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

## Standard X-ray Diffraction Powder Patterns

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# Standard X-ray Diffraction Powder Patterns Section 20 — Data for 71 Substances

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JCPDS®

International Centre for  
Diffraction Data

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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

#### Monograph 25

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

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

# STANDARD X-RAY DIFFRACTION POWDER PATTERNS

## Section 20 --- Data for 71 Substances

by

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Standard x-ray powder diffraction patterns are presented for 71 substances. These patterns, useful for identification, were obtained by manual or automated diffractometer methods, or were calculated from published crystal structure data. The lattice constants from the experimental work were refined by least-squares methods, and reflections were assigned Miller indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

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

### INTRODUCTION

The Powder Diffraction File (PDF) is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the JCPDS--International Centre for Diffraction Data<sup>1</sup>, the PDF is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the JCPDS, the program at the National Bureau of Standards contributes new or improved data to the PDF. Our work also aids in the development of diffraction techniques. This report presents information for one calculated and 70 experimental patterns, and is the thirtieth of the series of Standard X-ray Diffraction Powder Patterns.

### 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]

<sup>1</sup>JCPDS--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.

<sup>2</sup>See 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.

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

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

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

Another internal standard, fluorophlogopite (FP), is available as Standard Reference Material 675 [1982]. The d(001) spacing was refined from multiple powder data measurements using SRM 640a (Si) and tungsten as internal standards [Hubbard,

1983]. The calculated  $2\theta$  values of the  $00\ell$  lines are given in Table 2.

Table 1

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

Table 2

| SRM 675, Fluorophlogopite (FP)   |           |
|--|-----------|
| $d_{001} = 9.98104\text{\AA}$<br>$\pm 0.00007$                                 |           |
| Calculated $2\theta$ Angles, $\text{CuK}\alpha_1 \lambda = 1.540598\text{\AA}$ |           |
| 00 $\ell$  | $2\theta$ |
| 1  | 8.853     |
| 2  | 17.759    |
| 3  | 26.774    |
| 4  | 35.962    |
| 5  | 45.397    |
| 6  | 55.169    |
| 7  | 65.399    |
| 8  | 76.255    |
| 10   | 101.025   |
| 11   | 116.193   |
| 12   | 135.674   |

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

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

The data were processed with the JCPDS-NBS POWDER-PATTERN system of programs [Pyrros and Hubbard, 1983]. First the raw data were processed by the program POWDER.PATTERN that locates peaks with the second derivative algorithm of Savitzky and Golay [1964]. A three point Newton-Gregory interpolation [Daniels, 1978] was used to locate the derivative minimum. For some patterns, weak peaks were read from strip chart recordings or were located with the interactive graphics program PLOT.PATTERN/INT. This program displays the spectrum on a Tektronix graphic terminal. The user can locate peaks by positioning a cursor at the peak. The peak position is defined either as the position of the cursor or as the minimum of the second derivative nearest to the cursor. The  $\text{K}\alpha_2$  peaks were occasionally read to assist in establishing a  $\text{K}\alpha_1$  peak position, but  $\text{K}\alpha_2$  peaks are not reported.

All patterns were plotted on paper with the plot program PLOT.PATTERN/HRD on a scale of one degree per inch and were visually inspected. The program POWDER.CALIBR was used to calculate a polynomial correction curve from the expected and observed  $2\theta$  peak positions of the internal standard reflections and to correct the observed  $2\theta$  values of the sample. At low angles,  $\text{K}\alpha_1$  and  $\text{K}\alpha_2$  peaks were unresolved for both the sample and the internal standard. Internal standard corrections were established from the theoretical values for  $\text{K}\alpha_1$  and were applied to the unresolved low angle peaks, as well as to the resolved  $\text{K}\alpha_1$  peaks in the higher angle regions. The program POWDER.EDTPKS was used to flag reflections to be used in the least-squares cell parameter refinement. Reflections due to  $\text{CuK}\alpha_2$  radiation were excluded from the refinement.

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

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

In most cases, preliminary lattice constants were available in the literature, and were used for the initial indexing and refinement. In cases where such data were not available, other methods were tried. If suitable single crystals were

available, the lattice constants were obtained by use of a four-circle diffractometer. Axial ratios and densities from Groth [1908] were sometimes useful. Cell constants were also found in some instances by use of Visser's computer program, Ito 9 [Visser, 1969].

A least squares program, JCPDS-NBS\*LSQ82, derived from the program of Evans, Appleman and Handwerker [1963], assigned  $hkl$ 's and refined the lattice constants. The cell refinement was based only upon corrected  $2\theta$  values ( $\theta_{corr}$ ) which could be indexed without ambiguity. The program minimized the value  $\sum(\theta_{corr} - \theta_{calc})^2$ . Generally, when two or more calculated  $2\theta$ 's were within 0.03 degrees of the corrected  $2\theta$ , unique indices were not assigned. The possible multiple indices are reported. A plus sign (+) indicates more than 2 possible indices. Multiple  $hkl$ 's were not utilized or reported in indexing cubic patterns. Instead, a single appropriate index was used.

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

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

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

**Figures of merit.** Several figures of merit ratings are available for assessing indexed powder data.  $M_{20}$  [de Wolff, 1968] is a criterion for the reliability of the unit cell and indexing.  $M_{20}$  is defined by:

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

where  $Q_{20}$  is the value of  $1/d^2$  for the 20th observed line (not counting unexplained lines),  $N_{20}$  is the number of different calculated Q values up to  $Q_{20}$ , and  $\bar{\varepsilon}$  is the average magnitude of the discrepancy in Q for these 20 lines. The number of unindexable lines occurring up to the 20th observed and indexed line is  $X_{20}$ . A value of  $M_{20} > 10$  will guarantee the essential correctness of the indexing provided there are not more than 2 spurious lines ( $X_{20} \leq 2$ ) [de Wolff, 1968]. In general, patterns reported in this publication had  $M_{20} > 20$  and  $X_{20} = 0$ .  $M_{20}$  is reported if a cell was derived

only through computer indexing from powder data, without further confirmation.

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

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

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 the discrepancy between observed and calculated  $2\theta$  values for each reported  $hkl$ . When multiple indices are reported for an observed reflection, then each possible  $\Delta 2\theta$  is included in the  $\overline{|\Delta 2\theta|}$ .  $N_{\text{poss}}$  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  $\mu\text{m}$ , as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position.

