0.6887

Volume

754.60 Å³

Density

(calculated) 2.183 g/cm³

Figure of merit

F₃₀ = 42.1(0.010,69)

Additional pattern

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

References

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

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | |
|---|----------------------------|--------|-------|
| d(Å) | I ^{rel} σ = ±3 | hkl | 2θ(°) |
| 15.07 | 100 | 2 0 0 | 5.86 |
| 7.53 | 8 | 4 0 0 | 11.75 |
| 5.604 | 8 | 2 1 0 | 15.80 |
| 5.175 | 3 | 3 1 0 | 17.12 |
| 4.706 | 57 | 4 1 0 | 18.84 |
| 4.261 | 4 | 5 1 0 | 20.83 |
| 4.124 | 8 | -1 0 1 | 21.53 |
| 3.855M | 61 | 6 1 0 | 23.05 |
| 3.855M | | -3 0 1 | 23.05 |
| 3.764 | 7 | 8 0 0 | 23.62 |

Iron Aluminum Oxide (Hercynite), FeAl_2O_4

Synonym

Iron aluminate

CAS registry no.

12068-49-4

Sample

The sample was prepared by grinding under acetone stoichiometric amounts of $\alpha\text{-Fe}_2\text{O}_3$ and $\gamma\text{-Al}_2\text{O}_3$ in an agate mortar. After drying, the mixture was transferred to an iron crucible for heat treatment in controlled atmosphere. The sample was heated at 1200 °C for 8 hours in an oxygen pressure $\leq 10^{-16}$ atm. followed by grinding and reheating for 8 hours at 1300 °C for 8 hours in an oxygen pressure $\leq 10^{-16}$ atm.

Color

Greenish gray

Structure

Cubic, $\text{Fd}3\text{m}$ (227), $Z = 8$. Isostructural with spinel (Holgersson, 1927). The structure of spinel was determined by Bragg (1915) and Nishikawa (1915).

Lattice constant of this sample

$a = 8.1534(1)\text{\AA}$

Volume

542.03\AA^3

Density

(calculated) 4.260 g/cm^3

Figure of merit

$F_{27} = 112.33(0.008, 32)$

Additional patterns

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

Clark, et al. (1931)

Fischer and Hoffmann (1955)

Krause and Thiel (1932)

References

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

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

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

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

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

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

| CuK α_1 $\lambda = 1.540598 \overset{\circ}{\text{\AA}}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.430825 \overset{\circ}{\text{\AA}}$ | | | | | |
|---|------------------|-----------|---|---|-------------------|
| $d(\overset{\circ}{\text{\AA}})$ | I^{rel} | hk ℓ | | | $2\theta(^\circ)$ |
| $\sigma = \pm 2$ | | | | | |
| 4.709 | 3 | 1 | 1 | 1 | 18.83 |
| 2.883 | 58 | 2 | 2 | 0 | 30.99 |
| 2.460 | 100 | 3 | 1 | 1 | 36.50 |
| 2.0382 | 17 | 4 | 0 | 0 | 44.41 |
| 1.8711 | 5 | 3 | 3 | 1 | 48.62 |
| | | | | | |
| 1.6649 | 16 | 4 | 2 | 2 | 55.12 |
| 1.5691 | 36 | 5 | 1 | 1 | 58.80 |
| 1.4414 | 42 | 4 | 4 | 0 | 64.61 |
| 1.2892 | 5 | 6 | 2 | 0 | 73.38 |
| 1.2434 | 8 | 5 | 3 | 3 | 76.56 |
| | | | | | |
| 1.2293 | 3 | 6 | 2 | 2 | 77.60 |
| 1.1769 | 2 | 4 | 4 | 4 | 81.77 |
| 1.1417 | 1 | 5 | 5 | 1 | 84.86 |
| 1.0897 | 5 | 6 | 4 | 2 | 89.97 |
| 1.0614 | 10 | 7 | 3 | 1 | 93.06 |
| | | | | | |
| 1.0191 | 5 | 8 | 0 | 0 | 98.20 |
| .9962 | 1L | 7 | 3 | 3 | 101.29 |
| .9608 | 3 | 6 | 6 | 0 | 106.59 |
| .9415 | 5 | 7 | 5 | 1 | 109.81 |
| .9353 | 1 | 6 | 6 | 2 | 110.89 |
| | | | | | |
| .9116 | 3 | 8 | 4 | 0 | 115.35 |
| .8949 | 2 | 9 | 1 | 1 | 118.80 |
| .8691 | 2 | 6 | 6 | 4 | 124.82 |
| .8547 | 5 | 9 | 3 | 1 | 128.64 |
| .8321 | 10 | 8 | 4 | 4 | 135.55 |
| | | | | | |
| .8195 | 1 | 7 | 7 | 1 | 140.10 |
| .7995 | 3 | 10 | 2 | 0 | 148.93 |

Iron Antimony Oxide, FeSbO₄

Synonym

Iron antimonate

Sample

The sample was prepared at NBS.

Chemical analysis

Chemical analysis showed 22.94 weight percent Fe, 49.47 weight percent Sb, and by difference, 27.59 weight percent oxygen. On this basis, the composition most nearly corresponds to the formula FeSbO₄.

Color

Medium yellowish brown

Structure

Tetragonal, P4₂/mm (136), Z = 1, iso-structural with rutile (Brandt, 1943).

Lattice constants of this sample

a = 4.6352(2) Å
c = 3.0733(2)

c/a = 0.6630

Volume

66.030 Å³

Density

(calculated) 6.076 g/cm³

Figure of merit

F₃₀ = 61.2(0.011,43)

Comment

PDF card 7-349 (Mason and Vitaliano, 1953) requires the value of c = 9.14 only because of its first reflection. The pattern may be a mixture of the rutile and trirutile phases of Fe_xSb_yO₄.

References

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Ag, a = 4.08651 Å | | | |
|--|----------------------------|-------|--------|
| d(Å) | I ^{rel} σ = ±2 | hkl | 2θ(°) |
| 3.279 | 100 | 1 1 0 | 27.17 |
| 2.562 | 71 | 1 0 1 | 34.99 |
| 2.318 | 17 | 2 0 0 | 38.82 |
| 2.242 | 8 | 1 1 1 | 40.19 |
| 2.0720 | 3 | 2 1 0 | 43.65 |
| 1.7185 | 56 | 2 1 1 | 53.26 |
| 1.6386 | 14 | 2 2 0 | 56.08 |
| 1.5367 | 6 | 0 0 2 | 60.17 |
| 1.4655 | 10 | 3 1 0 | 63.42 |
| 1.3912 | 12 | 1 1 2 | 67.24 |
| 1.3802 | 14 | 3 0 1 | 67.85 |
| 1.3231 | 1L | 3 1 1 | 71.21 |
| 1.2806 | 4 | 2 0 2 | 73.96 |
| 1.2344 | 1L | 2 1 2 | 77.22 |
| 1.1858 | 7 | 3 2 1 | 81.02 |
| 1.1585 | 3 | 4 0 0 | 83.35 |
| 1.1211 | 4 | 2 2 2 | 86.80 |
| 1.0925 | 3 | 3 3 0 | 89.67 |
| 1.0606 | 5 | 3 1 2 | 93.15 |
| 1.0559 | 5 | 4 1 1 | 93.69 |
| 1.0364 | 2 | 4 2 0 | 96.02 |
| 1.0004 | 2 | 1 0 3 | 100.71 |
| .9253 | 2 | 4 0 2 | 112.71 |
| .9183 | 4 | 2 1 3 | 114.03 |
| .9091 | 2 | 5 1 0 | 115.84 |
| .8903 | 3 | 3 3 2 | 119.82 |
| .8877 | 5 | 4 3 1 | 120.40 |
| .8593 | 3 | 4 2 2 | 127.38 |
| .8538 | 2 | 3 0 3 | 128.89 |
| .8288 | 4 | 5 2 1 | 136.68 |
| .8194 | 1L | 4 4 0 | 140.11 |
| .8012 | 2 | 3 2 3 | 148.06 |

Iron Chromium Oxide (Chromite), FeCr_2O_4

Synonym

Iron chromite

CAS registry no.

12068-77-8

Sample

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

Color

Dark reddish brown

Structure

Cubic, $\text{Fd}3\text{m}$ (227), $Z = 8$. Isostructural with spinel, Holgersson (1927).

Lattice constant of this sample

$a = 8.3790(2)\text{\AA}$

Volume

588.27\AA^3

Density

(calculated) 5.055 g/cm^3

Polymorphism

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

Figure of merit

$F_{27} = 87.8(0.009, 34)$

Additional patterns

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

Holgersson (1927)

Hilty, et al. (1955)

References

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

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

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

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

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

| $\text{CuK}\alpha_1$ $\lambda = 1.540598\text{\AA}$; temp. $25 \pm 1^\circ\text{C}$ Internal standard Ag, $a = 4.08651\text{\AA}$ | | | |
|---|------------------|--------|---------------------|
| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
| $\sigma = \pm 3$ | | | |
| 4.839 | 13 | 1 1 1 | 18.32 |
| 2.962 | 33 | 2 2 0 | 30.15 |
| 2.526 | 100 | 3 1 1 | 35.51 |
| 2.418 | 7 | 2 2 2 | 37.15 |
| 2.0943 | 22 | 4 0 0 | 43.16 |
| 1.7105 | 11 | 4 2 2 | 53.53 |
| 1.6125 | 39 | 5 1 1 | 57.07 |
| 1.4812 | 48 | 4 4 0 | 62.67 |
| 1.4162 | 2 | 5 3 1 | 65.90 |
| 1.3247 | 3 | 6 2 0 | 71.11 |
| 1.2777 | 10 | 5 3 3 | 74.15 |
| 1.2632 | 5 | 6 2 2 | 75.15 |
| 1.2095 | 3 | 4 4 4 | 79.12 |
| 1.1734 | 1 | 7 1 1 | 82.06 |
| 1.1197 | 4 | 6 4 2 | 86.94 |
| 1.0907 | 12 | 7 3 1 | 89.86 |
| 1.0476 | 5 | 8 0 0 | 94.67 |
| .9873 | 2 | 8 2 2 | 102.56 |
| .9675 | 10 | 7 5 1 | 105.53 |
| .9612 | 2 | 6 6 2 | 106.53 |
| .9367 | 2 | 8 4 0 | 110.64 |
| .8931 | 1 | 6 6 4 | 119.19 |
| .8783 | 5 | 9 3 1 | 122.58 |
| .8552 | 12 | 8 4 4 | 128.50 |
| .8217 | 1 | 10 2 0 | 139.27 |
| .8101 | 7 | 9 5 1 | 143.95 |
| .8063 | 1L | 10 2 2 | 145.65 |

Lithium Zirconium Oxide, Li_2ZrO_3

Synonyms

Lithium zirconate
Dilithium zirconium trioxide

CAS registry no.

12031-83-3

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

a = 5.4266(5) Å
b = 9.0310(8)
c = 5.4227(7)
β = 112.720(8)°

a/b = 0.6009
c/b = 0.6005

Volume

245.13 Å³

Density

(calculated) 4.148 g/cm³

Figure of merit

F₃₀ = 62.6(0.011,43)

Additional pattern

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

References

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | | | |
|---|------------------|-----|---|---|-------|
| d(Å) | I ^{rel} | hkl | | | 2θ(°) |
| σ = ±4 | | | | | |
| 4.512 | 18 | 0 | 2 | 0 | 19.66 |
| 4.377 | 100 | 1 | 1 | 0 | 20.27 |
| 4.037 | 39 | -1 | 1 | 1 | 22.00 |
| 3.351 | 56 | 0 | 2 | 1 | 26.58 |
| 2.852 | 13 | 1 | 1 | 1 | 31.34 |
| 2.580M | 23 | 1 | 3 | 0 | 34.74 |
| 2.580M | | -1 | 1 | 2 | 34.74 |
| 2.504+ | 24 | -1 | 3 | 1 | 35.84 |
| 2.504+ | | 2 | 0 | 0 | 35.84 |
| 2.313 | 19 | -2 | 2 | 1 | 38.90 |
| 2.258M | 33 | -2 | 0 | 2 | 39.90 |
| 2.258M | | 0 | 4 | 0 | 39.90 |
| 2.189M | 7 | 2 | 2 | 0 | 41.21 |
| 2.189M | | 0 | 2 | 2 | 41.21 |
| 2.127 | 46 | 1 | 3 | 1 | 42.46 |
| 2.0590 | 17 | 0 | 4 | 1 | 43.94 |
| 2.0197 | 4 | -2 | 2 | 2 | 44.84 |
| 2.0070 | 1L | -1 | 3 | 2 | 45.14 |
| 1.9115 | 12 | 1 | 1 | 2 | 47.53 |
| 1.7952 | 9 | 2 | 2 | 1 | 50.82 |
| 1.7702M | 5 | -3 | 1 | 1 | 51.59 |
| 1.7702M | | -1 | 1 | 3 | 51.59 |
| 1.7300 | 4 | -2 | 4 | 1 | 52.88 |
| 1.6991M | 20 | -3 | 1 | 2 | 53.92 |
| 1.6991M | | 1 | 5 | 0 | 53.92 |
| 1.6764+ | 10 | -1 | 5 | 1 | 54.71 |
| 1.6764+ | | 2 | 4 | 0 | 54.71 |
| 1.6408M | 8 | 3 | 1 | 0 | 56.00 |
| 1.6408M | | 1 | 3 | 2 | 56.00 |
| 1.6151 | 13 | -2 | 2 | 3 | 56.97 |
| 1.5969 | 3 | -2 | 4 | 2 | 57.68 |
| 1.5643 | 7 | 0 | 2 | 3 | 59.00 |
| 1.5481+ | 32 | -3 | 3 | 1 | 59.68 |
| 1.5481+ | | 1 | 5 | 1 | 59.68 |
| 1.5048 | 10 | 0 | 6 | 0 | 61.58 |
| 1.5019 | 13 | 2 | 0 | 2 | 61.71 |
| 1.4998M | 10 | -3 | 3 | 2 | 61.81 |
| 1.4998M | | -1 | 5 | 2 | 61.81 |
| 1.4849 | 2 | -3 | 1 | 3 | 62.50 |
| 1.4785 | 5 | 2 | 4 | 1 | 62.80 |
| 1.4414 | 1L | 0 | 6 | 1 | 64.61 |
| 1.4257 | 1 | 2 | 2 | 2 | 65.41 |
| 1.4081M | 3 | 3 | 1 | 1 | 66.33 |
| 1.4081M | | 1 | 1 | 3 | 66.33 |
| 1.3727 | 5 | -2 | 4 | 3 | 68.27 |

Lithium Zirconium Oxide, Li_2ZrO_3 - (continued)

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

Magnesium Arsenate Hydrate (Hoernesite), $\text{Mg}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$

Synonym

Magnesium arsenate octahydrate

CAS registry no.

37541-75-6

Sample

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

Color

Colorless

Structure

Monoclinic, $I2/m$ (12), $Z = 2$. Isostructural with vivianite. (Wolfe, 1940) The structure of vivianite, $\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$, is discussed by Mori and Ito (1950).

Lattice constants of this sample

$a = 10.137(2)\text{Å}$
 $b = 13.455(2)$
 $c = 4.7542(10)$
 $\beta = 101.73(2)^\circ$

$a/b = 0.7530$

$c/b = 0.3533$

Volume

634.9 Å^3

Density

(calculated) 2.589 g/cm³

Figure of merit

$F_{30} = 32.0(0.019, 45)$

Additional pattern

PDF card 19-752 (Koritnij and Süssse, 1966)

References

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

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ Å}; \text{ temp. } 25 \pm 1 \text{ °C}$ Internal standard Si, $a = 5.43088 \text{ Å}$ | | | |
|--|------------------|-------|---------------------|
| $d(\text{Å})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
| $\sigma = \pm 3$ | | | |
| 7.97 | 31 | 1 1 0 | 11.09 |
| 6.73 | 100 | 0 2 0 | 13.14 |
| 4.399 | 48 | 0 1 1 | 20.17 |
| 3.992 | 26 | 2 2 0 | 22.25 |
| 3.916 | 16 | 1 0 1 | 22.69 |

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

Magnesium Arsenate Hydrate (Hoernesite), $\text{Mg}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$ - (continued)

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

Magnesium Phosphate (Farringtonite), $\text{Mg}_3(\text{PO}_4)_2$

Synonyms

Magnesium orthophosphate
Trimagnesium biphosphate

CAS registry no.

10043-83-1

Sample

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

Color

Colorless

Structure

Monoclinic, $\text{P2}_1/\text{n}$ (14), $Z = 2$. The structure of $\text{Mg}_3(\text{PO}_4)_2$ was determined by Nord and Kierkegaard (1968).