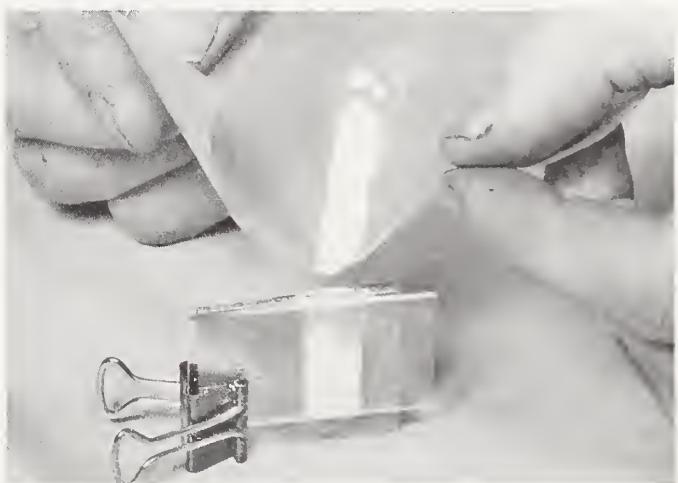


Figure 1.

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,  $\sigma$ , in the relative intensity values was calculated from the values of the five strongest lines, excluding the line with  $I_{rel}=100$ .

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

and

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

where

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

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

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

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

#### UNITS

In this publication the Ångström unit ( $1\text{\AA} = 100 \text{ pm}$ ) 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  $\text{\AA}^3$  ( $1\text{\AA}^3 = 1 \times 10^{-30} \text{ m}^3$ ). Densities are reported in  $\text{g/cm}^3$  ( $1 \text{ gm/cm}^3 = 10^3 \text{ kg/m}^3$ ).

#### ACKNOWLEDGMENTS

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Barium Cadmium Phosphate, BaCd(PO<sub>3</sub>)<sub>4</sub>

**Synonym**

Barium cadmium metaphosphate

**Sample**

The sample was made by heating Ba(OH)<sub>2</sub>·8H<sub>2</sub>O, CdCO<sub>3</sub>, and (NH<sub>4</sub>)<sub>2</sub>HPO<sub>4</sub> at 500 °C overnight. It was reground, heated at 700 °C for 2 days followed by heating at 800 °C overnight.

**Color**

Colorless

**Structure**

Monoclinic, P2<sub>1</sub>/n (14). The structure of BaCd(PO<sub>3</sub>)<sub>4</sub> was determined by Averbuch-Pouchot et al. (1975). This phase is isostructural with other phases with Mn, Ca, and Ag in place of Cd.

**Crystallographic constants of this sample**

$$a = 14.954(2) \text{ Å}$$

$$b = 9.2066(11)$$

$$c = 7.2290(11)$$

$$\beta = 90.82(2)^\circ$$

$$a/b = 1.6243$$

$$c/b = 0.7852$$

$$Z = 4$$

$$V = 995.15 \text{ Å}^3$$

$$\text{Density (calc)} = 3.775 \text{ g/cm}^3$$

**Figure of merit**

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

**Additional patterns**

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

**References**

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

Barium Cadmium Phosphate, BaCd(PO<sub>3</sub>)<sub>4</sub> - (continued)

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

# Barium Titanium Oxide, BaTiO<sub>3</sub>

## Synonym

Barium titanate

## CAS registry no.

12047-27-7

## Sample

The sample was prepared by heating BaTiO<sub>3</sub> at 1550 °C for one hour and quenching it in water.

## Color

Light gray

## Structure

Hexagonal, P6<sub>3</sub>/mmc (194). The structure was determined by Burbank and Evans (1948).

## Crystallographic constants of this sample

$$a = 5.72481(11) \text{ \AA}$$

$$c = 13.9673(3)$$

$$c/a = 2.4398$$

$$Z = 6$$

$$V = 396.43 \text{ \AA}^3$$

$$\text{Density (calc)} = 5.862 \text{ g/cm}^3$$

## Figure of merit

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

## Polymorphism

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

## Additional patterns

PDF card 8-372 (Rase and Roy, 1955)

Dickson et al. (1961)

Arend and Kihlborg (1969)

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = $26 \pm 2$ °C<br>Internal standards Si, SRM 640a<br>Fluorophlogopite, SRM 675 |                                      |       |   |                      |
|--|--------------------------------------|-------|---|----------------------|
| $d(\text{\AA})$  | $I^{\text{rel}}$<br>$\sigma = \pm 1$ | $hkl$ |   | $2\theta (\text{°})$ |
| 6.989  | 2                                    | 0     | 0 | 2                    |
| 4.674  | 2                                    | 1     | 0 | 1                    |
| 4.043  | 9                                    | 1     | 0 | 2                    |
| 3.492  | 1L                                   | 0     | 0 | 4                    |
| 3.394  | 26                                   | 1     | 0 | 3                    |
| 2.863  | 100                                  | 1     | 1 | 0                    |
| 2.855  | 91                                   | 1     | 0 | 4                    |
| 2.649  | 1L                                   | 1     | 1 | 2                    |
| 2.4408   | 6                                    | 2     | 0 | 1                    |
| 2.4337   | 4                                    | 1     | 0 | 5                    |
| 2.3365   | 16                                   | 2     | 0 | 2                    |
| 2.3290   | 15                                   | 0     | 0 | 6                    |
| 2.2136   | 3                                    | 1     | 1 | 4                    |
| 2.1882   | 22                                   | 2     | 0 | 3                    |
| 2.1073   | 1L                                   | 1     | 0 | 6                    |
| 2.0214   | 33                                   | 2     | 0 | 4                    |
| 1.8539   | 13                                   | 2     | 0 | 5                    |
| 1.8514   | 10                                   | 1     | 0 | 7                    |
| 1.8102   | 5                                    | 2     | 1 | 2                    |
| 1.8061   | 8                                    | 1     | 1 | 6                    |
| 1.7466   | 2                                    | 0     | 0 | 8                    |
| 1.7389   | 8                                    | 2     | 1 | 3                    |
| 1.6513   | 32                                   | 2     | 1 | 4                    |
| 1.6470   | 29                                   | 1     | 0 | 8                    |
| 1.5544   | 9                                    | 2     | 0 | 7                    |
| 1.4942   | 1                                    | 3     | 0 | 4                    |
| 1.4908   | 6                                    | 1     | 1 | 8                    |
| 1.4813   | 3                                    | 1     | 0 | 9                    |
| 1.4595   | 1L                                   | 2     | 1 | 6                    |
| 1.4312   | 15                                   | 2     | 2 | 0                    |
| 1.4277   | 12                                   | 2     | 0 | 8                    |
| 1.3686   | 3                                    | 3     | 1 | 1                    |
| 1.3658   | 8                                    | 2     | 1 | 7                    |
| 1.3494   | 4                                    | 3     | 1 | 2                    |
| 1.3475   | 4                                    | 3     | 0 | 6                    |
| 1.3443   | 4                                    | 1     | 0 | 10                   |
| 1.3243   | 1L                                   | 2     | 2 | 4                    |
| 1.3188   | 5                                    | 3     | 1 | 3                    |
| 1.3154   | 6                                    | 2     | 0 | 9                    |
| 1.2793   | 11                                   | 3     | 1 | 4                    |
| 1.2772   | 5                                    | 2     | 1 | 8                    |
| 1.2552   | 1L                                   | 1     | 1 | 10                   |
| 1.2340   | 1                                    | 3     | 1 | 5                    |
| 1.2301   | 2                                    | 1     | 0 | 11                   |
| 1.2190   | 6                                    | 2     | 2 | 6                    |

Barium Titanium Oxide, BaTiO<sub>3</sub> - (continued)

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

# Barium Titanium Oxide, BaTi<sub>2</sub>O<sub>5</sub>

## Synonyms

Barium titanate  
Barium metadititanate

## Sample

The sample was prepared by fusing an equimolar mixture of BaTiO<sub>3</sub> and TiO<sub>2</sub> at 1375 °C for one hour, then quenching in water.

## Color

Light gray

## Structure

Monoclinic, C2/m (12). The structure of BaTi<sub>2</sub>O<sub>5</sub> was determined by Harrison (1956).

## Crystallographic constants of this sample

a = 16.9140(12) Å  
b = 3.9345(3)  
c = 9.4122(7)  
β = 103.114(6)°

a/b = 4.2989

c/b = 2.3922

Z = 6

V = 610.04 Å<sup>3</sup>

Density (calc) = 5.112 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 90.6(0.0077,43)

## Additional pattern

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

## References

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

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

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 26±2 °C |                  |        |        |  |
|--|------------------|--------|--------|--|
| Internal standards W, a = 4.0861 Å                 |                  |        |        |  |
| Fluorophlogopite, SRM 675                          |                  |        |        |  |
| d(Å)   | I <sup>rel</sup> | hkl    | 2θ(°)  |  |
|  | σ = ±3           |        |        |  |
| 8.25   | 9                | 2 0 0  | 10.718 |  |
| 6.976  | 7                | -2 0 1 | 12.680 |  |
| 4.585  | 19               | 0 0 2  | 19.344 |  |
| 4.460  | 4                | -2 0 2 | 19.893 |  |
| 4.123  | 28               | -4 0 1 | 21.537 |  |
| 3.827  | 7                | 1 1 0  | 23.225 |  |
| 3.668  | 6                | 2 0 2  | 24.246 |  |
| 3.473  | 100              | 4 0 1  | 25.632 |  |
| 3.152  | 86               | -3 1 1 | 28.287 |  |
| 3.105  | 35               | -2 0 3 | 28.727 |  |
| 3.056  | 23               | 0 0 3  | 29.200 |  |
| 3.016  | 76               | -1 1 2 | 29.596 |  |
| 2.904  | 59               | 3 1 1  | 30.764 |  |
| 2.864  | 62               | 1 1 2  | 31.207 |  |
| 2.802  | 28               | -3 1 2 | 31.909 |  |
| 2.772  | 69               | -4 0 3 | 32.266 |  |
| 2.746  | 28               | 6 0 0  | 32.581 |  |
| 2.674  | 17               | 2 0 3  | 33.480 |  |
| 2.634  | 4                | -6 0 2 | 34.008 |  |
| 2.552  | 28               | -5 1 1 | 35.141 |  |
| 2.525  | 8                | 5 1 0  | 35.520 |  |
| 2.479  | 9                | 6 0 1  | 36.201 |  |
| 2.451  | 5                | -1 1 3 | 36.627 |  |
| 2.3957   | 5                | -5 1 2 | 37.511 |  |
| 2.3717   | 33               | -3 1 3 | 37.906 |  |
| 2.3333   | 27               | 5 1 1  | 38.554 |  |
| 2.3292   | 26               | 1 1 3  | 38.624 |  |
| 2.2910   | 16               | 0 0 4  | 39.294 |  |
| 2.2237   | 15               | 4 0 3  | 40.535 |  |
| 2.1504   | 6                | 6 0 2  | 41.981 |  |
| 2.1377   | 9                | -5 1 3 | 42.242 |  |
| 2.1138   | 3                | -8 0 1 | 42.743 |  |
| 2.0891   | 57               | 2 0 4  | 43.274 |  |
| 2.0758   | 17               | 3 1 3  | 43.566 |  |
| 2.0610   | 70               | -8 0 2 | 43.893 |  |
| 2.0200   | 35               | 7 1 0  | 44.833 |  |
| 2.0137   | 32               | -1 1 4 | 44.982 |  |
| 1.9960   | 25               | -6 0 4 | 45.401 |  |
| 1.9674   | 53               | 0 2 0  | 46.100 |  |
| 1.9221M  | 7                | 1 1 4  | 47.252 |  |
| 1.9221M  |                  | -8 0 3 | 47.252 |  |
| 1.9175   | 6                | 8 0 1  | 47.372 |  |
| 1.8823   | 5                | -2 0 5 | 48.313 |  |
| 1.8666   | 5                | -5 1 4 | 48.747 |  |
| 1.8600   | 5                | -7 1 3 | 48.929 |  |

Barium Titanium Oxide, BaTi<sub>2</sub>O<sub>5</sub> - (continued)

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

Barium Titanium Oxide, BaTi<sub>4</sub>O<sub>9</sub>

**Synonym**

Barium tetratitanate

**CAS registry no.**

12009-31-3

**Sample**

The sample was prepared using BaTiO<sub>3</sub> and TiO<sub>2</sub> (rutile). The reactants in a 1:3 molar ratio were blended by grinding under acetone. The following heating schedule, with periodic grinding, yielded a nearly single phase product, containing less than 1% of an extra phase: 800 °C for 20 hours; 1175 °C for 25 hours; 1250 °C for 20 hours; 1325 °C for 4 days.