Lattice constants of this sample

$a = 7.5995(8) \text{ \AA}$
 $b = 8.2355(8)$
 $c = 5.0762(5)$
 $\beta = 94.062(9)^\circ$

$a/b = 0.9228$

$c/b = 0.6164$

Volume

317.42 \AA^3

Density

(calculated) 2.750 g/cm^3

Polymorphism

Berak (1958) suggests a second form of $\text{Mg}_3(\text{PO}_4)_2$ stable above about 1000 °C.

Figure of merit

$F_{30} = 57.0(0.011, 47)$

Additional patterns

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

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

References

Berak, J. (1958). Roczn. Chem. 32, 19.

Du Fresne, E. R. and Roy, S. K. (1961).

Geochim. Cosmochim. Acta 24, 198.

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

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | | |
|--|--------------------------------------|--------|-------------------|--|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^\circ)$ | |
| 5.576 | 10 | 1 1 0 | 15.88 | |
| 4.356 | 30 | -1 0 1 | 20.37 | |
| 4.312 | 24 | 0 1 1 | 20.58 | |
| 4.118 | 30 | 0 2 0 | 21.56 | |
| 4.077 | 28 | 1 0 1 | 21.78 | |
| 3.852 | 84 | -1 1 1 | 23.07 | |
| 3.792 | 6 | 2 0 0 | 23.44 | |
| 3.657 | 28 | 1 1 1 | 24.32 | |
| 3.619 | 6 | 1 2 0 | 24.58 | |
| 3.443 | 100 | 2 1 0 | 25.86 | |
| 3.195 | 14 | 0 2 1 | 27.90 | |
| 2.992 | 21 | -1 2 1 | 29.84 | |
| 2.896 | 4 | 1 2 1 | 30.85 | |
| 2.790 | 16 | 2 2 0 | 32.05 | |
| 2.764 | 3 | 2 1 1 | 32.36 | |
| 2.533 | 22 | 0 0 2 | 35.41 | |
| 2.498 | 23 | -2 2 1 | 35.92 | |
| 2.414M | 32 | 3 1 0 | 37.22 | |
| 2.414M | | 0 3 1 | 37.22 | |
| 2.322 | 8 | -1 3 1 | 38.75 | |
| 2.240 | 5 | -3 1 1 | 40.22 | |
| 2.222 | 4 | 2 3 0 | 40.57 | |
| 2.177 | 3 | -2 0 2 | 41.45 | |
| 2.158 | 1L | 0 2 2 | 41.83 | |
| 2.125 | 22 | 3 1 1 | 42.51 | |
| 2.108 | 9 | -1 2 2 | 42.87 | |
| 2.0679 | 10 | -2 3 1 | 43.74 | |
| 2.0599 | 8 | 0 4 0 | 43.92 | |
| 2.0417 | 13 | 1 2 2 | 44.33 | |
| 1.9866 | 2 | 1 4 0 | 45.63 | |
| 1.9256 | 3 | -2 2 2 | 47.16 | |
| 1.9077 | 2 | 0 4 1 | 47.63 | |
| 1.8950 | 7 | 4 0 0 | 47.97 | |
| 1.8597 | 7 | 3 3 0 | 48.94 | |
| 1.8275 | 9 | 2 2 2 | 49.86 | |
| 1.8108 | 1L | -3 1 2 | 50.35 | |
| 1.7860 | 3 | 1 3 2 | 51.10 | |
| 1.7753 | 8 | -3 3 1 | 51.43 | |
| 1.7224M | 7 | -2 4 1 | 53.13 | |
| 1.7224M | | 4 2 0 | 53.13 | |
| 1.6976 | 4 | 4 1 1 | 53.97 | |
| 1.6918M | 10 | -3 2 2 | 54.17 | |
| 1.6918M | | 3 1 2 | 54.17 | |
| 1.6860 | 1L | 2 4 1 | 54.37 | |
| 1.6727 | 1L | -1 0 3 | 54.84 | |

Magnesium Phosphate (Farringtonite), $\text{Mg}_3(\text{PO}_4)_2$ - (continued)

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

Manganese Tartrate, $C_4H_4MnO_6$

Sample

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

Color

Pale greenish yellow

Structure

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

Lattice constants of this sample

$a = 9.4388(8) \text{ \AA}$
 $b = 11.6925(13)$
 $c = 5.0706(4)$

$a/b = 0.8073$
 $c/b = 0.4337$

Volume

559.61 \AA^3

Density

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

Figures of merit

$F_{30} = 57.1(0.011, 49)$
 $M_{20} = 40.5$

Additional pattern

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

References

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

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

| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
|------------------|------------------|-------|---------------------|
| $\sigma = \pm 2$ | | | |
| 3.008 | 1L | 2 3 0 | 29.68 |
| 2.923 | 8 | 0 4 0 | 30.56 |
| 2.794 | 1L | 1 4 0 | 32.01 |
| 2.673 | 27 | 3 0 1 | 33.50 |
| 2.585 | 49 | 2 3 1 | 34.67 |
| 2.536 | 4 | 0 0 2 | 35.36 |
| 2.485 | 16 | 2 4 0 | 36.12 |
| 2.446M | 72 | 3 3 0 | 36.71 |
| 2.446M | | 1 4 1 | 36.71 |
| 2.430 | 31 | 3 2 1 | 36.96 |
| 2.398 | 5 | 1 1 2 | 37.48 |
| 2.359 | 1L | 4 0 0 | 38.12 |
| 2.327 | 2 | 0 2 2 | 38.66 |
| 2.270 | 11 | 1 5 0 | 39.68 |
| 2.233M | 16 | 2 0 2 | 40.36 |
| 2.233M | | 2 4 1 | 40.36 |
| 2.188 | 5 | 4 2 0 | 41.23 |
| 2.124 | 3 | 0 5 1 | 42.52 |
| 2.105 | 10 | 4 1 1 | 42.94 |
| 2.086 | 29 | 2 2 2 | 43.34 |
| 2.0733M | 14 | 1 3 2 | 43.62 |
| 2.0733M | | 1 5 1 | 43.62 |
| 1.9727 | 8 | 3 4 1 | 45.97 |
| 1.9466 | 13 | 3 1 2 | 46.62 |
| 1.9361 | 19 | 2 5 1 | 46.89 |
| 1.9153 | 14 | 0 4 2 | 47.43 |
| 1.8755M | 12 | 3 5 0 | 48.50 |
| 1.8755M | | 4 3 1 | 48.50 |
| 1.8361 | 7 | 4 4 0 | 49.61 |
| 1.7857 | 1 | 1 6 1 | 51.11 |
| 1.7744 | 3 | 2 4 2 | 51.46 |
| 1.7699 | 3 | 5 0 1 | 51.60 |
| 1.7606M | 6 | 3 3 2 | 51.89 |
| 1.7606M | | 3 5 1 | 51.89 |
| 1.7273M | 16 | 4 0 2 | 52.97 |
| 1.7273M | | 4 4 1 | 52.97 |
| 1.6985 | 10 | 5 3 0 | 53.94 |
| 1.6927 | 14 | 5 2 1 | 54.14 |
| 1.6638 | 3 | 1 0 3 | 55.16 |
| 1.6563M | 4 | 3 6 0 | 55.43 |
| 1.6563M | | 4 2 2 | 55.43 |
| 1.6446 | 8 | 1 7 0 | 55.86 |
| 1.6000 | 7 | 1 2 3 | 57.56 |
| 1.5861M | 7 | 0 7 1 | 58.11 |
| 1.5861M | | 5 4 0 | 58.11 |
| 1.5780 | 6 | 4 5 1 | 58.44 |
| 1.5735 | 5 | 6 0 0 | 58.62 |
| 1.5509 | 2 | 0 3 3 | 59.56 |
| 1.5450 | 1L | 0 6 2 | 59.81 |
| 1.5191 | 4 | 6 2 0 | 60.94 |

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^{\circ} \text{C}$ Internal standard Si, $a = 5.430825 \text{ \AA}$ | | | |
|---|------------------|-------|---------------------|
| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
| $\sigma = \pm 2$ | | | |
| 7.34 | 14 | 1 1 0 | 12.04 |
| 5.843 | 65 | 0 2 0 | 15.15 |
| 4.716 | 12 | 2 0 0 | 18.80 |
| 4.653 | 53 | 0 1 1 | 19.06 |
| 4.467 | 100 | 1 0 1 | 19.86 |
| 3.673 | 57 | 2 2 0 | 24.21 |
| 3.604 | 20 | 1 3 0 | 24.68 |
| 3.549 | 98 | 1 2 1 | 25.07 |
| 3.313 | 18 | 2 1 1 | 26.89 |
| 3.092 | 3 | 0 3 1 | 28.85 |

Manganese Tartrate, $C_4H_4MnO_6$ - (continued)

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

Molybdenum Silicide, Mo₅Si₃

CAS registry no.
12033-40-8

Sample

Stoichiometric amounts of Mo and Si₃N₄ were mixed, pelleted and heated in a crucible to 1600 °C for 1 hour while lying on a pellet of previously made Mo₅Si₃ which was put on a piece of Mo.

Color

Olive black

Structure

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

Lattice constants of this sample

a = 9.6483(6) Å
c = 4.9135(5)

c/a = 0.5093

Volume

457.40 Å³

Density

(calculated) 8.190 g/cm³

Figure of merit

F₃₀ = 98.6(0.009,35)

Additional patterns

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

Nowotny et al. (1956)

References

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

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | |
|---|----------------------------|-------|-------|
| d(Å) | I ^{rel} σ = ±2 | hkl | 2θ(°) |
| 6.820 | 1 | 1 1 0 | 12.97 |
| 4.826 | 2 | 2 0 0 | 18.37 |
| 3.413 | 5 | 2 2 0 | 26.09 |
| 3.242 | 25 | 2 1 1 | 27.49 |
| 3.052 | 21 | 3 1 0 | 29.24 |
| 2.457 | 25 | 0 0 2 | 36.54 |
| 2.412 | 16 | 4 0 0 | 37.25 |
| 2.351 | 71 | 3 2 1 | 38.26 |
| 2.311 | 12 | 1 1 2 | 38.94 |
| 2.2740 | 10 | 3 3 0 | 39.60 |
| 2.1903 | 38 | 2 0 2 | 41.18 |
| 2.1578 | 59 | 4 2 0 | 41.83 |
| 2.1130 | 100 | 4 1 1 | 42.76 |
| 1.9940 | 57 | 2 2 2 | 45.45 |
| 1.7955 | 2 | 4 3 1 | 50.81 |
| 1.7209 | 2 | 4 0 2 | 53.18 |
| 1.6835 | 8 | 5 2 1 | 54.46 |
| 1.6544 | 1 | 5 3 0 | 55.50 |
| 1.6087 | 2 | 6 0 0 | 57.22 |
| 1.5314 | 4 | 2 1 3 | 60.40 |
| 1.5254 | 10 | 6 2 0 | 60.66 |
| 1.5103 | 1L | 6 1 1 | 61.33 |
| 1.4991 | 11 | 5 1 2 | 61.84 |
| 1.4406 | 11 | 5 4 1 | 64.65 |
| 1.4012 | 11 | 4 4 2 | 66.70 |
| 1.3971 | 18 | 3 2 3 | 66.92 |
| 1.3804 | 12 | 6 3 1 | 67.84 |
| 1.3724 | 11 | 5 3 2 | 68.29 |
| 1.3643 | 17 | 7 1 0 | 68.75 |
| 1.3453 | 24 | 6 0 2 | 69.86 |
| 1.3418 | 33 | 4 1 3 | 70.07 |
| 1.2797 | 2 | 7 2 1 | 74.02 |
| 1.2283 | 9 | 0 0 4 | 77.68 |
| 1.2086M | 2 | 1 1 4 | 79.19 |
| 1.2086M | | 5 2 3 | 79.19 |
| 1.1979 | 1 | 6 5 1 | 80.04 |
| 1.1932 | 6 | 7 1 2 | 80.42 |
| 1.1751 | 11 | 6 4 2 | 81.92 |
| 1.1698 | 10 | 8 2 0 | 82.37 |
| 1.1631 | 2 | 7 4 1 | 82.95 |
| 1.1391M | 3 | 3 1 4 | 85.10 |
| 1.1391M | | 6 1 3 | 85.10 |
| 1.1369 | 8 | 6 6 0 | 85.30 |
| 1.1259 | 4 | 7 3 2 | 86.34 |
| 1.1087 | 4 | 5 4 3 | 88.02 |
| 1.1004 | 11 | 8 3 1 | 88.86 |
| 1.0945 | 4 | 4 0 4 | 89.46 |

Nickel Arsenate Hydrate (Annabergite), $\text{Ni}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$

Synonym

Nickel orthoarsenate octahydrate

CAS registry no.

54469-74-1

Sample

The sample was prepared at NBS. A solution of 2 gms $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ in 1 liter H_2O was added dropwise to a solution of 2 gms Na_2HAsO_4 in $1\frac{1}{2}$ liters of warm H_2O . The combined solution was held at 70 to 80 °C for 3 weeks. The crystals were filtered off and washed with H_2O and $\text{C}_2\text{H}_5\text{OH}$.

Color

Light yellow green

Structure

Monoclinic, I2/m (12), $Z = 2$ (Barth, 1937). It is isostructural with vivianite, $\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$. The structure of vivianite was discussed by Mori and Ito (1950).

Lattice constants of this sample

$a = 10.054(2) \text{ \AA}$
 $b = 13.303(3)$
 $c = 4.7159(10)$
 $\beta = 102.10(2)^\circ$

$a/b = 0.7558$

$c/b = 0.3545$

Volume

616.73 \AA^3

Density

(calculated) 3.221 g/cm^3

Figure of merit

$F_{30} = 55.6(0.012, 44)$

Additional pattern

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

References

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

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

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal std. Fluorophlogopite SRM 675 | | | | |
|---|--------------------------------------|--------|-------------------|--|
| d(\AA) | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^\circ)$ | |
| 7.91 | 33 | 1 1 0 | 11.17 | |
| 6.66 | 100 | 0 2 0 | 13.29 | |
| 4.919 | 11 | 2 0 0 | 18.02 | |
| 4.562 | 4 | -1 0 1 | 19.44 | |
| 4.363 | 20 | 0 1 1 | 20.34 | |
| 4.044 | 6 | 1 3 0 | 21.96 | |
| 3.954 | 8 | 2 2 0 | 22.47 | |
| 3.879 | 16 | 1 0 1 | 22.91 | |
| 3.765 | 3 | -1 2 1 | 23.61 | |
| 3.639 | 8 | -2 1 1 | 24.44 | |
| 3.347 | 5 | 1 2 1 | 26.61 | |
| 3.326 | 4 | 0 4 0 | 26.78 | |
| 3.198 | 43 | 0 3 1 | 27.88 | |
| 2.982M | 52 | -3 0 1 | 29.94 | |
| 2.982M | | 2 1 1 | 29.94 | |
| 2.756 | 12 | 2 4 0 | 32.46 | |
| 2.721 | 30 | -3 2 1 | 32.89 | |
| 2.687 | 21 | -1 4 1 | 33.32 | |
| 2.635 | 14 | 3 3 0 | 34.00 | |
| 2.568 | 1 | 1 5 0 | 34.91 | |
| 2.523 | 8 | 1 4 1 | 35.55 | |
| 2.440 | 17 | 3 0 1 | 36.80 | |
| 2.321 | 10 | -1 1 2 | 38.76 | |
| 2.304M | 16 | 4 2 0 | 39.07 | |
| 2.304M | | 0 5 1 | 39.07 | |
| 2.217 | 3 | 0 6 0 | 40.66 | |
| 2.178M | 8 | 0 2 2 | 41.43 | |
| 2.178M | | -2 5 1 | 41.43 | |
| 2.155 | 1 | -2 2 2 | 41.89 | |
| 2.102 | 1 | -4 3 1 | 43.00 | |
| 2.079 | 7 | -3 1 2 | 43.49 | |
| 2.066 | 8 | 3 5 0 | 43.79 | |
| 2.021 | 1 | 2 6 0 | 44.80 | |
| 1.9919 | 2 | -1 6 1 | 45.50 | |
| 1.9678 | 3 | 3 4 1 | 46.09 | |
| 1.9463 | 6 | 5 1 0 | 46.63 | |
| 1.9322 | 6 | 1 3 2 | 46.99 | |
| 1.9006 | 9 | -3 3 2 | 47.82 | |
| 1.8240 | 3 | 4 3 1 | 49.96 | |
| 1.7756 | 2 | -4 5 1 | 51.42 | |
| 1.7572 | 3 | 0 7 1 | 52.00 | |
| 1.6915 | 1 | -5 4 1 | 54.18 | |
| 1.6713 | 8 | 1 5 2 | 54.89 | |
| 1.6629 | 10 | 0 8 0 | 55.19 | |
| 1.6505 | 11 | -3 5 2 | 55.64 | |

Nickel Arsenate Hydrate (Annabergite), $\text{Ni}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$ - (continued)

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

Nickel Molybdenum Oxide, NiMoO₄

Synonyms

Molybdenum nickel tetraoxide
Nickel molybdate

Sample

The sample was prepared at NBS. Stoichiometric amounts of NiO and MoO₃ were heated at 800 °C for 2 hours, then ground and reheated at 800 °C for 6 hours.

Color

Brilliant yellow green

Structure

Monoclinic, I2/m (12), Z = 8, isostructural with low temperature CoMoO₄ (Smith, 1962).

Lattice constants of this sample

a = 9.509(2) Å
b = 8.759(2)
c = 7.6678(15)
β = 113.13(2)°

a/b = 1.0856
c/b = 0.8754

Volume

587.3 Å³

Density

(calculated) 4.946 g/cm³

Polymorphism

Sleight and Chamberland (1968) report 3 polymorphs. The one described here occurs at low temperature when the heated reactants are cooled slowly. A second polymorph exists only at temperatures above 690 °C, and is isostructural with MnMoO₄. A third polymorph, isostructural with NiWO₄, can be prepared hydrothermally at 700 °C with pressures above 3 kbars.

Figure of merit

F₃₀ = 27.7(0.017,63)

Additional patterns

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

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

References

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | | |
|---|----------------------------|--------|-------|--|
| d(Å) | I ^{rel} σ = ±2 | hkl | 2θ(°) | |
| 6.19 | 80 | 1 1 0 | 14.29 | |
| 5.50 | 4 | 0 1 1 | 16.11 | |
| 4.665 | 11 | 1 0 1 | 19.01 | |
| 4.373M | 1 | 0 2 0 | 20.29 | |
| 4.373M | | 2 0 0 | 20.29 | |
| 4.085 | 3 | -2 1 1 | 21.74 | |
| 3.711 | 15 | -1 2 1 | 23.96 | |
| 3.513 | 48 | -1 1 2 | 25.33 | |
| 3.166 | 5 | -3 0 1 | 28.16 | |
| 3.095 | 100 | 2 2 0 | 28.82 | |
| 3.002 | 2 | 2 1 1 | 29.74 | |
| 2.769M | 15 | 1 3 0 | 32.31 | |
| 2.769M | | 3 1 0 | 32.31 | |
| 2.746 | 46 | 0 2 2 | 32.58 | |
| 2.727 | 36 | -3 1 2 | 32.82 | |
| 2.465 | 1L | -2 3 1 | 36.42 | |
| 2.331M | 8 | 2 0 2 | 38.59 | |
| 2.331M | | -3 0 3 | 38.59 | |
| 2.323 | 10 | -1 3 2 | 38.74 | |
| 2.307 | 4 | -4 0 2 | 39.01 | |
| 2.284 | 1 | -4 1 1 | 39.42 | |
| 2.188M | 14 | 0 4 0 | 41.23 | |
| 2.188M | | 4 0 0 | 41.23 | |
| 2.154 | 1L | 2 3 1 | 41.90 | |
| 2.094 | 5 | 3 2 1 | 43.17 | |
| 2.090 | 5 | -1 4 1 | 43.26 | |
| 2.062 | 45 | 3 3 0 | 43.87 | |
| 1.998 | 1 | -4 1 3 | 45.36 | |
| 1.982 | 3 | 1 4 1 | 45.74 | |
| 1.957M | 4 | 2 4 0 | 46.37 | |
| 1.957M | | 4 2 0 | 46.37 | |
| 1.916 | 24 | -2 0 4 | 47.40 | |
| 1.847M | 1 | -5 1 2 | 49.30 | |
| 1.847M | | 4 1 1 | 49.30 | |
| 1.836 | 3 | -1 1 4 | 49.60 | |
| 1.828 | 2 | -3 1 4 | 49.85 | |
| 1.801 | 2 | -3 4 1 | 50.63 | |
| 1.759 | 1L | 2 1 3 | 51.94 | |
| 1.727 | 2 | -5 2 1 | 52.98 | |
| 1.716 | 10 | 5 1 0 | 53.34 | |

Nickel Molybdenum Oxide, NiMoO₄ - (continued)

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

Nickel Phosphate Hydrate, $\text{Ni}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$

Synonym

Nickel orthophosphate octahydrate

CAS registry no.

19033-89-7

Sample

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

Color

Very light yellowish green.

Structure

Monoclinic, $\text{I}2/\text{m}$ (12), $Z = 2$. Vivianite structure, from the similarity of cell size, space group and chemistry. The structure of vivianite, $\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$, is discussed by Mori and Ito (1950).

Lattice constants of this sample

$a = 9.846(4) \text{ \AA}$
 $b = 13.203(4)$
 $c = 4.6342(15)$
 $\beta = 102.27(3)^\circ$

$a/b = 0.7457$
 $c/b = 0.3510$

Volume

588.67 \AA^3

Density

(calculated) 2.878 g/cm^3

Figure of merit

$F_{30} = 31.9(0.016, 58)$

Additional pattern

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

References

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | | |
|---|------------------|-----|---|---|-------|
| Internal standard Ag, a = 4.08651 Å | | | | | |
| d(Å) | I ^{rel} | hkl | | | 2θ(°) |
| σ = ±3 | | | | | |
| 7.77 | 36 | 1 | 1 | 0 | 11.38 |
| 6.62 | 100 | 0 | 2 | 0 | 13.36 |
| 4.808 | 61 | 2 | 0 | 0 | 18.44 |
| 4.480 | 32 | -1 | 0 | 1 | 19.80 |
| 4.277 | 10 | 0 | 1 | 1 | 20.75 |
| 4.005 | 20 | 1 | 3 | 0 | 22.18 |
| 3.799 | 50 | 1 | 0 | 1 | 23.40 |
| 3.576 | 8 | -2 | 1 | 1 | 24.88 |
| 3.297 | 2 | 0 | 4 | 0 | 27.02 |
| 3.159 | 33 | 0 | 3 | 1 | 28.23 |
| 2.924 | 72 | -3 | 0 | 1 | 30.55 |
| 2.722 | 6 | 2 | 4 | 0 | 32.88 |
| 2.675 | 46 | -3 | 2 | 1 | 33.47 |
| 2.657 | 35 | -1 | 4 | 1 | 33.71 |
| 2.591 | 10 | 3 | 3 | 0 | 34.59 |
| 2.548 | 2 | 1 | 5 | 0 | 35.19 |
| 2.491 | 19 | 1 | 4 | 1 | 36.03 |
| 2.389 | 27 | 3 | 0 | 1 | 37.62 |
| 2.283M | 17 | -1 | 1 | 2 | 39.44 |
| 2.283M | | 0 | 5 | 1 | 39.44 |
| 2.241 | 2 | -2 | 0 | 2 | 40.20 |
| 2.189 | 18 | -3 | 4 | 1 | 41.20 |
| 2.153 | 14 | -2 | 5 | 1 | 41.93 |
| 2.122 | 5 | -2 | 2 | 2 | 42.56 |
| 2.079 | 3 | 1 | 1 | 2 | 43.49 |
| 2.039 | 11 | 3 | 5 | 0 | 44.39 |
| 1.975 | 1 | -1 | 6 | 1 | 45.92 |
| 1.938 | 3 | 4 | 1 | 1 | 46.83 |
| 1.901 | 19 | 1 | 3 | 2 | 47.81 |
| 1.872 | 6 | -3 | 3 | 2 | 48.61 |
| 1.857 | 5 | -4 | 0 | 2 | 49.01 |
| 1.789 | 3 | 4 | 3 | 1 | 51.00 |
| 1.6503M | 5 | 0 | 8 | 0 | 55.65 |
| 1.6503M | | 5 | 0 | 1 | 55.65 |

Nickel Sulfate Hydrate (Nickel-hexahydrate), β -NiSO₄·6H₂O

Synonym

Nickel sulfate hexahydrate

CAS registry no.

10101-97-0

Sample

The sample was prepared by slow evaporation from a solution of nickel sulfate in an aqueous solution of H₃PO₄.

Color

Strong green

Structure

Monoclinic, A2/a (15), Z = 8. Isostructural with other divalent hexahydrate sulfates (Sutor, 1959). The structure of MgSO₄·6H₂O was discussed by Ide (1938).

Lattice constants of this sample

a = 24.188(5) Å
b = 7.2410(14)
c = 9.895(2)
β = 98.41(2)°

a/b = 3.3404
c/b = 1.3665

Volume

1714.4 Å³

Density

(calculated) 2.037 g/cm³

Polymorphism

NiSO₄·6H₂O also occurs in a tetragonal form as the mineral retgersite.

Figure of merit

F₃₀ = 52.3(0.013,45)

Additional patterns

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

PDF card 26-1288 (Nawaz, 1973)

References

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

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

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å | | | |
|--|----------------------------|--------|-------|
| d(Å) | I ^{rel} σ = ±3 | hkl | 2θ(°) |
| 5.98 | 5 | 4 0 0 | 14.80 |
| 5.824 | 20 | 0 1 1 | 15.20 |
| 5.538 | 6 | 1 1 1 | 15.99 |
| 5.424 | 21 | -2 1 1 | 16.33 |
| 5.061 | 21 | 2 1 1 | 17.51 |
| 4.900M | 51 | -3 1 1 | 18.09 |
| 4.900M | | 0 0 2 | 18.09 |
| 4.782 | 24 | -2 0 2 | 18.54 |
| 4.519 | 6 | 3 1 1 | 19.63 |
| 4.367 | 100 | -4 1 1 | 20.32 |
| 4.314 | 21 | 2 0 2 | 20.57 |
| 4.096 | 22 | -4 0 2 | 21.68 |
| 4.003 | 60 | 4 1 1 | 22.19 |
| 3.865 | 4 | -5 1 1 | 22.99 |
| 3.625 | 14 | 0 2 0 | 24.54 |
| 3.576 | 9 | 1 2 0 | 24.88 |
| 3.544M | 20 | 5 1 1 | 25.11 |
| 3.544M | | 4 0 2 | 25.11 |
| 3.466 | 3 | 2 2 0 | 25.68 |
| 3.432 | 8 | -6 1 1 | 25.94 |
| 3.340 | 8 | -6 0 2 | 26.67 |
| 3.162 | 7 | 6 1 1 | 28.20 |
| 3.068 | 2 | -7 1 1 | 29.08 |
| 3.001 | 6 | -1 1 3 | 29.75 |
| 2.992 | 11 | 8 0 0 | 29.84 |
| 2.979 | 17 | -2 1 3 | 29.97 |
| 2.916M | 26 | -1 2 2 | 30.63 |
| 2.916M | | -3 1 3 | 30.63 |
| 2.890M | 38 | 6 0 2 | 30.92 |
| 2.890M | | 5 2 0 | 30.92 |
| 2.860 | 1 | 1 2 2 | 31.25 |
| 2.818 | 8 | -4 1 3 | 31.73 |
| 2.801 | 1 | 2 1 3 | 31.92 |
| 2.774 | 9 | 2 2 2 | 32.25 |
| 2.737 | 2 | -8 0 2 | 32.69 |
| 2.711 | 1L | -4 2 2 | 33.02 |
| 2.690 | 5 | -5 1 3 | 33.28 |
| 2.681 | 5 | 6 2 0 | 33.39 |
| 2.660 | 5 | 3 2 2 | 33.66 |
| 2.588 | 1L | -5 2 2 | 34.63 |
| 2.570 | 9 | 8 1 1 | 34.88 |
| 2.553 | 2 | -6 1 3 | 35.12 |
| 2.471 | 12 | -2 0 4 | 36.33 |
| 2.454 | 3 | -6 2 2 | 36.59 |
| 2.408 | 2 | -7 1 3 | 37.31 |

Nickel Sulfate Hydrate (Nickel-hexahydrate), β -NiSO₄·6H₂O - (continued)

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

Niobium, Nb

Synonym

Columbium

CAS registry no.

7440-03-1

Sample

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

Color

Dark gray

Structure

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

Lattice constant of this sample

$a = 3.30332(13)\text{\AA}$

Volume

36.046\AA^3

Density

(calculated) 8.560 g/cm^3

Figure of merit

$F_g = 102.8(0.010, 8)$

Additional patterns

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

Nadler and Kempter (1959)

References

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

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

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

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

| CuK α_1 $\lambda = 1.540598\text{\AA}$; temp. $25 \pm 1\text{ }^\circ\text{C}$ Internal standard W, $a = 3.16524\text{\AA}$ | | | |
|--|--------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^\circ)$ |
| 2.336 | 100 | 1 1 0 | 38.51 |
| 1.6519 | 18 | 2 0 0 | 55.59 |
| 1.3484 | 28 | 2 1 1 | 69.68 |
| 1.1678 | 8 | 2 2 0 | 82.54 |
| 1.0446 | 11 | 3 1 0 | 95.02 |
| .9535 | 3 | 2 2 2 | 107.78 |
| .8830 | 13 | 3 2 1 | 121.48 |
| .8258 | 2 | 4 0 0 | 137.74 |

Potassium Barium Phosphate, KBaPO_4

Synonym

Potassium barium orthophosphate

CAS registry no.

25640-29-3

Sample

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

Color.

Colorless

Structure

Orthorhombic, Pnam (62), Z = 4. (Struck and White, 1962). Isostructural with $\beta\text{-K}_2\text{SO}_4$, arcanite.

Lattice constants of this sample

a = 7.7084(5) Å
b = 9.9783(8) Å
c = 5.6649(5) Å

a/b = 0.7725
c/b = 0.5677

Volume

435.73 Å³

Density

(calculated) 4.137 g/cm³

Polymorphism

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

Figure of merit

$F_{30} = 111.6(0.008, 35)$

Additional patterns

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

Wanmaker and Spier (1962)

Majling, et al. (1979) calculated pattern

References

Klement, R. and Uffelman, R. (1941). *Naturwissenschaften* **29**, 300.

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

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

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

| CuK α_1 $\lambda = 1.540598$ Å; temp. 25±1 °C Internal standard Si, a = 5.430825 Å | | | | |
|--|--------------------------------------|-------|---------------------|--|
| d(Å) | I ^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^{\circ})$ | |
| 6.100 | 8 | 1 1 0 | 14.51 | |
| 4.990 | 18 | 0 2 0 | 17.76 | |
| 4.927 | 33 | 0 1 1 | 17.99 | |
| 4.189 | 4 | 1 2 0 | 21.19 | |
| 4.153 | 3 | 1 1 1 | 21.38 | |
| 3.854 | 6 | 2 0 0 | 23.06 | |
| 3.594 | 4 | 2 1 0 | 24.75 | |
| 3.368 | 40 | 1 2 1 | 26.44 | |
| 3.186 | 3 | 2 0 1 | 27.98 | |
| 3.052M | 94 | 1 3 0 | 29.24 | |
| 3.052M | | 2 2 0 | 29.24 | |
| 3.036 | 100 | 2 1 1 | 29.40 | |
| 2.868 | 41 | 0 3 1 | 31.16 | |
| 2.832 | 39 | 0 0 2 | 31.57 | |
| 2.685M | 4 | 1 3 1 | 33.34 | |
| 2.685M | | 2 2 1 | 33.34 | |
| 2.569 | 6 | 1 1 2 | 34.90 | |
| 2.518 | 4 | 2 3 0 | 35.63 | |
| 2.488 | 19 | 3 1 0 | 36.07 | |
| 2.463 | 2 | 0 2 2 | 36.45 | |
| 2.3732 | 2 | 1 4 0 | 37.88 | |
| 2.3464 | 3 | 1 2 2 | 38.33 | |
| 2.3008 | 5 | 2 3 1 | 39.12 | |
| 2.2823M | 14 | 3 2 0 | 39.45 | |
| 2.2823M | | 2 0 2 | 39.45 | |
| 2.2768 | 13 | 3 1 1 | 39.55 | |
| 2.2250 | 7 | 2 1 2 | 40.51 | |
| 2.1888 | 33 | 1 4 1 | 41.21 | |
| 2.1187 | 3 | 3 2 1 | 42.64 | |
| 2.0939 | 4 | 2 4 0 | 43.17 | |
| 2.0765M | 54 | 1 3 2 | 43.55 | |
| 2.0765M | | 2 2 2 | 43.55 | |
| 2.0335 | 15 | 3 3 0 | 44.52 | |
| 1.9646 | 1L | 2 4 1 | 46.17 | |
| 1.9318 | 14 | 1 5 0 | 47.00 | |
| 1.9271 | 14 | 4 0 0 | 47.12 | |
| 1.9134 | 1L | 3 3 1 | 47.48 | |
| 1.8817M | 4 | 0 5 1 | 48.33 | |
| 1.8817M | | 2 3 2 | 48.33 | |
| 1.8693 | 7 | 3 1 2 | 48.67 | |
| 1.8557 | 4 | 0 1 3 | 49.05 | |
| 1.8237 | 1L | 4 0 1 | 49.97 | |
| 1.7942 | 16 | 4 1 1 | 50.85 | |
| 1.7724 | 1L | 2 5 0 | 51.52 | |
| 1.7218 | 5 | 1 2 3 | 53.15 | |

Potassium Barium Phosphate, KBaPO_4 - (continued)

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

Potassium Calcium Phosphate, KCaPO_4

Synonym

Potassium calcium orthophosphate

CAS registry no.