**Color**

Colorless

**Structure**

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

**Crystallographic constants of this sample**

$$a = 6.2940(5) \text{ \AA}$$

$$b = 14.5324(11)$$

$$c = 3.7972(3)$$

$$a/b = 0.4331$$

$$c/b = 0.2613$$

$$Z = 2$$

$$V = 347.32 \text{ \AA}^3$$

$$\text{Density (calc)} = 4.522 \text{ g/cm}^3$$

**Figure of merit**

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

**Additional pattern**

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

**References**

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

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $26 \pm 1 \text{ }^\circ\text{C}$<br>Internal standards Ag, $a = 4.08651 \text{ \AA}$<br>Fluorophlogopite, SRM 675 |                                      |         |   |   |                      |
|--|--------------------------------------|---------|---|---|----------------------|
| $d(\text{\AA})$  | $I^{\text{rel}}$<br>$\sigma = \pm 3$ | $h k l$ |   |   | $2\theta ({}^\circ)$ |
| 7.267  | 1L                                   | 0       | 2 | 0 | 12.170               |
| 6.295  | 1L                                   | 1       | 0 | 0 | 14.057               |
| 5.777  | 15                                   | 1       | 1 | 0 | 15.324               |
| 4.758  | 16                                   | 1       | 2 | 0 | 18.634               |
| 3.840  | 36                                   | 1       | 3 | 0 | 23.141               |
| 3.675  | 5                                    | 0       | 1 | 1 | 24.198               |
| 3.631  | 5                                    | 0       | 4 | 0 | 24.494               |
| 3.250  | 21                                   | 1       | 0 | 1 | 27.417               |
| 3.173  | 18                                   | 1       | 1 | 1 | 28.098               |
| 3.147M   | 67                                   | 1       | 4 | 0 | 28.341               |
| 3.147M   |                                      | 2       | 0 | 0 | 28.341               |
| 3.077  | 2                                    | 2       | 1 | 0 | 28.999               |
| 2.988  | 93                                   | 0       | 3 | 1 | 29.874               |
| 2.968  | 100                                  | 1       | 2 | 1 | 30.089               |
| 2.888  | 1L                                   | 2       | 2 | 0 | 30.936               |
| 2.700  | 1                                    | 1       | 3 | 1 | 33.155               |
| 2.639M   | 68                                   | 2       | 3 | 0 | 33.942               |
| 2.639M   |                                      | 1       | 5 | 0 | 33.942               |
| 2.4225+  | 17                                   | 2       | 0 | 1 | 37.081               |
| 2.4225+  |                                      | 1       | 4 | 1 | 37.081               |
| 2.3899   | 10                                   | 2       | 1 | 1 | 37.606               |
| 2.3779   | 8                                    | 2       | 4 | 0 | 37.803               |
| 2.3080   | 11                                   | 0       | 5 | 1 | 38.994               |
| 2.2975   | 8                                    | 2       | 2 | 1 | 39.179               |
| 2.2604   | 8                                    | 1       | 6 | 0 | 39.848               |
| 2.1666M  | 22                                   | 1       | 5 | 1 | 41.653               |
| 2.1666M  |                                      | 2       | 3 | 1 | 41.653               |
| 2.1337   | 1L                                   | 2       | 5 | 0 | 42.325               |
| 2.0989   | 1L                                   | 3       | 0 | 0 | 43.061               |
| 2.0159M  | 26                                   | 2       | 4 | 1 | 44.929               |
| 2.0159M  |                                      | 3       | 2 | 0 | 44.929               |
| 1.9716   | 1                                    | 1       | 7 | 0 | 45.996               |
| 1.9422   | 5                                    | 1       | 6 | 1 | 46.732               |
| 1.9250   | 15                                   | 3       | 3 | 0 | 47.177               |
| 1.9200   | 10                                   | 2       | 6 | 0 | 47.305               |
| 1.8985   | 30                                   | 0       | 0 | 2 | 47.876               |
| 1.8611   | 5                                    | 2       | 5 | 1 | 48.900               |
| 1.8368M  | 7                                    | 0       | 2 | 2 | 49.590               |
| 1.8368M  |                                      | 3       | 0 | 1 | 49.590               |
| 1.8220M  | 13                                   | 3       | 1 | 1 | 50.021               |
| 1.8220M  |                                      | 0       | 7 | 1 | 50.021               |
| 1.8167+  | 15                                   | 3       | 4 | 0 | 50.175               |
| 1.8167+  |                                      | 0       | 8 | 0 | 50.175               |
| 1.8042   | 3                                    | 1       | 1 | 2 | 50.548               |
| 1.7805   | 10                                   | 3       | 2 | 1 | 51.268               |

Barium Titanium Oxide, BaTi<sub>4</sub>O<sub>9</sub> - (continued)

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

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

# Barium Titanium Phosphate, $\text{BaTi}_4(\text{PO}_4)_6$

## Sample

The sample was prepared by heating stoichiometric proportions of  $\text{BaCO}_3$ ,  $\text{TiO}_2$  (anatase), and  $(\text{NH}_4)_2\text{HPO}_4$  at 500 °C. The phase was then reground and heated at 1200 °C for 3 days.

## Color

Bluish white

## Structure

Rhombohedral,  $\bar{R}\bar{3}c$  (167). Similar to  $\text{BaZr}_4(\text{PO}_4)_6$ ,  $\text{NaZr}_2(\text{PO}_4)_3$ , and other phosphates of this type. The structure of  $\text{NaZr}_2(\text{PO}_4)_3$  was determined by Hagman and Kierkegaard (1968).

Crystallographic constants of this sample  
(Hexagonal axes)

$$\begin{aligned} a &= 8.3483(2) \text{ \AA} \\ c &= 23.0193(9) \end{aligned}$$

$$c/a = 2.7574$$

$$\begin{aligned} Z &= 3 \\ V &= 1389.37 \text{ \AA}^3 \end{aligned}$$

$$\text{Density (calc)} = 3.222 \text{ g/cm}^3$$

## Figure of merit

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

## Additional pattern

PDF card 12-685 (Harrison, 1960)