18901-69-4

Sample

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

Color

Colorless

Structure

Hexagonal, $\text{P}\bar{3}\text{m1}$ (164), $Z = 2$. (Bredig, 1941)
Isostructural with apthitalite, $(\text{K},\text{Na})_3\text{Na}(\text{SO}_4)_2$
The structure of apthitalite was determined by Gossner (1928).

Lattice constants of this sample

$a = 5.5085(4)\text{Å}$
 $c = 7.5020(8)$

$c/a = 1.3619$

Volume

197.14 Å^3

Density

(calculated) 2.934 g/cm^3

Polymorphism

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

Figure of merit

$F_{27} = 38.1(0.011,65)$

Additional patterns

PDF card 3-619 (Bredig, 1942)

Wanmaker and Spier (1962)

References

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

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

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

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

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

| $\text{CuK}\alpha_1$ $\lambda = 1.540598\text{ Å}$; temp. $25\pm 1\text{ °C}$ Internal standard Si, $a = 5.430825\text{ Å}$ | | | |
|---|--------------------------------------|-------|---------------------|
| $d(\text{Å})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ |
| 4.024 | 8 | 1 0 1 | 22.07 |
| 3.750 | 12 | 0 0 2 | 23.71 |
| 2.949 | 100 | 1 0 2 | 30.28 |
| 2.754 | 100 | 1 1 0 | 32.49 |
| 2.386 | 2 | 2 0 0 | 37.67 |
| 2.272 | 17 | 2 0 1 | 39.64 |
| 2.0125 | 39 | 2 0 2 | 45.01 |
| 1.8762 | 6 | 0 0 4 | 48.48 |
| 1.8038 | 2 | 2 1 0 | 50.56 |
| 1.7450 | 3 | 1 0 4 | 52.39 |
| 1.7255 | 2 | 2 0 3 | 53.03 |
| 1.6251 | 14 | 2 1 2 | 56.59 |
| 1.5906 | 12 | 3 0 0 | 57.93 |
| 1.5497 | 12 | 1 1 4 | 59.61 |
| 1.4643 | 1L | 3 0 2 | 63.48 |
| 1.3770 | 9 | 2 2 0 | 68.03 |
| 1.2929 | 1 | 2 2 2 | 73.14 |
| 1.2478 | 4 | 3 1 2 | 76.24 |
| 1.2128 | 3 | 3 0 4 | 78.86 |
| 1.2097 | 2 | 1 0 6 | 79.10 |
| 1.1365 | 1 | 4 0 2 | 85.34 |
| 1.1101 | 1 | 2 2 4 | 87.88 |
| 1.1073 | 1 | 2 0 6 | 88.16 |
| 1.0507 | 1 | 3 2 2 | 94.30 |
| 1.0410 | 2 | 4 1 0 | 95.46 |
| 1.0275 | 1L | 2 1 6 | 97.13 |
| 1.0030 | 1L | 4 1 2 | 100.35 |

Potassium Strontium Phosphate, KSrPO_4

Synonym

Potassium strontium orthophosphate

CAS registry no.

53201-92-6

Sample

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

Color

Colorless

Structure

Orthorhombic, Pnam (62), $Z = 4$. Iso-structural with arcanite, $\beta\text{-K}_2\text{SO}_4$. (Klement and Kresse, 1961) The structure of arcanite was determined by Robinson, (1958). This phase of KSrPO_4 can also be indexed on a hexagonal cell with $a = 11.124$ and $c = 7.350$, this being similar to the high form of K_2SO_4 , but with a doubled a .

Lattice constants of this sample

$a = 7.3507(7) \text{ \AA}$
 $b = 9.6340(9)$
 $c = 5.5621(6)$

$a/b = 0.7630$
 $c/b = 0.5773$

Volume

393.89 \AA^3

Density

(calculated) 3.738 g/cm^3

Polymorphism

KSrPO_4 is reported to have several other forms (Klement and Uffelman, 1941).

Figure of merit

$F_{30} = 82.0(0.008, 45)$

Additional patterns

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

Wanmaker and Spier, 1962

References

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

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

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | | |
|---|------------------|-----|---|---|-------|
| Internal standard Si, a = 5.430825 Å | | | | | |
| d(Å) | I ^{rel} | hkℓ | | | 2θ(°) |
| σ = ±1 | | | | | |
| 5.836 | 5 | 1 | 1 | 0 | 15.17 |
| 4.813M | 19 | 0 | 2 | 0 | 18.42 |
| 4.813M | | 0 | 1 | 1 | 18.42 |
| 4.028M | 8 | 1 | 2 | 0 | 22.05 |
| 4.028M | | 1 | 1 | 1 | 22.05 |
| 3.433 | 2 | 2 | 1 | 0 | 25.93 |
| 3.263 | 27 | 1 | 2 | 1 | 27.31 |
| 3.066 | 5 | 2 | 0 | 1 | 29.10 |
| 2.943 | 32 | 1 | 3 | 0 | 30.35 |
| 2.922M | 100 | 2 | 2 | 0 | 30.57 |
| 2.922M | | 2 | 1 | 1 | 30.57 |
| 2.780M | 93 | 0 | 3 | 1 | 32.17 |
| 2.780M | | 0 | 0 | 2 | 32.17 |
| 2.587 | 3 | 2 | 2 | 1 | 34.65 |
| 2.512 | 4 | 1 | 1 | 2 | 35.72 |
| 2.418 | 8 | 2 | 3 | 0 | 37.15 |
| 2.4107M | 5 | 0 | 4 | 0 | 37.27 |
| 2.4107M | | 0 | 2 | 2 | 37.27 |
| 2.3744 | 19 | 3 | 1 | 0 | 37.86 |
| 2.2890M | 10 | 1 | 4 | 0 | 39.33 |
| 2.2890M | | 1 | 2 | 2 | 39.33 |
| 2.2177M | 10 | 2 | 3 | 1 | 40.65 |
| 2.2177M | | 2 | 0 | 2 | 40.65 |
| 2.1843M | 6 | 3 | 2 | 0 | 41.30 |
| 2.1843M | | 3 | 1 | 1 | 41.30 |
| 2.1613 | 7 | 2 | 1 | 2 | 41.76 |
| 2.1168 | 24 | 1 | 4 | 1 | 42.68 |
| 2.0330 | 6 | 3 | 2 | 1 | 44.53 |
| 2.0214 | 22 | 1 | 3 | 2 | 44.80 |
| 2.0150M | 36 | 2 | 4 | 0 | 44.95 |
| 2.0150M | | 2 | 2 | 2 | 44.95 |
| 1.9478 | 9 | 3 | 3 | 0 | 46.59 |
| 1.8942 | 1 | 2 | 4 | 1 | 47.99 |
| 1.8639 | 8 | 1 | 5 | 0 | 48.82 |
| 1.8378M | 6 | 3 | 3 | 1 | 49.56 |
| 1.8378M | | 4 | 0 | 0 | 49.56 |
| 1.8251 | 6 | 2 | 3 | 2 | 49.93 |
| 1.8203+ | 6 | 0 | 4 | 2 | 50.07 |
| 1.8203+ | | 0 | 1 | 3 | 50.07 |
| 1.8061M | 7 | 3 | 1 | 2 | 50.49 |
| 1.8061M | | 4 | 1 | 0 | 50.49 |
| 1.7447 | 1 | 4 | 0 | 1 | 52.40 |
| 1.7167+ | 11 | 4 | 2 | 0 | 53.32 |
| 1.7167+ | | 4 | 1 | 1 | 53.32 |
| 1.7064 | 1 | 2 | 5 | 0 | 53.67 |

Potassium Strontium Phosphate, KSrPO_4 - (continued)

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

Silver Telluride (Hessite), Ag₂Te

CAS registry no.
12002-98-1

Sample

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

Color

Unground: medium gray
Ground: dark gray

Structure

Monoclinic, P2₁/n (13), Z = 8. The space group was assumed from absences in the present powder data. The cell having "b" equal to half our value below would not allow an index for the very weak line at d = 8.91. This reflection appeared consistently in patterns from randomly oriented samples, but only appeared intermittently from non-randomly oriented mountings. Frueh (1959) gave the space group P2₁/n with b' = b/2.

Lattice constants of this sample

a = 8.1698(15) Å
b = 8.940(2)
c = 8.0653(15)
β = 112.793(15)°

a/b = 0.9138
c/b = 0.9022

Volume

543.07 Å³

Density

(calculated) 8.399 g/cm³

Polymorphism

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

Figure of merit

F₃₀ = 23.1(0.015,89)

Additional patterns

PDF card 12-695 (Thompson, 1949)

Frueh (1959)

Tokody (1932)

References

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

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.430825 Å | | | | |
|---|------------------|--------|-------|--|
| d(Å) | I ^{rel} | hkl | 2θ(°) | |
| σ = ±3 | | | | |
| 8.91 | 5 | 0 1 0 | 9.92 | |
| 6.76 | 10 | -1 0 1 | 13.08 | |
| 4.492 | 8 | 1 0 1 | 19.75 | |
| 3.764 | 5 | 2 0 0 | 23.62 | |
| 3.726 | 7 | -1 2 1 | 23.86 | |
| 3.382 | 8 | -2 0 2 | 26.33 | |
| 3.169 | 24 | 1 2 1 | 28.14 | |
| 3.003 | 52 | -2 2 1 | 29.73 | |
| 2.983M | 59 | -1 2 2 | 29.93 | |
| 2.983M | | 0 3 0 | 29.93 | |
| 2.880 | 100 | 2 2 0 | 31.03 | |
| 2.857 | 24 | 0 2 2 | 31.28 | |
| 2.695 | 10 | -2 2 2 | 33.21 | |
| 2.453 | 6 | 2 2 1 | 36.60 | |
| 2.444 | 6 | 1 2 2 | 36.75 | |
| 2.323M | 41 | 0 3 2 | 38.73 | |
| 2.323M | | -3 2 1 | 38.73 | |
| 2.301 | 96 | -1 2 3 | 39.12 | |
| 2.254 | 58 | -3 0 3 | 39.97 | |
| 2.246M | 61 | -3 2 2 | 40.11 | |
| 2.246M | | 2 0 2 | 40.11 | |
| 2.235+ | 30 | 0 4 0 | 40.33 | |
| 2.235+ | | -2 2 3 | 40.33 | |
| 2.189 | 30 | 3 2 0 | 41.21 | |
| 2.167 | 12 | 0 2 3 | 41.65 | |
| 2.141+ | 54 | 3 0 1 | 42.17 | |
| 2.141+ | | 0 4 1 | 42.17 | |
| 2.122M | 22 | 1 0 3 | 42.57 | |
| 2.122M | | -1 4 1 | 42.57 | |
| 2.026 | 15 | -4 0 2 | 44.70 | |
| 2.012 | 6 | -3 2 3 | 45.03 | |
| 2.002M | 4 | -2 0 4 | 45.25 | |
| 2.002M | | 1 4 1 | 45.25 | |
| 1.958M | 6 | -3 3 2 | 46.33 | |
| 1.958M | | -2 4 1 | 46.33 | |
| 1.953M | 5 | -2 1 4 | 46.45 | |
| 1.953M | | -1 4 2 | 46.45 | |
| 1.930 | 10 | 3 2 1 | 47.04 | |
| 1.884 | 1L | 4 0 0 | 48.27 | |
| 1.863 | 3 | -2 4 2 | 48.84 | |
| 1.858 | 5 | 0 0 4 | 48.98 | |
| 1.845 | 2 | -4 2 2 | 49.36 | |
| 1.821M | 4 | -1 2 4 | 50.06 | |
| 1.821M | | 0 1 4 | 50.06 | |
| 1.7737 | 11 | 1 4 2 | 51.48 | |
| 1.7355M | 2 | -3 2 4 | 52.70 | |
| 1.7355M | | 4 2 0 | 52.70 | |
| 1.6950 | 9 | -3 4 2 | 54.06 | |
| 1.6904 | 9 | -4 0 4 | 54.22 | |
| 1.6020 | 6 | -5 0 1 | 57.48 | |

Silver Telluride (Hessite), Ag₂Te - (continued)

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

Sodium Barium Phosphate, NaBaPO₄

Synonym

Sodium barium orthophosphate

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

CAS registry no.

53201-91-5

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

Sample

The sample was prepared at NBS. Na₂CO₃ and 2BaHPO₄ were ground together, heated up gradually to 800 °C, re-ground, returned to oven at 800 °C, heated to 1000 °C, and held there for 1 hour.

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

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

Color

Colorless

Optical data

Low double refraction with an average value ~1.612.

Structure

Hexagonal, P₃m1 (164), Z = 2, isostructural with apthitalite, (K,Na)₃Na(SO₄)₂. The structure was determined by Calvo and Faggiani (1975).

Lattice constants of this sample

a = 5.6181(3) Å
c = 7.2636(5)

c/a = 1.2929

Volume

198.55 Å³

Density

(calculated) 4.270 g/cm³

Polymorphism

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

Figure of merit

F₃₀ = 82.1(0.010,38)

Additional patterns

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

Majling et al. (1979) (calculated pattern)

Comment

A pattern given by Kolsi et al., (1981) is called monoclinic but can be indexed with the hexagonal cell here which has $\frac{1}{2}$ the volume of the monoclinic cell.

References

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

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

Klement, R. and Uffelman, R. (1941). *Naturwissenschaften* **29**, 300.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | | |
|---|------------------|-----|---|---|-------|
| Internal std. Fluorophlogopite SRM 675 | | | | | |
| d(Å) | I ^{rel} | hkl | | | 2θ(°) |
| σ = ±3 | | | | | |
| 7.27 | 4 | 0 | 0 | 1 | 12.17 |
| 4.868 | 3 | 1 | 0 | 0 | 18.21 |
| 4.044 | 59 | 1 | 0 | 1 | 21.96 |
| 3.632 | 1 | 0 | 0 | 2 | 24.49 |
| 2.910 | 100 | 1 | 0 | 2 | 30.70 |
| | | | | | |
| 2.808 | 100 | 1 | 1 | 0 | 31.84 |
| 2.620 | 8 | 1 | 1 | 1 | 34.20 |
| 2.423 | 22 | 0 | 0 | 3 | 37.08 |
| 2.307 | 32 | 2 | 0 | 1 | 39.01 |
| 2.222 | 7 | 1 | 1 | 2 | 40.57 |
| | | | | | |
| 2.1672 | 6 | 1 | 0 | 3 | 41.64 |
| 2.0210 | 50 | 2 | 0 | 2 | 44.81 |
| 1.8337 | 25 | 1 | 1 | 3 | 49.68 |
| 1.8155 | 3 | 0 | 0 | 4 | 50.21 |
| 1.7824 | 11 | 2 | 1 | 1 | 51.21 |
| | | | | | |
| 1.7008 | 13 | 1 | 0 | 4 | 53.86 |
| 1.6405 | 24 | 2 | 1 | 2 | 56.01 |
| 1.6219 | 14 | 3 | 0 | 0 | 56.71 |
| 1.5826 | 1 | 3 | 0 | 1 | 58.25 |
| 1.5247 | 3 | 1 | 1 | 4 | 60.69 |
| | | | | | |
| 1.4802 | 1 | 3 | 0 | 2 | 62.72 |
| 1.4641 | 2 | 2 | 1 | 3 | 63.49 |
| 1.4548 | 10 | 2 | 0 | 4 | 63.94 |
| 1.4045 | 12 | 2 | 2 | 0 | 66.52 |
| 1.3920 | 5 | 1 | 0 | 5 | 67.20 |
| | | | | | |
| 1.3472 | 6 | 3 | 0 | 3 | 69.75 |
| 1.3265 | 3 | 3 | 1 | 1 | 71.00 |
| 1.2920 | 10 | 2 | 1 | 4 | 73.20 |
| 1.2651 | 8 | 3 | 1 | 2 | 75.02 |
| 1.2474 | 3 | 2 | 0 | 5 | 76.27 |
| | | | | | |
| 1.2148 | 5 | 2 | 2 | 3 | 78.71 |
| 1.2095 | 2 | 3 | 0 | 4 | 79.12 |
| 1.1996 | 2 | 4 | 0 | 1 | 79.90 |
| 1.1786 | 1 | 3 | 1 | 3 | 81.62 |
| 1.1748 | 1 | 1 | 0 | 6 | 81.94 |

Sodium Barium Phosphate, NaBaPO₄ - (continued)

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

Sodium Strontium Phosphate, NaSrPO₄

Synonym

Sodium strontium orthophosphate

CAS registry no.

19553-80-1

Sample

The sample was made at NBS by heating a 2:2:1 molar mixture of (NH₄)₂HPO₄, SrCO₃, and Na₂CO₃ at 1000 °C for 2 days.

Color

Colorless

Structure

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

Lattice constants of this sample

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

a/b = 3.7602

c/b = 3.1766

Volume

1871.21 Å³

Density

(calculated) 2.919 g/cm³

Polymorphism

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

Figure of merit

F₃₀ = 43.4(0.011,63)M₂₀ = 20.6

Additional pattern

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

References

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

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

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

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.430825 Å | | | |
|---|----------------------------|--------|-------|
| d(Å) | I ^{rel} σ = ±5 | hkl | 2θ(°) |
| 9.98 | 2 | 2 0 0 | 8.85 |
| 8.43M | 10 | 0 0 2 | 10.48 |
| 8.43M | | -1 0 2 | 10.48 |
| 7.20 | 2 | -2 0 2 | 12.28 |
| 6.66 | 4 | 3 0 0 | 13.28 |
| 5.886 | 1L | 2 0 2 | 15.04 |
| 5.836 | 1 | -3 0 2 | 15.17 |
| 5.166 | 9 | 0 1 1 | 17.15 |
| 5.078 | 1 | -1 1 1 | 17.45 |
| 4.930 | 1 | 1 1 1 | 17.98 |
| 4.779 | 3 | 3 0 2 | 18.55 |
| 4.709 | 4 | -2 1 1 | 18.83 |
| 4.478 | 6 | 2 1 1 | 19.81 |
| 4.209M | 5 | -3 1 1 | 21.09 |
| 4.209M | | -2 0 4 | 21.09 |
| 3.996 | 3 | 5 0 0 | 22.23 |
| 3.961M | 7 | 3 1 1 | 22.43 |
| 3.961M | | 4 0 2 | 22.43 |
| 3.931 | 8 | -5 0 2 | 22.60 |
| 3.906 | 11 | 0 1 3 | 22.75 |
| 3.828 | 5 | -2 1 3 | 23.22 |
| 3.632 | 7 | 2 0 4 | 24.49 |
| 3.602M | 12 | -4 0 4 | 24.70 |
| 3.602M | | -3 1 3 | 24.70 |
| 3.484 | 10 | 4 1 1 | 25.55 |
| 3.356 | 6 | 5 0 2 | 26.54 |
| 3.330 | 9 | 6 0 0 | 26.75 |
| 3.180 | 4 | 3 1 3 | 28.04 |
| 2.922 | 30 | -6 0 4 | 30.57 |
| 2.903 | 44 | 6 0 2 | 30.78 |
| 2.886M | 55 | 4 1 3 | 30.96 |
| 2.886M | | -6 1 1 | 30.96 |
| 2.866M | 62 | 0 1 5 | 31.18 |
| 2.866M | | -2 0 6 | 31.18 |
| 2.805 | 2 | -3 0 6 | 31.88 |
| 2.772 | 11 | 1 1 5 | 32.27 |
| 2.732 | 100 | -6 1 3 | 32.75 |
| 2.715 | 48 | 0 2 0 | 32.97 |
| 2.646 | 1L | 5 0 4 | 33.85 |
| 2.615 | 7 | 5 1 3 | 34.26 |
| 2.585M | 5 | 0 2 2 | 34.67 |
| 2.585M | | -1 2 2 | 34.67 |
| 2.576 | 6 | 2 0 6 | 34.80 |
| 2.550 | 4 | -5 1 5 | 35.17 |
| 2.514 | 1 | 3 2 0 | 35.68 |

Sodium Strontium Phosphate, NaSrPO₄ - (continued)

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

Sodium Titanium Phosphate, $\text{NaTi}_2(\text{PO}_4)_3$

Synonyms

Sodium titanium orthophosphate
NTP

CAS registry no.
22239-24-3

Sample

The sample was made at NBS by heating a 1:2:2 molar mixture of $\text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O}$, $(\text{NH}_4)_2\text{HPO}_4$, and TiO_2 (anatase) at 1000 °C. It was then re-ground and heated at 1200° C for 18 hours.

Color

Colorless

Structure

Rhombohedral, $R\bar{3}c$ (167). Isostructural with $\text{NaZr}_2(\text{PO}_4)_3$ and other similar phosphates. The structure of $\text{NaZr}_2(\text{PO}_4)_3$ was determined by Hagman and Kierkegaard (1968).

Lattice constants of this sample

Hexagonal axes

$a = 8.4912(3)\text{Å}$
 $c = 21.7858(12)$

$c/a = 2.5657$
 $Z = 6$

Volume

1360.35 Å^3

Density

(calculated) 2.957 g/cm^3

Polymorphism

Götz and Niebergall (1969) report a cubic form of $\text{NaTi}_2(\text{PO}_4)_3$ in the ternary system $\text{NaPO}_3\text{-NaF-TiO}_2$.

Figure of merit

$F_{30} = 112.7(0.007,36)$

Additional patterns

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

Chernorukov (1978)

References

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

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

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

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | | |
|---|------------------|-----|---|----|-------|
| Internal standard Si, a = 5.430825 Å | | | | | |
| d(Å) | I ^{rel} | hkl | | | 2θ(°) |
| σ = ±2 | | | | | |
| 6.095 | 14 | 0 | 1 | 2 | 14.52 |
| 4.377 | 20 | 1 | 0 | 4 | 20.27 |
| 4.245 | 32 | 1 | 1 | 0 | 20.91 |
| 3.666 | 100 | 1 | 1 | 3 | 24.26 |
| 3.632 | 10 | 0 | 0 | 6 | 24.49 |
| 3.485 | 4 | 2 | 0 | 2 | 25.54 |
| 3.048 | 28 | 0 | 2 | 4 | 29.28 |
| 2.759M | 64 | 1 | 1 | 6 | 32.42 |
| 2.759M | | 2 | 1 | 1 | 32.42 |
| 2.694 | 2 | 1 | 2 | 2 | 33.23 |
| 2.5532 | 1 | 0 | 1 | 8 | 35.12 |
| 2.4761 | 2 | 2 | 1 | 4 | 36.25 |
| 2.4520 | 16 | 3 | 0 | 0 | 36.62 |
| 2.1883 | 2 | 2 | 0 | 8 | 41.22 |
| 2.1032 | 7 | 1 | 1 | 9 | 42.97 |
| 2.0733 | 2 | 2 | 1 | 7 | 43.62 |
| 2.0378 | 5 | 2 | 2 | 3 | 44.42 |
| 2.0322M | 6 | 3 | 0 | 6 | 44.55 |
| 2.0322M | | 1 | 3 | 1 | 44.55 |
| 2.0053 | 1 | 3 | 1 | 2 | 45.18 |
| 1.9455 | 15 | 1 | 2 | 8 | 46.65 |
| 1.9100 | 3 | 1 | 3 | 4 | 47.57 |
| 1.8740 | 2 | 0 | 2 | 10 | 48.54 |
| 1.8473 | 2 | 3 | 1 | 5 | 49.29 |
| 1.8330 | 16 | 2 | 2 | 6 | 49.70 |
| 1.8152 | 5 | 0 | 0 | 12 | 50.22 |
| 1.8128 | 6 | 0 | 4 | 2 | 50.29 |
| 1.7419 | 1L | 4 | 0 | 4 | 52.49 |
| 1.7144 | 9 | 2 | 1 | 10 | 53.40 |
| 1.7058 | 7 | 1 | 3 | 7 | 53.69 |
| 1.6821 | 1L | 3 | 2 | 1 | 54.51 |
| 1.6674 | 1 | 2 | 3 | 2 | 55.03 |
| 1.6328 | 6 | 3 | 1 | 8 | 56.30 |
| 1.6115 | 5 | 3 | 2 | 4 | 57.11 |
| 1.6048 | 11 | 4 | 1 | 0 | 57.37 |
| 1.5959 | 2 | 2 | 2 | 9 | 57.72 |
| 1.5733 | 2 | 2 | 3 | 5 | 58.63 |
| 1.5670 | 4 | 4 | 1 | 3 | 58.89 |
| 1.5236 | 5 | 0 | 4 | 8 | 60.74 |
| 1.4889 | 6 | 1 | 3 | 10 | 62.31 |
| 1.4678 | 6 | 4 | 1 | 6 | 63.31 |
| 1.4589 | 2 | 3 | 0 | 12 | 63.74 |
| 1.4331 | 5 | 2 | 0 | 14 | 65.03 |
| 1.4199 | 4 | 0 | 5 | 4 | 65.71 |
| 1.4153 | 3 | 3 | 3 | 0 | 65.95 |
| 1.4051 | 2 | 4 | 0 | 10 | 66.49 |
| 1.3890 | 1L | 3 | 3 | 3 | 67.36 |
| 1.3798 | 1 | 2 | 2 | 12 | 67.87 |
| 1.3741 | 3 | 1 | 1 | 15 | 68.19 |
| 1.3583 | 3 | 1 | 2 | 14 | 69.10 |

Sodium Titanium Phosphate, $\text{NaTi}_2(\text{PO}_4)_3$ - (continued)

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

Sodium Zirconium Phosphate, $\text{NaZr}_2(\text{PO}_4)_3$

Synonyms

Sodium zirconium orthophosphate
NZP

CAS registry no.

19527-81-2

Sample

The sample was made at NBS by heating a 1:2:2 molar mixture of $\text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O}$, $(\text{NH}_4)_2\text{HPO}_4$, and ZrO_2 , slowly up to 1000 °C. It was then re-ground and heated to 1200 °C overnight.

Color

Colorless

Structure

Rhombohedral, $R\bar{3}c(167)$. Isostructural with $\text{NaTi}_2(\text{PO}_4)_3$ and many other similar phosphates. The structure has been determined by Hagman and Kierkegaard, (1968) and confirmed by Hong (1976).

Lattice constants of this sample

Hexagonal axes

$a = 8.8048(4)\text{Å}$
 $c = 22.7572(14)\text{Å}$

 $c/a = 2.5846$ $Z = 6$

Volume

 1527.88 Å^3

Density

(calculated) 3.198 g/cm³

Figure of merit

 $F_{30} = 103.6(0.007,43)$

Additional patterns

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

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

Majling, et al. (1979) calculated pattern

References

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

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

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

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

| CuK α_1 $\lambda = 1.540598\text{ Å}$; temp. $25 \pm 1\text{ °C}$ Internal standard Si, $a = 5.430825\text{ Å}$ | | | |
|--|--------------------------------------|--------|---------------------|
| $d(\text{Å})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ |
| 6.325 | 22 | 0 1 2 | 13.99 |
| 4.556 | 75 | 1 0 4 | 19.47 |
| 4.399 | 97 | 1 1 0 | 20.17 |
| 3.807 | 100 | 1 1 3 | 23.35 |
| 3.614 | 1 | 2 0 2 | 24.61 |
| 3.166 | 54 | 0 2 4 | 28.16 |
| 2.873 | 94 | 1 1 6 | 31.10 |
| 2.666 | 3 | 0 1 8 | 33.59 |
| 2.571 | 24 | 2 1 4 | 34.87 |
| 2.5419 | 42 | 3 0 0 | 35.28 |
| 2.2801 | 7 | 2 0 8 | 39.49 |
| 2.2016 | 6 | 2 2 0 | 40.96 |
| 2.1929 | 3 | 1 1 9 | 41.13 |
| 2.1802 | 3 | 1 0 10 | 41.38 |
| 2.1568 | 2 | 2 1 7 | 41.85 |
| 2.1116 | 10 | 3 0 6 | 42.79 |
| 2.0797 | 3 | 3 1 2 | 43.48 |
| 2.0248 | 21 | 1 2 8 | 44.72 |
| 1.9824 | 12 | 1 3 4 | 45.73 |
| 1.9542 | 6 | 0 2 10 | 46.43 |
| 1.9039 | 29 | 2 2 6 | 47.73 |
| 1.8802 | 5 | 0 4 2 | 48.37 |
| 1.8078 | 1 | 4 0 4 | 50.44 |
| 1.7860 | 22 | 2 1 10 | 51.10 |
| 1.7727 | 4 | 1 3 7 | 51.51 |
| 1.6967 | 9 | 3 1 8 | 54.00 |
| 1.6719 | 14 | 3 2 4 | 54.87 |
| 1.6638 | 25 | 4 1 0 | 55.16 |
| 1.6328 | 1 | 2 3 5 | 56.30 |
| 1.6251 | 2 | 4 1 3 | 56.59 |
| 1.5894 | 5 | 0 1 14 | 57.98 |
| 1.5834 | 4 | 0 4 8 | 58.22 |
| 1.5490 | 12 | 1 3 10 | 59.64 |
| 1.5401 | 1 | 3 2 7 | 60.02 |
| 1.5236 | 14 | 4 1 6 | 60.74 |
| 1.5197 | 1 | 3 0 12 | 60.91 |
| 1.4950 | 7 | 2 0 14 | 62.03 |
| 1.4787 | 4 | 3 1 11 | 62.79 |
| 1.4730 | 6 | 0 5 4 | 63.06 |
| 1.4676 | 7 | 3 3 0 | 63.32 |
| 1.4610 | 4 | 4 0 10 | 63.64 |
| 1.4406 | 1 | 3 3 3 | 64.65 |
| 1.4340 | 3 | 1 1 15 | 64.98 |
| 1.4157 | 9 | 1 2 14 | 65.93 |
| 1.3969 | 5 | 2 4 4 | 66.93 |

Sodium Zirconium Phosphate, $\text{NaZr}_2(\text{PO}_4)_3$ - (continued)

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

Yttrium Chromium Oxide, YCrO₃

Synonym

Yttrium orthochromite

Sample

The sample was prepared at NBS by T. Negas.

Color

Medium yellowish green

Structure

Orthorhombic, Pnma (62), Z = 4, isostructural with GdFeO₃ (Geller and Wood, 1956). The structure of GdFeO₃ was determined by Geller (1956).