## References

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$ ; mean $T = 26.0 \text{ }^\circ\text{C}$<br>Internal standard Si, SRM 640a |                  |       |   |                      |
|--|------------------|-------|---|----------------------|
| $d(\text{\AA})$  | $I^{\text{rel}}$ | $hkl$ |   | $2\theta ({}^\circ)$ |
| $\sigma = \pm 3$   |                  |       |   |                      |
| 6.124  | 5                | 0     | 1 | 2                    |
| 4.502  | 4                | 1     | 0 | 4                    |
| 4.176  | 59               | 1     | 1 | 0                    |
| 3.667  | 100              | 1     | 1 | 3                    |
| 3.449  | 12               | 2     | 0 | 2                    |
| 3.061  | 16               | 0     | 2 | 4                    |
| 2.8245   | 93               | 1     | 1 | 6                    |
| 2.7132   | 12               | 2     | 1 | 1                    |
| 2.6731   | 12               | 0     | 1 | 8                    |
| 2.6584   | 14               | 1     | 2 | 2                    |
| 2.4682   | 2                | 2     | 1 | 4                    |
| 2.4098   | 22               | 3     | 0 | 0                    |
| 2.3502   | 3                | 1     | 2 | 5                    |
| 2.2511   | 5                | 2     | 0 | 8                    |
| 2.1934   | 5                | 1     | 0 | 10                   |
| 2.1809   | 8                | 1     | 1 | 9                    |
| 2.1014   | 2                | 2     | 1 | 7                    |
| 2.0872   | 2                | 2     | 2 | 0                    |
| 2.0409   | 13               | 3     | 0 | 6                    |
| 2.0137   | 3                | 2     | 2 | 3                    |
| 1.9976   | 2                | 1     | 3 | 1                    |
| 1.9815   | 12               | 1     | 2 | 8                    |
| 1.9411   | 2                | 0     | 2 | 10                   |
| 1.9176   | 4                | 0     | 0 | 12                   |
| 1.8938   | 1L               | 1     | 3 | 4                    |
| 1.8331   | 30               | 2     | 2 | 6                    |
| 1.7854   | 1                | 0     | 4 | 2                    |
| 1.7602   | 6                | 2     | 1 | 10                   |
| 1.7430   | 3                | 1     | 1 | 12                   |
| 1.7240   | 3                | 4     | 0 | 4                    |
| 1.7119   | 6                | 1     | 3 | 7                    |
| 1.6613   | 1L               | 1     | 2 | 11                   |
| 1.6451   | 10               | 3     | 1 | 8                    |
| 1.6412   | 4                | 2     | 3 | 2                    |
| 1.6169   | 1                | 2     | 2 | 9                    |
| 1.6032   | 2                | 0     | 1 | 14                   |
| 1.5935   | 1                | 3     | 2 | 4                    |
| 1.5776   | 13               | 4     | 1 | 0                    |
| 1.5605   | 1                | 2     | 3 | 5                    |
| 1.5452   | 3                | 4     | 1 | 3                    |
| 1.5306   | 6                | 0     | 4 | 8                    |
| 1.5121   | 5                | 1     | 3 | 10                   |
| 1.5008   | 11               | 3     | 0 | 12                   |
| 1.4969   | 11               | 2     | 0 | 14                   |
| 1.4808   | 2                | 3     | 2 | 7                    |

Barium Titanium Phosphate,  $\text{BaTi}_4(\text{PO}_4)_6$  - (continued)

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

Barium Zirconium Phosphate, BaZr<sub>4</sub>(PO<sub>4</sub>)<sub>6</sub>

**Synonym**

Barium zirconium orthophosphate

CAS registry no.  
6792-89-8

**Sample**

The sample was made by heating a 1:4:6 molar mixture of BaCO<sub>3</sub>, ZrO<sub>2</sub>, and (NH<sub>4</sub>)<sub>2</sub>HPO<sub>4</sub> at 500 °C. This was followed by grinding and heating to 1600 °C for 1 day.

**Color**

Colorless

**Structure**

Rhombohedral, R\*\* (166). The structure was similar to that of NaZr<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> (Chernorukov et al., 1978).

Crystallographic constants of this sample  
(Hexagonal axes)

$$a = 8.6468(5) \text{ \AA}$$

$$c = 23.984(2)$$

$$c/a = 2.7737$$

$$Z = 3$$

$$V = 1552.97 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.439 \text{ g/cm}^3$$

**Figure of merit**

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

**Reference**

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

| <sup>o</sup><br>CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 25.0 °C |                  |       |        |  |
|--|------------------|-------|--------|--|
| Internal standards Si, SRM 640a  |                  |       |        |  |
| Fluorophlogopite, SRM 675  |                  |       |        |  |
| d( $\text{\AA}$ )  | I <sup>rel</sup> | hkl   | 2θ(°)  |  |
| $\sigma = \pm 4$   |                  |       |        |  |
| 8.01   | 1L               | 0 0 3 | 11.039 |  |
| 7.16   | 1                | 1 0 1 | 12.353 |  |
| 6.359  | 1                | 0 1 2 | 13.915 |  |
| 4.681  | 7                | 1 0 4 | 18.942 |  |
| 4.324  | 36               | 1 1 0 | 20.522 |  |
| 4.040  | 2                | 0 1 5 | 21.986 |  |
| 3.999  | 1                | 0 0 6 | 22.213 |  |
| 3.804  | 40               | 1 1 3 | 23.368 |  |
| 3.695  | 3                | 0 2 1 | 24.063 |  |
| 3.576  | 2                | 2 0 2 | 24.876 |  |

| d( $\text{\AA}$ ) | I <sup>rel</sup> | hkl              |  |  | 2θ(°)  |
|-------------------|------------------|------------------|--|--|--------|
|                   |                  | $\sigma = \pm 4$ |  |  |        |
| 3.176             | 20               | 0 2 4            |  |  | 28.071 |
| 3.114             | 2                | 1 0 7            |  |  | 28.647 |
| 2.936             | 100              | 1 1 6            |  |  | 30.422 |
| 2.811             | 8                | 2 1 1            |  |  | 31.810 |
| 2.784             | 7                | 0 1 8            |  |  | 32.126 |
| 2.755             | 2                | 1 2 2            |  |  | 32.473 |
| 2.559             | 2                | 2 1 4            |  |  | 35.032 |
| 2.496             | 30               | 3 0 0            |  |  | 35.952 |
| 2.437             | 2                | 1 2 5            |  |  | 36.850 |
| 2.384             | 1                | 3 0 3            |  |  | 37.709 |
| 2.340             | 6                | 2 0 8            |  |  | 38.435 |
| 2.2684            | 4                | 1 1 9            |  |  | 39.703 |
| 2.1829            | 4                | 2 1 7            |  |  | 41.328 |
| 2.1613            | 6                | 2 2 0            |  |  | 41.760 |
| 2.1173            | 14               | 3 0 6            |  |  | 42.669 |
| 2.0865            | 2                | 2 2 3            |  |  | 43.330 |
| 2.0683            | 4                | 1 3 1            |  |  | 43.731 |
| 2.0581            | 11               | 1 2 8            |  |  | 43.960 |
| 2.0193            | 4                | 0 2 10           |  |  | 44.849 |
| 1.9977            | 2                | 0 0 12           |  |  | 45.360 |
| 1.9625            | 2                | 1 3 4            |  |  | 46.221 |
| 1.9014            | 28               | 2 2 6            |  |  | 47.798 |
| 1.8501            | 1L               | 0 4 2            |  |  | 49.209 |
| 1.8295            | 12               | 2 1 10           |  |  | 49.801 |
| 1.8140            | 2                | 1 1 12           |  |  | 50.255 |
| 1.7760            | 2                | 1 3 7            |  |  | 51.409 |
| 1.7072            | 6                | 3 1 8            |  |  | 53.642 |
| 1.6788            | 2                | 2 2 9            |  |  | 54.623 |
| 1.6702            | 4                | 0 1 14           |  |  | 54.929 |
| 1.6513            | 4                | 3 2 4            |  |  | 55.613 |
| 1.6339            | 14               | 4 1 0            |  |  | 56.257 |
| 1.6167            | 1L               | 2 3 5            |  |  | 56.909 |
| 1.6008            | 1L               | 4 1 3            |  |  | 57.526 |
| 1.5877            | 2                | 0 4 8            |  |  | 58.048 |
| 1.5700            | 6                | 1 3 10           |  |  | 58.766 |
| 1.5602            | 9                | 3 0 12           |  |  | 59.172 |
| 1.5573            | 9                | 2 0 14           |  |  | 59.292 |
| 1.5356            | 2                | 3 2 7            |  |  | 60.214 |
| 1.5126            | 15               | 4 1 6            |  |  | 61.230 |
| 1.4995            | 1                | 1 1 15           |  |  | 61.823 |
| 1.4905            | 1L               | 2 3 8            |  |  | 62.235 |
| 1.4863            | 1                | 5 0 2            |  |  | 62.432 |
| 1.4756            | 2                | 4 0 10           |  |  | 62.934 |
| 1.4657            | 10               | 1 2 14           |  |  | 63.413 |
| 1.4531            | 2                | 0 5 4            |  |  | 64.026 |
| 1.4411            | 5                | 3 3 0            |  |  | 64.625 |