Lattice constants of this sample

 $a = 5.5237(3) \text{ \AA}$
 $b = 7.5343(5)$
 $c = 5.2427(3)$
 $a/b = 0.7331$
 $c/b = 0.6958$

Volume

 218.19 \AA^3

Density

(calculated) 5.751 g/cm³

Figure of merit

 $F_{30} = 116.2(0.008, 31)$

Additional patterns

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

Geller and Wood (1956)

Keith and Roy (1954)

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

References

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

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

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

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

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

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Ag, $a = 4.08651 \text{ \AA}$ | | | | |
|--|--------------------------------------|-------|-------------------|--|
| d(\AA) | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^\circ)$ | |
| 4.306 | 2 | 0 1 1 | 20.61 | |
| 3.805 | 5 | 1 0 1 | 23.36 | |
| 3.770 | 5 | 0 2 0 | 23.58 | |
| 3.396 | 22 | 1 1 1 | 26.22 | |
| 2.762 | 22 | 2 0 0 | 32.39 | |
| 2.676 | 100 | 1 2 1 | 33.46 | |
| 2.621 | 27 | 0 0 2 | 34.18 | |
| 2.593 | 11 | 2 1 0 | 34.56 | |
| 2.443 | 1L | 2 0 1 | 36.76 | |
| 2.3678 | 2 | 1 0 2 | 37.97 | |
| 2.3248 | 1 | 2 1 1 | 38.70 | |
| 2.2647 | 5 | 0 3 1 | 39.77 | |
| 2.2592 | 9 | 1 1 2 | 39.87 | |
| 2.2276 | 6 | 2 2 0 | 40.46 | |
| 2.1509 | 9 | 0 2 2 | 41.97 | |
| 2.0967 | 11 | 1 3 1 | 43.11 | |
| 2.0497 | 3 | 2 2 1 | 44.15 | |
| 2.0049 | 2 | 1 2 2 | 45.19 | |
| 1.9013 | 24 | 2 0 2 | 47.80 | |
| 1.8831 | 18 | 0 4 0 | 48.29 | |
| 1.8582 | 8 | 2 3 0 | 48.98 | |
| 1.8434 | 13 | 2 1 2 | 49.40 | |
| 1.7516 | 1L | 2 3 1 | 52.18 | |
| 1.7376 | 2 | 3 0 1 | 52.63 | |
| 1.7230 | 2 | 1 3 2 | 53.11 | |
| 1.7020 | 1 | 0 1 3 | 53.82 | |
| 1.6933 | 20 | 3 1 1 | 54.12 | |
| 1.6878 | 1 | 1 4 1 | 54.31 | |
| 1.6665 | 1L | 1 0 3 | 55.06 | |
| 1.6264 | 3 | 1 1 3 | 56.54 | |
| 1.5772 | 9 | 3 2 1 | 58.47 | |
| 1.5564 | 11 | 2 4 0 | 59.33 | |
| 1.5291 | 17 | 0 4 2 | 60.50 | |
| 1.5238 | 27 | 1 2 3 | 60.73 | |
| 1.5157 | 6 | 2 3 2 | 61.09 | |
| 1.5066 | 1L | 3 0 2 | 61.50 | |
| 1.4764 | 1 | 2 0 3 | 62.90 | |
| 1.4482 | 1L | 0 5 1 | 64.27 | |
| 1.4344 | 1L | 0 3 3 | 64.96 | |
| 1.4286 | 8 | 3 3 1 | 65.26 | |
| 1.4008 | 1 | 1 5 1 | 66.72 | |
| 1.3883 | 1L | 1 3 3 | 67.40 | |
| 1.3809 | 1L | 4 0 0 | 67.81 | |
| 1.3752 | 1L | 2 2 3 | 68.13 | |
| 1.3583 | 3 | 4 1 0 | 69.10 | |

Yttrium Chromium Oxide, YCrO₃ - (continued)

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

Zinc Arsenate Hydrate (Koettigite), $\text{Zn}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$

Synonyms

Zinc arsenate octahydrate
Zinc orthoarsenate octahydrate

Sample

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

Spectrographic analysis

Major impurities

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

Color

Colorless

Structure

Monoclinic, $I2/m$ (12), $Z = 2$. Vivianite structure (Wolfe, 1940). The structure of vivianite ($\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$) was discussed by Mori and Ito (1950).

Lattice constants of this sample

$a = 10.118(2)\text{\AA}$
 $b = 13.431(2)$
 $c = 4.7615(12)$
 $\beta = 101.81(2)^\circ$

$a/b = 0.7533$

$c/b = 0.3545$

Volume

633.37 \AA^3

Density

(calculated) 3.241 g/cm^3

Comment

Note the similarity between the data above and the data for the phase $\text{Co}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$ also appearing in this Monograph.

Figure of merit

$F_{30} = 67.1(0.010, 44)$

Additional pattern

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

References

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

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

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

| CuK α_1 $\lambda = 1.540598\text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$ | | | |
|---|------------------|--------|---------------------|
| Internal standard Si, $a = 5.43088\text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
| $\sigma = \pm 2$ | | | |
| 7.97 | 24 | 1 1 0 | 11.09 |
| 6.72 | 100 | 0 2 0 | 13.17 |
| 4.951 | 10 | 2 0 0 | 17.90 |
| 4.595 | 5 | -1 0 1 | 19.30 |
| 4.403 | 14 | 0 1 1 | 20.15 |

Zinc Sulfate Hydrate (Gunningite), $\text{ZnSO}_4 \cdot \text{H}_2\text{O}$

Synonym

Zinc sulfate monohydrate

CAS registry no.

7446-19-7

Sample

The sample was made by allowing $\text{ZnSO}_4 \cdot 6\text{H}_2\text{O}$ to stay in dry air for several days.

Color

Colorless

Structure

Monoclinic, $A2/a$ (15), $Z = 4$. Isostructural with kieserite ($\text{MgSO}_4 \cdot \text{H}_2\text{O}$), (Pistorius, 1961).

The structure of kieserite was determined by Leonhardt and Weiss (1957).

Lattice constants of this sample

$a = 7.5079(6) \text{ \AA}$

$b = 7.5871(6)$

$c = 6.9355(6)$

$\beta = 116.248(7)^\circ$

Volume

354.3 \AA^3

Density

(calculated) 3.364 g/cm^3

Figure of merit

$F_{30} = 122.5(0.006, 38)$

Additional pattern

PDF card 12-781 (Pistorius)

References

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

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

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ } ^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | | | |
|---|------------------|-------|---|---|---------------------|
| $d(\text{\AA})$ | I^{rel} | hkl | | | $2\theta(^{\circ})$ |
| $\sigma = \pm 1$ | | | | | |
| 4.810 | 39 | 0 | 1 | 1 | 18.43 |
| 4.759 | 39 | -1 | 1 | 1 | 18.63 |
| 3.794 | 11 | 0 | 2 | 0 | 23.43 |
| 3.404 | 100 | 1 | 1 | 1 | 26.16 |
| 3.348 | 23 | -2 | 1 | 1 | 26.60 |
| 3.307 | 28 | 1 | 2 | 0 | 26.94 |
| 3.056 | 47 | -2 | 0 | 2 | 29.20 |
| 2.5595 | 16 | -1 | 2 | 2 | 35.03 |
| 2.5185 | 46 | 2 | 2 | 0 | 35.62 |
| 2.4051 | 3 | 0 | 2 | 2 | 37.36 |

| $d(\text{\AA})$ | I^{rel} | hkl | | | $2\theta(^{\circ})$ |
|------------------|------------------|-------|---|---|---------------------|
| $\sigma = \pm 1$ | | | | | |
| 2.3989 | 3 | 2 | 1 | 1 | 37.46 |
| 2.3805 | 5 | -2 | 2 | 2 | 37.76 |
| 2.3678 | 6 | -3 | 1 | 1 | 37.97 |
| 2.3370 | 13 | -1 | 3 | 1 | 38.49 |
| 2.1888 | 18 | -1 | 1 | 3 | 41.21 |
| | | | | | |
| 2.1064 | 9 | 1 | 3 | 1 | 42.90 |
| 2.0934 | 4 | -2 | 3 | 1 | 43.18 |
| 2.0536 | 10 | 1 | 2 | 2 | 44.06 |
| 2.0223 | 2 | -3 | 2 | 2 | 44.78 |
| 1.9674 | 14 | -3 | 1 | 3 | 46.10 |
| | | | | | |
| 1.9318 | 2 | 3 | 2 | 0 | 47.00 |
| 1.9036 | 7 | 2 | 0 | 2 | 47.74 |
| 1.8979 | 5 | 0 | 4 | 0 | 47.89 |
| 1.8105 | 9 | 3 | 1 | 1 | 50.36 |
| 1.7912 | 1 | -4 | 1 | 1 | 50.94 |
| | | | | | |
| 1.7886 | 1 | 2 | 3 | 1 | 51.02 |
| 1.7753 | 1 | -3 | 3 | 1 | 51.43 |
| 1.7330 | 3 | -2 | 0 | 4 | 52.78 |
| 1.7011 | 7 | 2 | 2 | 2 | 53.85 |
| 1.6964 | 5 | -1 | 3 | 3 | 54.01 |
| | | | | | |
| 1.6909 | 1L | -4 | 1 | 3 | 54.20 |
| 1.6835 | 4 | 4 | 0 | 0 | 54.46 |
| 1.6738 | 15 | -4 | 2 | 2 | 54.80 |
| 1.6522 | 8 | 2 | 4 | 0 | 55.58 |
| 1.6193 | 10 | 0 | 4 | 2 | 56.81 |
| | | | | | |
| 1.6035 | 1 | 0 | 3 | 3 | 57.42 |
| 1.5861 | 9 | -3 | 3 | 3 | 58.11 |
| 1.5765 | 4 | -2 | 2 | 4 | 58.50 |
| 1.5557 | 6 | 0 | 0 | 4 | 59.36 |
| 1.5420 | 3 | -1 | 2 | 4 | 59.94 |
| | | | | | |
| 1.5383 | 1 | 4 | 2 | 0 | 60.10 |
| 1.5279M | 3 | -3 | 2 | 4 | 60.55 |
| 1.5279M | | -4 | 0 | 4 | 60.55 |
| 1.5006 | 7 | 3 | 3 | 1 | 61.77 |
| 1.4857 | 1L | -3 | 4 | 2 | 62.46 |
| | | | | | |
| 1.4726 | 1 | -1 | 5 | 1 | 63.08 |
| 1.4518 | 3 | 1 | 3 | 3 | 64.09 |
| 1.4486 | 2 | 3 | 4 | 0 | 64.25 |
| 1.4390 | 3 | 0 | 2 | 4 | 64.73 |
| 1.4364 | 4 | -5 | 1 | 3 | 64.86 |
| | | | | | |
| 1.4301 | 1 | -5 | 1 | 1 | 65.18 |
| 1.4172M | 3 | -4 | 2 | 4 | 65.85 |
| 1.4172M | | 3 | 2 | 2 | 65.85 |
| 1.4094 | 3 | 1 | 5 | 1 | 66.26 |
| 1.3962 | 1 | -5 | 2 | 2 | 66.97 |
| | | | | | |
| 1.3541 | 1 | -3 | 1 | 5 | 69.34 |
| 1.3302 | 2 | -4 | 4 | 2 | 70.77 |
| 1.3024 | 1 | 1 | 2 | 4 | 72.52 |
| 1.2795 | 5 | -2 | 4 | 4 | 74.03 |
| 1.2693 | 2 | 5 | 2 | 0 | 74.73 |

Zinc Sulfate Hydrate (Gunningite), $\text{ZnSO}_4 \cdot \text{H}_2\text{O}$ - (continued)

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

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

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

Synonyms

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

CAS registry no.
24486-13-3

Structure

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

Atom positions

All atoms were in general positions 8(c).

Lattice constants

$a = 7.157 \text{ \AA}$
 $b = 30.881$
 $c = 10.871$

(published values: 7.157 \AA , 30.879 , 10.870 for $CuK\alpha = 1.54178$; Williams, 1973)

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

Volume
 2402.7 \AA^3

Density

(calculated) 1.384 g/cm^3

Thermal parameters

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

Scattering factors

Zero ionization (International Tables, 1962)

Scale factors

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

Comment

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

Additional patterns

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

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

References

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

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

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

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

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

| Calculated Pattern (Peak heights) | | | |
|-----------------------------------|------------------|--------|---------------------|
| $\lambda = 1.540598 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
| 15.44 | 100 | 0 2 0 | 5.72 |
| 8.87 | 1 | 0 2 1 | 9.96 |
| 7.72 | 30 | 0 4 0 | 11.46 |
| 5.863 | 90 | 1 1 1 | 15.10 |
| 5.569 | 7 | 1 2 1 | 15.90 |
| 5.434 | 45 | 0 0 2 | 16.30 |
| 5.163 | 12 | 1 3 1 | 17.16 |
| 4.726 | 9 | 1 4 1 | 18.76 |
| 4.653 | 2 | 0 6 1 | 19.06 |
| 4.283 | 2 | 1 1 2 | 20.72 |
| 3.897 | 80 | 1 6 1 | 22.80 |
| 3.773 | 2 | 1 4 2 | 23.56 |
| 3.736 | 3 | 0 6 2 | 23.80 |
| 3.548 | 15 | 1 7 1 | 25.08 |
| 3.485 | 8 | 2 2 0 | 25.54 |
| 3.378 | 6 | 2 3 0 | 26.36 |
| 3.312 | 1 | 1 6 2 | 26.90 |
| 3.243+ | 1 | 1 8 1 | 27.48 |
| 3.164 | 1 | 1 2 3 | 28.18 |
| 3.085+ | 13 | 1 3 3 | 28.92 |
| 2.976+ | 22 | 1 9 1 | 30.00 |
| 2.938 | 2 | 2 6 0 | 30.40 |
| 2.864+ | 12 | 1 5 3 | 31.20 |
| 2.779+ | 27 | 2 7 0 | 32.18 |
| 2.743+ | 2 | 1 10 1 | 32.62 |
| 2.685 | 5 | 0 10 2 | 33.34 |
| 2.624 | 4 | 2 8 0 | 34.14 |
| 2.608 | 7 | 1 7 3 | 34.36 |
| 2.585 | 6 | 2 6 2 | 34.68 |
| 2.477+ | 2 | 2 9 0 | 36.24 |
| 2.3624 | 1 | 2 8 2 | 38.06 |
| 2.3376 | 2 | 2 10 0 | 38.48 |
| 2.3248+ | 2 | 0 12 2 | 38.70 |
| 2.2224 | 5 | 0 8 4 | 40.56 |
| 2.2088 | 2 | 2 11 0 | 40.82 |

+ More than one hkl possible

Phenobarbital Hydrate, $C_{12}H_{12}N_2O_3 \cdot H_2O$ - (continued)

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

| Calculated Pattern (Integrated) | | | |
|---------------------------------|------------------|-------|---------------------|
| $\lambda=1.540598\text{\AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
| 15.44 | 100 | 0 2 0 | 5.72 |
| 8.891 | 1 | 0 2 1 | 9.94 |
| 7.722 | 31 | 0 4 0 | 11.45 |
| 5.870 | 97 | 1 1 1 | 15.08 |
| 5.573 | 5 | 1 2 1 | 15.89 |
| 5.437 | 48 | 0 0 2 | 16.29 |
| 5.169 | 11 | 1 3 1 | 17.14 |
| 5.148 | 3 | 0 6 0 | 17.21 |
| 5.128 | 2 | 0 2 2 | 17.28 |
| 4.7263 | 10 | 1 4 1 | 18.76 |
| 4.6526 | 1 | 0 6 1 | 19.06 |
| 4.2875 | 2 | 1 1 2 | 20.70 |
| 3.9904 | 1 | 1 3 2 | 22.26 |
| 3.9005 | 93 | 1 6 1 | 22.78 |
| 3.7763 | 1 | 1 4 2 | 23.54 |
| 3.7372 | 3 | 0 6 2 | 23.79 |
| 3.5787 | 2 | 2 0 0 | 24.86 |
| 3.5492 | 17 | 1 7 1 | 25.07 |
| 3.4863 | 9 | 2 2 0 | 25.53 |
| 3.3796 | 8 | 2 3 0 | 26.35 |

| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
|-----------------|------------------|--------|---------------------|
| 3.3129 | 1 | 1 6 2 | 26.89 |
| 3.2431 | 1 | 1 8 1 | 27.48 |
| 3.1641 | 1 | 1 2 3 | 28.18 |
| 3.1112 | 1 | 2 4 1 | 28.67 |
| 3.0880 | 6 | 0 10 0 | 28.89 |
| 3.0849 | 10 | 1 3 3 | 28.92 |
| 2.9820 | 8 | 1 4 3 | 29.94 |
| 2.9762 | 19 | 1 9 1 | 30.00 |
| 2.9752 | 2 | 2 1 2 | 30.01 |
| 2.9379 | 2 | 2 6 0 | 30.40 |
| 2.8707 | 4 | 2 3 2 | 31.13 |
| 2.8644 | 12 | 1 5 3 | 31.20 |
| 2.7870 | 23 | 2 4 2 | 32.09 |
| 2.7794 | 19 | 2 7 0 | 32.18 |
| 2.7437 | 2 | 1 10 1 | 32.61 |
| 2.7380 | 1 | 1 6 3 | 32.68 |
| 2.6853 | 6 | 0 10 2 | 33.34 |
| 2.6242 | 4 | 2 8 0 | 34.14 |
| 2.6079 | 8 | 1 7 3 | 34.36 |
| 2.5845 | 7 | 2 6 2 | 34.68 |
| 2.4788 | 1 | 1 8 3 | 36.21 |
| 2.4768 | 2 | 2 9 0 | 36.24 |
| 2.3630 | 2 | 2 8 2 | 38.05 |
| 2.3382 | 2 | 2 10 0 | 38.47 |
| 2.3260 | 1 | 0 12 2 | 38.68 |
| 2.3237 | 1 | 3 1 1 | 38.72 |
| 2.2224 | 7 | 0 8 4 | 40.56 |
| 2.2088 | 1 | 2 11 0 | 40.82 |
| 2.1642 | 3 | 2 0 4 | 41.70 |
| 2.1431 | 2 | 2 2 4 | 42.13 |
| 2.0893 | 2 | 2 12 0 | 43.27 |
| 2.0756 | 2 | 1 1 5 | 43.57 |
| 2.0616 | 2 | 1 2 5 | 43.88 |
| 2.0133 | 2 | 1 12 3 | 44.99 |
| 1.9948 | 1 | 3 8 1 | 45.43 |
| 1.9792 | 2 | 2 13 0 | 45.81 |
| 1.9287 | 1 | 1 6 5 | 47.08 |
| 1.9275 | 7 | 3 9 1 | 47.11 |
| 1.8600 | 1 | 3 10 1 | 48.93 |
| 1.8220 | 2 | 1 14 3 | 50.02 |
| 1.7929 | 1 | 3 11 1 | 50.89 |
| 1.7747 | 1 | 2 14 2 | 51.45 |
| 1.7629 | 1 | 4 3 0 | 51.82 |
| 1.7156 | 1 | 0 18 0 | 53.36 |
| 1.6988 | 1 | 2 16 0 | 53.93 |
| 1.6402 | 1 | 0 8 6 | 56.02 |
| 1.6048 | 2 | 3 1 5 | 57.37 |

INORGANIC NAMES

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| | | |
|--|-----|-----|
| Aluminum, Al | 1 | 11 |
| Aluminum antimony, AlSb | 4 | 72 |
| Aluminum bismuth oxide, Al ₄ Bi ₂ O ₉ | 11m | 5 |
| Aluminum borate, Al ₁₈ B ₄ O ₃₃ | 17m | 5 |
| Aluminum chloride, AlCl ₃ | 9m | 61 |
| Aluminum chloride hydrate (chloraluminite), AlCl ₃ ·6H ₂ O | 7 | 3 |
| Aluminum copper, Al ₄ Cu ₉ | 11m | 79 |
| Aluminum fluoride hydroxide silicate, topaz, Al ₂ (F,OH) ₂ SiO ₄ | 1m | 4 |
| Aluminum iron, AlFe | 18m | 5 |
| Aluminum iron antimony oxide, bahianite, Al _{5.66} Fe _{0.09} Sb _{2.95} O ₁₆ | 16m | 87 |
| Aluminum iron oxide, AlFeO ₃ | 15m | 7 |
| Aluminum lithium, Al ₄ Li ₉ | 10m | 98 |
| Aluminum nickel, AlNi | 6m | 82 |
| Aluminum nitride, AlN | 12m | 5 |
| Aluminum nitrate hydrate, Al(NO ₃) ₃ ·9H ₂ O | 11m | 6 |
| Aluminum oxide (corundum), α-Al ₂ O ₃ .. | 9 | 3 |
| Aluminum oxide hydrate (boehmite), α-Al ₂ O ₃ ·H ₂ O | 3 | 38 |
| Aluminum oxide hydrate, diaspore, β-Al ₂ O ₃ ·H ₂ O | 3 | 41 |
| Aluminum phosphate, Al(PO ₃) ₃ | 2m | 3 |
| Aluminum phosphate (berlinite), AlPO ₄ (trigonal) | 10 | 3 |
| Aluminum phosphate, AlPO ₄ (orthorhombic) | 10 | 4 |
| Aluminum plutonium, Al ₃ Pu | 15m | 77 |
| Aluminum rhenium, AlRe | 15m | 79 |
| Aluminum rhenium, Al ₁₂ Re | 15m | 80 |
| Aluminum rhodium, AlRh | 15m | 82 |
| Aluminum ruthenium, AlRu | 15m | 83 |
| Aluminum ruthenium, Al ₆ Ru | 15m | 84 |
| Aluminum samarium, AlSm ₂ | 15m | 86 |
| Aluminum samarium, AlSm ₃ | 15m | 88 |
| Aluminum samarium, Al ₂ Sm | 15m | 90 |
| Aluminum samarium, Al ₃ Sm | 15m | 91 |
| Aluminum silicate (mullite), Al ₆ Si ₂ O ₁₃ | 3m | 3 |
| Aluminum sulfate, Al ₂ (SO ₄) ₃ | 15m | 8 |
| Aluminum technetium, Al ₆ Tc | 15m | 93 |
| Aluminum terbium, Al ₂ Tb | 15m | 95 |
| Aluminum terbium, Al ₂ Tb ₃ | 15m | 96 |
| Aluminum thorium uranium, Al ₆ ThU | 15m | 98 |
| Aluminum tungsten, Al ₅ W, δ-phase | 15m | 100 |
| Aluminum tungsten oxide, Al ₂ (WO ₄) ₃ .. | 11m | 7 |
| Aluminum vanadium, Al ₁₀ V | 15m | 102 |
| Aluminum vanadium, Al _{10.25} V | 15m | 104 |
| Aluminum vanadium, Al ₂₃ V ₄ | 15m | 106 |
| Aluminum vanadium, Al ₄₅ V ₇ , α'-phase . | 15m | 108 |
| Aluminum ytterbium, Al ₂ Yb | 15m | 111 |
| Aluminum yttrium, Al ₃ Y | 15m | 112 |
| Aluminum yttrium oxide, AlYO ₃ | 19m | 7 |
| Aluminum yttrium oxide, Al ₂ Y ₄ O ₉ | 19m | 9 |
| Aluminum yttrium oxide, Al ₅ Y ₃ O ₁₂ ... | 19m | 11 |

| | | |
|---|-----|----|
| Ammonium aluminum fluoride, (NH ₄) ₃ AlF ₆ | 9m | 5 |
| Ammonium aluminum selenate hydrate, NH ₄ Al(SeO ₄) ₂ ·12H ₂ O | 9m | 6 |
| Ammonium aluminum sulfate, NH ₄ Al(SO ₄) ₂ | 10m | 5 |
| Ammonium aluminum sulfate hydrate (tschermigite), NH ₄ Al(SO ₄) ₂ ·12H ₂ O | 6 | 3 |
| Ammonium azide, NH ₄ N ₃ | 9 | 4 |
| Ammonium beryllium fluoride, (NH ₄) ₂ BeF ₄ | 3m | 5 |
| Ammonium borate hydrate, NH ₄ B ₅ O ₈ ·4H ₂ O | 17m | 7 |
| Ammonium boron fluoride, NH ₄ BF ₄ ... | 3m | 6 |
| Ammonium bromide, NH ₄ Br | 2 | 49 |
| Ammonium cadmium bromide, (NH ₄) ₄ CdBr ₆ | 15m | 9 |
| Ammonium cadmium chloride, NH ₄ CdCl ₃ | 5m | 6 |
| Ammonium cadmium phosphate hydrate, NH ₄ CdPO ₄ ·H ₂ O | 19m | 13 |
| Ammonium cadmium sulfate, (NH ₄) ₂ Cd ₂ (SO ₄) ₃ | 7m | 5 |
| Ammonium cadmium sulfate hydrate, (NH ₄) ₂ Cd(SO ₄) ₂ ·6H ₂ O | 8m | 5 |
| Ammonium calcium sulfate, (NH ₄) ₂ Ca ₂ (SO ₄) ₃ | 8m | 7 |
| Ammonium cerium nitrate, (NH ₄) ₂ Ce(NO ₃) ₆ | 18m | 6 |
| Ammonium chlorate, NH ₄ ClO ₄ (orthorhombic) | 7 | 6 |
| Ammonium chloride (salammoniac), NH ₄ Cl | 1 | 59 |
| Ammonium chromium sulfate hydrate, NH ₄ Cr(SO ₄) ₂ ·12H ₂ O | 6 | 7 |
| Ammonium cobalt (II) chloride, NH ₄ CoCl ₃ | 6m | 5 |
| Ammonium cobalt fluoride, NH ₄ CoF ₃ | 8m | 9 |
| Ammonium copper bromide hydrate, (NH ₄) ₂ CuBr ₄ ·2H ₂ O | 10m | 6 |
| Ammonium copper chloride, NH ₄ CuCl ₃ | 7m | 7 |
| Ammonium copper chloride hydrate, (NH ₄) ₂ CuCl ₄ ·2H ₂ O | 12m | 6 |
| Ammonium copper fluoride, NH ₄ CuF ₃ | 11m | 8 |
| Ammonium gallium sulfate hydrate, NH ₄ Ga(SO ₄) ₂ ·12H ₂ O | 6 | 9 |
| Ammonium germanium fluoride, (NH ₄) ₂ GeF ₆ | 6 | 8 |
| Ammonium hydrogen arsenate, NH ₄ H ₂ AsO ₄ | 16m | 9 |
| Ammonium hydrogen carbonate (teschemacherite), (NH ₄)HCO ₃ | 9 | 5 |
| Ammonium hydrogen phosphate, NH ₄ H ₂ PO ₄ | 4 | 64 |
| Ammonium iodate, NH ₄ IO ₃ | 10m | 7 |
| Ammonium iodide, NH ₄ I | 4 | 56 |
| Ammonium iridium chloride, (NH ₄) ₂ IrCl ₆ | 8 | 6 |
| Ammonium iron chloride hydrate, (NH ₄) ₂ FeCl ₅ ·H ₂ O | 14m | 7 |
| Ammonium iron fluoride, (NH ₄) ₃ FeF ₆ | 9m | 9 |
| Ammonium iron sulfate, NH ₄ Fe(SO ₄) ₂ | 10m | 8 |
| Ammonium iron sulfate hydrate, NH ₄ Fe(SO ₄) ₂ ·12H ₂ O | 6 | 10 |
| Ammonium lead chloride, (NH ₄) ₂ PbCl ₆ | 11m | 10 |
| Ammonium magnesium aluminum fluoride, NH ₄ MgAlF ₆ | 10m | 9 |

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

m - Monograph 25.

A mineral name in () indicates a synthetic sample.

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| Ammonium magnesium chromium oxide hydrate, $(\text{NH}_4)_2\text{Mg}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 10 |
| Ammonium magnesium phosphate hydrate (struvite), $\text{NH}_4\text{MgPO}_4 \cdot 6\text{H}_2\text{O}$ | 3m | 41 |
| Ammonium manganese chloride hydrate, $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$ | 11m | 11 |
| Ammonium manganese(II) fluoride, NH_4MnF_3 | 5m | 8 |
| Ammonium manganese sulfate, $(\text{NH}_4)_2\text{Mn}_2(\text{SO}_4)_3$ | 7m | 8 |
| Ammonium manganese sulfate hydrate, $(\text{NH}_4)_2\text{Mn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 12 |
| Ammonium mercury chloride, NH_4HgCl_3 | 8m | 14 |
| Ammonium molybdenum oxide phosphate hydrate, $(\text{NH}_4)_3(\text{MoO}_3)_{12}\text{PO}_4 \cdot 4\text{H}_2\text{O}$.. | 8 | 10 |
| Ammonium nickel(II) chloride, NH_4NiCl_3 | 6m | 6 |
| Ammonium nickel chromium oxide hydrate, $(\text{NH}_4)_2\text{Ni}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 16 |
| Ammonium nickel sulfate hydrate, $(\text{NH}_4)_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 17m | 9 |
| Ammonium nitrate (nitrammite), NH_4NO_3 | 7 | 4 |
| Ammonium osmium bromide, $(\text{NH}_4)_2\text{OsBr}_6$ | 3 | 71 |
| Ammonium osmium chloride, $(\text{NH}_4)_2\text{OsCl}_6$ | 1m | 6 |
| Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_4$ | 6 | 6 |
| Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_6$ | 8 | 7 |
| Ammonium platinum bromide, $(\text{NH}_4)_2\text{PtBr}_6$ | 9 | 6 |
| Ammonium platinum chloride, $(\text{NH}_4)_2\text{PtCl}_6$ | 5 | 3 |
| Ammonium potassium iron chloride hydrate (kremersite), $(\text{NH}_4, \text{K})_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ | 14m | 8 |
| Ammonium rhenium oxide, NH_4ReO_4 ... | 9 | 7 |
| Ammonium selenium bromide, $(\text{NH}_4)_2\text{SeBr}_6$ | 8 | 4 |
| Ammonium silicon fluoride (cryptohalite), $(\text{NH}_4)_2\text{SiF}_6$ | 5 | 5 |
| Ammonium strontium chromium oxide, $(\text{NH}_4)_2\text{Sr}(\text{CrO}_4)_2$ | 14m | 9 |
| Ammonium strontium sulfate, $(\text{NH}_4)_2\text{Sr}(\text{SO}_4)_2$ | 15m | 11 |
| Ammonium sulfate (mascagnite), $(\text{NH}_4)_2\text{SO}_4$ | 9 | 8 |
| Ammonium sulfate, $(\text{NH}_4)_2\text{S}_2\text{O}_3$ | 17m | 11 |
| Ammonium sulfate, $(\text{NH}_4)_2\text{S}_2\text{O}_8$ | 17m | 13 |
| Ammonium tellurium bromide, $(\text{NH}_4)_2\text{TeBr}_6$ | 8 | 5 |
| Ammonium tellurium chloride, $(\text{NH}_4)_2\text{TeCl}_6$ | 8 | 8 |
| Ammonium tin chloride, $(\text{NH}_4)_2\text{SnCl}_6$ | 5 | 4 |
| Ammonium tin fluoride, NH_4SnF_3 | 18m | 8 |
| Ammonium titanium fluoride, $(\text{NH}_4)_2\text{TiF}_6$ | 16m | 10 |
| Ammonium vanadium oxide, NH_4VO_3 ... | 8 | 9 |
| Ammonium zinc chloride, $(\text{NH}_4)_3\text{ZnCl}_5$ | 15m | 12 |
| Ammonium zinc fluoride, NH_4ZnF_3 ... | 8m | 18 |
| Ammonium zirconium fluoride, $(\text{NH}_4)_3\text{ZrF}_7$ | 6 | 14 |
| Antimony cobalt, CoSb | 15m | 121 |
| Antimony cobalt, CoSb_2 | 15m | 122 |
| Antimony cobalt titanium, CoSbTi .. | 15m | 124 |

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| Antimony cobalt vanadium, CoSbV ... | 15m | 125 |
| Antimony dysprosium, DySb | 4m | 41 |
| Antimony erbium, ErSb | 4m | 41 |
| Antimony(III) fluoride, SbF_3 | 2m | 4 |
| Antimony gadolinium, GdSb | 4m | 42 |
| Antimony gallium, GaSb | 6 | 30 |
| Antimony gold (aurostibite), AuSb_2 | 7 | 18 |
| Antimony indium, InSb | 4 | 73 |
| Antimony(III) iodide, SbI_3 | 6 | 16 |
| Antimony iron titanium oxide hydroxide, derbylite, $\text{SbFe}_4\text{Ti}_3\text{O}_{13}(\text{OH})$ | 16m | 89 |
| Antimony lanthanum, LaSb | 4m | 42 |
| Antimony neodymium, NdSb | 4m | 43 |
| Antimony(III) oxide (senarmontite), Sb_2O_3 (cubic) | 3 | 31 |
| Antimony(III) oxide, valentinite, Sb_2O_3 (orthorhombic) | 10 | 6 |
| Antimony(IV) oxide (cervantite), Sb_2O_4 | 10 | 8 |
| Antimony oxide, Sb_6O_{13} | 16m | 14 |
| Antimony praseodymium, PrSb | 4m | 43 |
| Antimony scandium, SbSc | 4m | 44 |
| Antimony selenide, Sb_2Se_3 | 3m | 7 |
| Antimony silver sulfide, AgSbS_2 (cubic) | 5m | 48 |
| Antimony silver sulfide (miargyrite), AgSbS_2 (monoclinic) | 5m | 49 |
| Antimony silver sulfide (pyrargyrite), Ag_3SbS_3 (trigonal) | 5m | 51 |
| Antimony silver telluride, AgSbTe_2 | 3m | 47 |
| Antimony(III) sulfide (stibnite), Sb_2S_3 | 5 | 6 |
| Antimony telluride, Sb_2Te_3 | 3m | 8 |
| Antimony terbium, SbTb | 5m | 61 |
| Antimony thorium, SbTh | 4m | 44 |
| Antimony thulium, SbTm | 4m | 45 |
| Antimony tin, SbSn | 16m | 15 |
| Antimony ytterbium, SbYb | 4m | 45 |
| Antimony yttrium, SbY | 4m | 46 |
| Arsenic, As | 3 | 6 |
| Arsenic bromide, AsBr_3 | 18m | 9 |
| Arsenic cerium, AsCe | 4m | 51 |
| Arsenic(III) iodide, AsI_3 | 13m | 7 |
| Arsenic oxide (arsenolite), As_2O_3 (cubic) | 1 | 51 |
| Arsenic oxide, claudetite, As_2O_3 (monoclinic) | 3m | 9 |
| Barium, Ba | 4 | 7 |
| Barium aluminum oxide, BaAl_2O_4 | 5m | 11 |
| Barium aluminum oxide, $\text{Ba}_3\text{Al}_2\text{O}_6$... | 12m | 7 |
| Barium aluminum titanium oxide, $\text{BaAl}_6\text{TiO}_{12}$ | 19m | 14 |
| Barium aluminum titanium oxide, $\text{Ba}_{1.23}\text{Al}_{2.46}\text{Ti}_{5.54}\text{O}_{16}$ | 18m | 10 |
| Barium aluminum titanium oxide, $\text{Ba}_3\text{Al}_{10}\text{TiO}_{20}$ | 19m | 16 |
| Barium arsenate, $\text{Ba}_3(\text{AsO}_4)_2$ | 2m | 6 |
| Barium borate, BaB_4O_7 | 4m | 6 |
| Barium borate, high form, BaB_2O_4 .. | 4m | 4 |
| Barium borate, $\text{BaB}_8\text{O}_{13}$ | 7m | 10 |
| Barium boride, BaB_6 | 19m | 18 |
| Barium bromate hydrate, $\text{Ba}(\text{BrO}_3)_2 \cdot \text{H}_2\text{O}$ | 8m | 19 |
| Barium bromide, BaBr_2 | 10m | 63 |