# Bismuth Germanium Oxide, $\text{Bi}_4(\text{GeO}_4)_3$

## Synonyms

Bismuth germanate, BGO  
Bismuth orthogermanate  
Germanium bismuthate

CAS registry no.  
12233-56-6

Sample  
The sample was donated by Harshaw Chemical Co.

Color  
Colorless

Structure  
Cubic,  $\bar{4}3d$  (220), isostructural with  $\text{Bi}_4(\text{SiO}_4)_3$ . The structure of  $\text{Bi}_4(\text{SiO}_4)_3$  was determined by Durif (1957).

Crystallographic constants of this sample  
 $a = 10.5187(2) \text{ \AA}$

$Z = 4$   
 $V = 1163.8 \text{ \AA}^3$   
Density (calc) =  $7.109 \text{ g/cm}^3$

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

## Additional patterns

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

## References

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

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = $24.9^\circ\text{C}$ |                  |       |                         |  |
|---|------------------|-------|-------------------------|--|
| Internal standard Si, SRM 640a  |                  |       |                         |  |
| d( $\text{\AA}$ )   | I <sup>rel</sup> | hkl   | 2 $\theta$ ( $^\circ$ ) |  |
| $\sigma = \pm 3$  |                  |       |                         |  |
| 4.293   | 62               | 2 1 1 | 20.673                  |  |
| 3.719   | 1                | 2 2 0 | 23.911                  |  |
| 3.326   | 94               | 3 1 0 | 26.786                  |  |
| 2.811   | 100              | 3 2 1 | 31.803                  |  |
| 2.631   | 14               | 4 0 0 | 34.052                  |  |
| 2.352   | 2                | 4 2 0 | 38.242                  |  |
| 2.2423  | 2                | 3 3 2 | 40.185                  |  |
| 2.1470  | 44               | 4 2 2 | 42.051                  |  |
| 2.0622  | 34               | 5 1 0 | 43.867                  |  |
| 1.9200  | 6                | 5 2 1 | 47.306                  |  |

| d( $\text{\AA}$ ) | I <sup>rel</sup> | hkl    | 2 $\theta$ ( $^\circ$ ) |  |
|-------------------|------------------|--------|-------------------------|--|
| $\sigma = \pm 3$  |                  |        |                         |  |
| 1.8594            | 2                | 4 4 0  | 48.946                  |  |
| 1.8038            | 18               | 5 3 0  | 50.560                  |  |
| 1.7059            | 38               | 6 1 1  | 53.685                  |  |
| 1.6626            | 14               | 6 2 0  | 55.203                  |  |
| 1.6226            | 22               | 5 4 1  | 56.685                  |  |
| 1.5505            | 15               | 6 3 1  | 59.577                  |  |
| 1.5183            | 6                | 4 4 4  | 60.975                  |  |
| 1.4874            | 21               | 7 1 0  | 62.382                  |  |
| 1.4585            | 2                | 6 4 0  | 63.759                  |  |
| 1.4313            | 8                | 7 2 1  | 65.120                  |  |
| 1.4053            | 7                | 6 4 2  | 66.478                  |  |
| 1.3809            | 1                | 7 3 0  | 67.813                  |  |
| 1.3360            | 3                | 6 5 1  | 70.422                  |  |
| 1.2947            | 8                | 7 4 1  | 73.022                  |  |
| 1.2758            | 1L               | 8 2 0  | 74.280                  |  |
| 1.2571            | 3                | 6 5 3  | 75.579                  |  |
| 1.2397            | 14               | 6 6 0  | 76.831                  |  |
| 1.2227            | 10               | 7 5 0  | 78.100                  |  |
| 1.1908            | 6                | 7 5 2  | 80.610                  |  |
| 1.1760            | 1                | 8 4 0  | 81.842                  |  |
| 1.1617            | 2                | 9 1 0  | 83.071                  |  |
| 1.1477            | 1L               | 8 4 2  | 84.319                  |  |
| 1.1343            | 9                | 7 6 1  | 85.551                  |  |
| 1.1213            | 2                | 6 6 4  | 86.779                  |  |
| 1.1088            | 9                | 9 3 0  | 88.007                  |  |
| 1.0850            | 3                | 7 6 3  | 90.461                  |  |
| 1.0736            | 4                | 8 4 4  | 91.698                  |  |
| 1.0626            | 10               | 9 4 1  | 92.923                  |  |
| 1.0415            | 6                | 10 1 1 | 95.393                  |  |
| 1.0314            | 1                | 10 2 0 | 96.632                  |  |
| 1.0216            | 2                | 9 5 0  | 97.873                  |  |
| 1.0029            | 9                | 10 3 1 | 100.355                 |  |
| .9852             | 2                | 8 7 1  | 102.869                 |  |
| .9766             | 1                | 10 4 0 | 104.136                 |  |
| .9683             | 1                | 9 6 1  | 105.402                 |  |
| .9602             | 4                | 10 4 2 | 106.681                 |  |
| .9523             | 6                | 11 1 0 | 107.966                 |  |
| .9371             | 1                | 10 5 1 | 110.568                 |  |
| .9298             | 1L               | 8 8 0  | 111.882                 |  |
| .9226             | 2                | 9 7 0  | 113.216                 |  |
| .9087             | 11               | 9 7 2  | 115.925                 |  |
| .9020             | 5                | 10 6 0 | 117.298                 |  |
| .8954             | 1                | 11 4 1 | 118.687                 |  |

# Bismuth Germanium Oxide, $\text{Bi}_{12}\text{GeO}_{20}$

CAS registry no.  
12233-73-7

## Sample

$\text{Bi}_2\text{O}_3$  and  $\text{GeO}_2$  were melted together in a 6 to 1 molar ratio and a single crystal was pulled from the melt by the Czochralski technique (Levin and Roth, 1964).

## Color

Single crystal: dark yellow  
Ground: yellowish white

## Structure

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

## Crystallographic constants of this sample

$a = 10.14558(14) \text{ \AA}^\circ$

$Z = 2$

$V = 144.31 \text{ \AA}^3$

Density (calc) = 9.223 g/cm<sup>3</sup>

## Figure of merit

$F_{30} = 117.3(0.0085, 30)$

## Additional patterns

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

## References

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

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

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 25.8 $^\circ\text{C}$ |                                      |     |   |                         |
|--|--------------------------------------|-----|---|-------------------------|
| Internal standard W, a = 3.16524 $\text{\AA}$                                    |                                      |     |   |                         |
| d( $\text{\AA}$ )  | I <sup>rel</sup><br>$\sigma = \pm 2$ | hkl |   | 2 $\theta$ ( $^\circ$ ) |
| 7.18   | 1                                    | 1   | 1 | 0                       |
| 5.072  | 2                                    | 2   | 0 | 0                       |
| 4.146  | 4                                    | 2   | 1 | 1                       |
| 3.587  | 22                                   | 2   | 2 | 0                       |
| 3.208  | 100                                  | 3   | 1 | 0                       |
|  |                                      |     |   | 27.785                  |
| 2.930  | 26                                   | 2   | 2 | 2                       |
| 2.712  | 76                                   | 3   | 2 | 1                       |
| 2.537  | 4                                    | 4   | 0 | 0                       |
| 2.391  | 12                                   | 3   | 3 | 0                       |
| 2.2681   | 12                                   | 4   | 2 | 0                       |
|  |                                      |     |   | 39.707                  |
| 2.1628   | 19                                   | 3   | 3 | 2                       |
| 2.0712   | 15                                   | 4   | 2 | 2                       |
| 1.9899   | 23                                   | 5   | 1 | 0                       |
| 1.8519   | 12                                   | 5   | 2 | 1                       |
| 1.7927   | 1                                    | 4   | 4 | 0                       |
|  |                                      |     |   | 50.894                  |
| 1.7396   | 46                                   | 5   | 3 | 0                       |
| 1.6910   | 25                                   | 6   | 0 | 0                       |
| 1.6460   | 36                                   | 5   | 3 | 2                       |
| 1.6036   | 1                                    | 6   | 2 | 0                       |
| 1.5656   | 6                                    | 5   | 4 | 1                       |
|  |                                      |     |   | 58.945                  |
| 1.5294   | 6                                    | 6   | 2 | 2                       |
| 1.4960   | 28                                   | 6   | 3 | 1                       |
| 1.4640   | 4                                    | 4   | 4 | 4                       |
| 1.4347   | 12                                   | 5   | 5 | 0                       |
| 1.4070   | 3                                    | 6   | 4 | 0                       |
|  |                                      |     |   | 66.387                  |
| 1.3807   | 8                                    | 7   | 2 | 1                       |
| 1.3559   | 5                                    | 6   | 4 | 2                       |
| 1.3320   | 2                                    | 7   | 3 | 0                       |
| 1.2887   | 7                                    | 6   | 5 | 1                       |
| 1.2683   | 1                                    | 8   | 0 | 0                       |
|  |                                      |     |   | 74.799                  |
| 1.2487   | 6                                    | 7   | 4 | 1                       |
| 1.2303   | 3                                    | 6   | 4 | 4                       |
| 1.2128   | 17                                   | 6   | 5 | 3                       |
| 1.1956   | 16                                   | 6   | 6 | 0                       |
| 1.1795   | 17                                   | 7   | 5 | 0                       |
|  |                                      |     |   | 81.549                  |
| 1.1640   | 1                                    | 6   | 6 | 2                       |
| 1.1489   | 6                                    | 7   | 5 | 2                       |
| 1.1343   | 2                                    | 8   | 4 | 0                       |
| 1.1205   | 4                                    | 9   | 1 | 0                       |
| 1.1071   | 6                                    | 8   | 4 | 2                       |
|  |                                      |     |   | 88.182                  |
| 1.0942   | 9                                    | 7   | 6 | 1                       |
| 1.0814   | 1                                    | 6   | 6 | 4                       |
| 1.0695   | 8                                    | 9   | 3 | 0                       |
| 1.0464   | 5                                    | 9   | 3 | 2                       |
| 1.0355   | 1L                                   | 8   | 4 | 4                       |
|  |                                      |     |   | 96.133                  |

Bismuth Germanium Oxide,  $\text{Bi}_{12}\text{GeO}_{20}$  ~ (continued)

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

# Bismuth Titanium Oxide, $\text{Bi}_{12}\text{TiO}_{20}$

CAS registry no.  
12441-73-5

### Sample

$\text{Bi}_2\text{O}_3$  and  $\text{TiO}_2$  were melted together in the ratio of 6 to 1 moles and a single crystal was pulled by the Czochralski technique (Levin and Roth, 1964).

### Color

Single crystal: dark red brown  
Ground: grayish yellow

### Structure

Cubic,  $I\bar{2}3$  (197). Assumed to be isomorphous with  $\text{Bi}_{12}\text{GeO}_{20}$  (Abrahams et al., 1967).