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| Lithium silver bromide, Li ₂ Ag ₈ Br | 12m | 55 | Magnesium iron hydroxide carbonate hydrate, pyroaurite, Mg ₆ Fe ₂ (OH) ₁₆ CO ₃ ·4H ₂ O (rhomb.) | 10m | 104 |
| Lithium silver bromide, Li ₄ Ag ₆ Br | 12m | 55 | Magnesium iron hydroxide carbonate hydrate, sjögrenite, Mg ₆ Fe ₂ (OH) ₁₆ CO ₃ ·4H ₂ O, (hexag.) ... | 10m | 103 |
| Lithium silver bromide, Li ₆ Ag ₄ Br | 12m | 55 | Magnesium lanthanum nitrate hydrate, Mg ₃ La ₂ (NO ₃) ₁₂ ·24H ₂ O | 1m | 22 |
| Lithium silver bromide, Li ₈ Ag ₂ Br | 12m | 55 | Magnesium manganese oxide, MgMn ₂ O ₄ | 10m | 35 |
| Lithium sodium aluminum fluoride, cryolithionite, Li ₃ Na ₃ Al ₂ F ₁₂ | 9m | 23 | Magnesium mercury, MgHg | 6m | 84 |
| Lithium sodium sulfate, LiNaSO ₄ ... | 6m | 24 | Magnesium molybdenum oxide, MgMoO ₄ | 7m | 28 |
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| Lithium sulfate hydrate, Li ₂ SO ₄ ·H ₂ O | 4m | 22 | Magnesium oxide (periclase), MgO .. | 1 | 37 |
| Lithium sulfide, Li ₂ S | 10m | 101 | Magnesium phosphate, Mg(PO ₃) ₂ | 13m | 26 |
| Lithium tantalum oxide, LiTaO ₃ | 14m | 20 | Magnesium phosphate, α-Mg ₂ P ₂ O ₇ | 18m | 41 |
| Lithium telluride, Li ₂ Te | 10m | 102 | Magnesium phosphate (farringtonite), Mg ₃ (PO ₄) ₂ | 19m | 55 |
| Lithium tin oxide, Li ₂ SnO ₃ | 16m | 45 | Magnesium selenide, MgSe | 5m | 70 |
| Lithium tungsten oxide, Li ₂ WO ₄ (trigonal) | 1m | 25 | Magnesium selenite hydrate, MgSeO ₃ ·6H ₂ O | 8m | 116 |
| Lithium tungsten oxide hydrate, Li ₂ WO ₄ ·0.5H ₂ O | 2m | 20 | Magnesium silicate, enstatite, MgSiO ₃ | 6 | 32 |
| Lithium uranium fluoride, LiUF ₅ ... | 7m | 131 | Magnesium silicate (forsterite), Mg ₂ SiO ₄ | 1 | 83 |
| Lithium zirconium oxide, Li ₂ ZrO ₃ .. | 19m | 51 | Magnesium sulfate hydrate (kieserite), MgSO ₄ ·H ₂ O | 16m | 46 |
| Lutetium arsenate, LuAsO ₄ | 5m | 36 | Magnesium sulfate hydrate (epsomite), MgSO ₄ ·7H ₂ O | 7 | 30 |
| Lutetium manganese oxide, LuMnO ₃ .. | 2m | 23 | Magnesium sulfide, MgS | 7 | 31 |
| Lutetium nitride, LuN | 4m | 62 | Magnesium sulfite hydrate, MgSO ₃ ·6H ₂ O | 9m | 26 |
| Lutetium oxide, Lu ₂ O ₃ | 1m | 27 | Magnesium tin, Mg ₂ Sn | 5 | 41 |
| Lutetium vanadium oxide, LuVO ₄ | 5m | 37 | Magnesium tin oxide, Mg ₂ SnO ₄ | 10m | 37 |
| Magnesium, Mg | 1 | 10 | Magnesium titanium oxide (geikielite), MgTiO ₃ | 5 | 43 |
| Magnesium aluminum oxide (spinel), MgAl ₂ O ₄ | 9m | 25 | Magnesium titanium oxide, Mg ₂ TiO ₄ | 12m | 25 |
| Magnesium aluminum silicate (low cordierite), Mg ₂ Al ₄ Si ₅ O ₁₈ (orthorhombic) | 1m | 28 | Magnesium tungsten oxide, MgWO ₄ ... | 13m | 27 |
| Magnesium aluminum silicate (indialite) Mg ₂ Al ₄ Si ₅ O ₁₈ (hexagonal) | 1m | 29 | Manganese, α-Mn (calculated pattern) | 7m | 142 |
| Magnesium aluminum silicate (pyrope), Mg ₃ Al ₂ (SiO ₄) ₂ | 4m | 24 | Manganese, α-Mn | 17m | 50 |
| Magnesium arsenate hydrate (hoernesite), Mg ₃ (AsO ₄) ₂ ·8H ₂ O | 19m | 53 | | | |
| Magnesium borate, MgB ₄ O ₇ | 17m | 47 | | | |
| Magnesium borate, Mg ₂ B ₂ O ₅ (triclinic) | 4m | 25 | | | |
| Magnesium bromide, MgBr ₂ | 4m | 62 | | | |
| Magnesium bromide hydrate, MgBr ₂ ·6H ₂ O | 11m | 35 | | | |
| Magnesium carbonate (magnesite), MgCO ₃ | 7 | 28 | | | |

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| Manganese, β -Mn | 18m | 43 |
| Manganese aluminum oxide (galaxite), MnAl ₂ O ₄ | 9 | 35 |
| Manganese bromide, MnBr ₂ | 4m | 63 |
| Manganese(II) carbonate (rhodochrosite), MnCO ₃ | 7 | 32 |
| Manganese chloride (scacchite), MnCl ₂ | 8m | 43 |
| Manganese chloride hydrate, MnCl ₂ ·2H ₂ O | 11m | 38 |
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| Manganese cobalt oxide, MnCo ₂ O ₄ ... | 9m | 30 |
| Manganese fluoride, MnF ₂ | 10m | 105 |
| Manganese iodide, MnI ₂ | 4m | 63 |
| Manganese iron oxide (jacobsite), MnFe ₂ O ₄ | 9 | 36 |
| Manganese(II) oxide (manganosite), MnO | 5 | 45 |
| Manganese oxide (pyrolusite), β -MnO ₂ | 10m | 39 |
| Manganese oxide (bixbyite), α -Mn ₂ O ₃ | 11m | 95 |
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| Mercury amide chloride, HgNH ₂ Cl ... | 10m | 40 |
| Mercury ammine chloride, Hg(NH ₃) ₂ Cl ₂ | 11m | 39 |
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| Mercury bromide, HgBr ₂ | 10m | 110 |
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| Mercury chloride, HgCl ₂ | 13m | 29 |
| Mercury chloride (calomel), Hg ₂ Cl ₂ | 13m | 30 |
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| Mercury(I) iodide, HgI | 4 | 49 |
| Mercury(II) iodide, HgI ₂ (tetragonal) | 7m | 32 |
| Mercury(II) oxide (montroydite), HgO | 9 | 39 |
| Mercury(II) selenide (tiemannite), HgSe | 7 | 35 |
| Mercury sulfate, HgSO ₄ | 16m | 50 |
| Mercury sulfate, Hg ₂ SO ₄ | 16m | 52 |
| Mercury(II) sulfide (cinnabar), HgS (hexagonal) | 4 | 17 |
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| Neodymium titanium oxide, Nd ₂ Ti ₂ O ₇ | 18m | 50 |
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| Nickel phosphate, Ni(PO ₃) ₂ | 14m | 22 |
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| Nickel silicon fluoride hydrate, NiSiF ₆ ·6H ₂ O | 8 | 38 |
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| Potassium barium phosphate, KBaPO ₄ | 19m | 68 |
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| | | | Rubidium copper chloride hydrate, $\text{Rb}_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$ | 10m | 47 |
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| Palladium, Pd | 1 | 21 |
| Palladseite, $\text{Pd}_{17}\text{Se}_{15}$ | 16m | 139 |
| Palmierite, $\text{K}_2\text{Pb}(\text{SO}_4)_2$ | 14m | 30 |
| Paraguanajuatite, Bi_2Se_3 | 18m | 16 |
| *Paratellurite, TeO_2 | 10 | 55 |
| Paratellurite, TeO_2 | 7 | 56 |
| Periclase, MgO | 1 | 37 |
| Perovskite, CaTiO_3 | 9m | 17 |
| *Phenakite, Be_2SiO_4 | 8 | 11 |
| Picromerite, $\text{K}_2\text{Mg}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 54 |
| *Pirssonite, $\text{Na}_2\text{Ca}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$ | 9m | 106 |
| Platinum, Pt | 1 | 31 |
| Portlandite, $\text{Ca}(\text{OH})_2$ | 1 | 58 |
| Potash alum, $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 36 |
| Powellite, CaMoO_4 | 6 | 22 |
| Pyrargyrite, Ag_3SbS_3 | 5m | 51 |
| Pyrite, FeS_2 | 5 | 29 |
| *Pyroaurite, $\text{Mg}_6\text{Fe}_2\text{CO}_3(\text{OH})_{16} \cdot 4\text{H}_2\text{O}$ | 10m | 104 |
| Pyrolusite, $\beta\text{-MnO}_2$ | 10m | 39 |
| Pyrope, $\text{Mg}_3\text{Al}_2(\text{SiO}_4)_3$ | 4m | 24 |
| Pyrophanite, MnTiO_3 | 15m | 42 |
| *Quartz, SiO_2 (α or low) | 3 | 24 |
| Quartz, low, $\alpha\text{-SiO}_2$ | 18m | 61 |
| Rammelsbergite, NiAs_2 | 10 | 42 |
| Retgersite, $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$ | 7 | 36 |
| Rhodochrosite, MnCO_3 | 7 | 32 |
| Rokunnite, $\text{FeCl}_2 \cdot 2\text{H}_2\text{O}$ | 11m | 32 |
| Romarchite, SnO | 4 | 28 |
| *Roscherite, (monoclinic), $\text{Be}_2\text{Ca}(\text{Fe}_{.3}\text{Mg}_{.7})_2\text{Al}_{.67}(\text{PO}_4)_3(\text{OH})_3 \cdot$ $2\text{H}_2\text{O}$ | 16m | 96 |
| *Roscherite, (triclinic), Be_4Ca_2 ($\text{Mn}_{3.91}\text{Mg}_{.04}\text{Ca}_{.05}$)($\text{Al}_{.13}\text{Fe}_{.42}\text{Mn}_{.12}$) (PO_4) $_6(\text{OH})_4 \cdot 6\text{H}_2\text{O}$ | 16m | 100 |
| Rutile, TiO_2 | 7m | 83 |
| Safflorite, CoFeAs_4 | 10 | 28 |
| Salammoniac, NH_4Cl | 1 | 59 |
| Sanbornite, $\beta\text{-BaSi}_2\text{O}_5$ | 13m | 10 |
| Sanmartinite, ZnWO_4 | 2m | 40 |
| Scacchite, MnCl_2 | 8m | 43 |
| *Scheelite, CaWO_4 | 6 | 23 |
| Schultenite, PbHAsO_4 | 14m | 18 |
| Selenium, Se | 5 | 54 |
| Selenolite, SeO_2 | 7m | 60 |
| Sellaite, MgF_2 | 4 | 33 |
| Senarmontite, Sb_2O_3 | 3 | 31 |
| Shcherbinaite, V_2O_5 | 8 | 66 |
| *Siderite, FeCO_3 | 15m | 32 |
| Silver, Ag | 1 | 23 |
| Silver, Ag (reference standard) ... | 8m | 2 |
| *Sjögrenite, $\text{Mg}_6\text{Fe}_2\text{CO}_3(\text{OH})_{16} \cdot 4\text{H}_2\text{O}$ | 10m | 103 |
| Skutterudite, CoAs_3 | 10 | 21 |
| *Smithsonite, ZnCO_3 | 8 | 69 |
| Soda alum, $\text{NaAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 15m | 68 |
| *Sodalite, $\text{Na}_8\text{Si}_6\text{Al}_6\text{O}_{24}\text{Cl}_2$ | 7m | 158 |
| Soda niter, NaNO_3 | 6 | 50 |
| Sphaerocobaltite, CoCO_3 | 10 | 24 |
| Sphalerite, ZnS | 2 | 16 |
| Spinel, MgAl_2O_4 | 9m | 25 |
| Stibnite, Sb_2S_3 | 5 | 6 |
| Stilleite, ZnSe | 3 | 23 |
| Stolzite, PbWO_4 | 5m | 34 |
| Strontianite, SrCO_3 | 3 | 56 |
| Struvite, $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ | 3m | 41 |
| Sulfur, S (orthorhombic) | 9 | 54 |
| Sylvite, KCl | 1 | 65 |
| Syngenite, $\text{K}_2\text{Ca}(\text{SO}_4)_2 \cdot \text{H}_2\text{O}$ | 14m | 25 |
| Szmikite, $\text{MnSO}_4 \cdot \text{H}_2\text{O}$ | 16m | 49 |

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| Tellurantimony, Sb_2Te_3 | 3m | 8 |
| *Tellurite, TeO_2 | 9 | 57 |
| Tellurium, Te | 1 | 26 |
| Tellurobismuthite, Bi_2Te_3 | 3m | 16 |
| Tenorite, CuO | 1 | 49 |
| Teschmacherite, NH_4HCO_3 | 9 | 5 |
| Thenardite, Na_2SO_4 | 2 | 59 |
| Thermonatrite, $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O}$ | 8 | 54 |
| *Thomsenolite, $\text{NaCaAlF}_6 \cdot \text{H}_2\text{O}$ | 8m | 132 |
| Thorianite, ThO_2 | 1 | 57 |
| Thortveitite, $\text{Sc}_2\text{Si}_2\text{O}_7$ | 7m | 58 |
| Tiemannite, HgSe | 7 | 35 |
| Tin, α -Sn (cubic) | 2 | 12 |
| Tin, β -Sn (tetragonal) | 1 | 24 |
| *Topaz, $\text{Al}_2\text{SiO}_4(\text{F},\text{OH})_2$ | 1m | 4 |
| Trevorite, NiFe_2O_4 | 10 | 44 |
| Trippkeite, CuAs_2O_4 | 16m | 120 |
| *Trona, $\text{Na}_3\text{H}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$ | 15m | 71 |
| Tschermigite, $\text{NH}_4\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$... | 6 | 3 |
| Tungstenite, WS_2 | 8 | 65 |
| Unnamed mineral, $\text{K}_{1.16}\text{Ba}_{.72}\text{Fe}_{.36}\text{Ti}_{5.58}\text{O}_{13}$ | 16m | 147 |
| Uraninite, UO_2 | 2 | 33 |
| Uvarovite, $\text{Ca}_3\text{Cr}_2(\text{SiO}_4)_3$ | 10 | 17 |
| *Valentinite, Sb_2O_3 | 10 | 6 |
| Vanthoffite, $\text{Na}_6\text{Mg}(\text{SO}_4)_4$ | 15m | 72 |
| Villiaumite, NaF | 1 | 63 |
| Vivianite, $\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$ | 16m | 38 |
| Wakefieldite, YVO_4 | 5m | 59 |
| Willemite, Zn_2SiO_4 | 7 | 62 |
| Witherite, BaCO_3 | 2 | 54 |
| Wulfenite, PbMoO_4 | 7 | 23 |
| Wurtzite, ZnS | 2 | 14 |
| *Xanthoconite, Ag_3AsS_3 | 8m | 126 |
| Xenotime, YPO_4 | 8 | 67 |
| Yavapaiite, $\text{KFe}(\text{SO}_4)_2$ | 16m | 59 |
| Zinc, Zn | 1 | 16 |
| Zincite, ZnO | 2 | 25 |
| Zinkosite, ZnSO_4 | 7 | 64 |
| *Zircon, ZrSiO_4 | 4 | 68 |
| Zircosulfate, $\text{Zr}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 7 | 66 |

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