### Crystallographic constants of this sample

$$a = 10.17391(13) \text{ \AA}$$

$$Z = 2$$

$$V = 1053.08 \text{ \AA}^3$$

$$\text{Density (calc)} = 9.069 \text{ g/cm}^3$$

### Figure of merit

$$F_{30} = 111.0(0.0090, 30)$$

### References

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 25.9 °C |                  |       |        |  |
|--|------------------|-------|--------|--|
| Internal standard W, a = 3.16524 $\text{\AA}$                      |                  |       |        |  |
| $d(\text{\AA})$  | I <sup>rel</sup> | hkl   | 2θ(°)  |  |
| $\sigma = \pm 3$   |                  |       |        |  |
| 7.19   | 1                | 1 1 0 | 12.296 |  |
| 5.080  | 3                | 2 0 0 | 17.444 |  |
| 4.152  | 4                | 2 1 1 | 21.381 |  |
| 3.595  | 23               | 2 2 0 | 24.747 |  |
| 3.218  | 100              | 3 1 0 | 27.701 |  |
| 2.936  | 25               | 2 2 2 | 30.424 |  |
| 2.720  | 77               | 3 2 1 | 32.901 |  |
| 2.543  | 3                | 4 0 0 | 35.263 |  |
| 2.398  | 11               | 3 3 0 | 37.482 |  |
| 2.2750   | 12               | 4 2 0 | 39.583 |  |
| 2.1691   | 20               | 3 3 2 | 41.603 |  |
| 2.0763   | 13               | 4 2 2 | 43.554 |  |
| 1.9959   | 20               | 5 1 0 | 45.403 |  |
| 1.8578   | 11               | 5 2 1 | 48.993 |  |
| 1.7982   | 1                | 4 4 0 | 50.729 |  |
| 1.7447   | 46               | 5 3 0 | 52.401 |  |
| 1.6959   | 22               | 6 0 0 | 54.028 |  |
| 1.6506   | 35               | 6 1 1 | 55.637 |  |
| 1.6090   | 1                | 6 2 0 | 57.207 |  |
| 1.5700   | 4                | 5 4 1 | 58.766 |  |

| $d(\text{\AA})$  | I <sup>rel</sup> | hkl    | 2θ(°)   |
|------------------|------------------|--------|---------|
| $\sigma = \pm 3$ |                  |        |         |
| 1.5335           | 6                | 6 2 2  | 60.307  |
| 1.4996           | 26               | 6 3 1  | 61.816  |
| 1.4687           | 3                | 4 4 4  | 63.268  |
| 1.4389           | 10               | 5 5 0  | 64.736  |
| 1.4107           | 2                | 6 4 0  | 66.192  |
| 1.3844           | 9                | 7 2 1  | 67.617  |
| 1.3599           | 4                | 6 4 2  | 69.002  |
| 1.3359           | 2                | 7 3 0  | 70.426  |
| 1.2920           | 6                | 6 5 1  | 73.196  |
| 1.2716           | 1                | 8 0 0  | 74.569  |
| 1.2522           | 5                | 7 4 1  | 75.929  |
| 1.2336           | 2                | 6 4 4  | 77.277  |
| 1.2158           | 16               | 6 5 3  | 78.626  |
| 1.1991           | 14               | 6 6 0  | 79.939  |
| 1.1827           | 13               | 7 5 0  | 81.277  |
| 1.1670           | 1                | 6 6 2  | 82.612  |
| 1.1519           | 4                | 7 5 2  | 83.941  |
| 1.1374           | 2                | 8 4 0  | 85.256  |
| 1.1235           | 4                | 9 1 0  | 86.569  |
| 1.1100           | 5                | 8 4 2  | 87.886  |
| 1.0972           | 8                | 7 6 1  | 89.189  |
| 1.0847           | 1                | 6 6 4  | 90.498  |
| 1.0724           | 5                | 9 3 0  | 91.824  |
| 1.0493           | 3                | 9 3 2  | 94.463  |
| 1.0384           | 1                | 8 4 4  | 95.770  |
| 1.0278           | 12               | 7 7 0  | 97.094  |
| 1.0174           | 3                | 10 0 0 | 98.423  |
| 1.0075           | 3                | 10 1 1 | 99.738  |
| .9976            | 3                | 10 2 0 | 101.089 |
| .9882            | 5                | 9 5 0  | 102.433 |
| .9792            | 2                | 10 2 2 | 103.752 |
| .9701            | 6                | 10 3 1 | 105.132 |
| .9529            | 3                | 8 7 1  | 107.877 |
| .9446            | 3                | 10 4 0 | 109.269 |
| .9365            | 5                | 9 6 1  | 110.673 |
| .9287            | 2                | 10 4 2 | 112.081 |
| .9211            | 4                | 11 1 0 | 113.501 |
| .9064            | 5                | 10 5 1 | 116.398 |
| .8923            | 3                | 9 7 0  | 119.364 |
| .8855            | 6                | 10 4 4 | 120.891 |
| .8789            | 9                | 9 7 2  | 122.442 |
| .8725            | 2                | 10 6 0 | 123.984 |
| .8661            | 4                | 11 4 1 | 125.586 |
| .8538            | 4                | 9 6 5  | 128.910 |
| .8478            | 3                | 12 0 0 | 130.612 |
| .8419            | 10               | 11 5 0 | 132.384 |
| .8307            | 4                | 10 7 1 | 136.025 |
| .8253            | 2                | 12 2 2 | 137.941 |
| .8198            | 3                | 12 3 1 | 139.973 |
| .8093            | 3                | 11 6 1 | 144.260 |
| .7993            | 2                | 9 9 0  | 149.017 |

# Boron Nitride, BN

CAS registry no.  
10294-33-4

## Sample

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

## Color

Colorless

## Structure

Hexagonal, P6<sub>3</sub>/mmc (194). The structure was determined by Pease (1952).

## Crystallographic constants of this sample

$$a = 2.50441(7) \text{ \AA}$$

$$c = 6.6562(4)$$

$$c/a = 2.6578$$

$$Z = 2$$

$$V = 36.158 \text{ \AA}^3$$

$$\text{Density (calc)} = 2.280 \text{ g/cm}^3$$

## Figure of merit

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

## Polymorphism

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

## Additional pattern

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

## References

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

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ mean } T = 26 \pm 2 \text{ }^\circ\text{C}$<br>Internal standard Si, SRM 640a |                  |       |                            |  |
|--|------------------|-------|----------------------------|--|
| $d(\text{\AA})$  | $I^{\text{rel}}$ | $hkl$ | $2\theta (\text{ }^\circ)$ |  |
| $\sigma = \pm 1$   |                  |       |                            |  |
| 3.328  | 100              | 0 0 2 | 26.765                     |  |
| 2.169  | 15               | 1 0 0 | 41.598                     |  |
| 2.0619   | 6                | 1 0 1 | 43.874                     |  |
| 1.8176   | 9                | 1 0 2 | 50.150                     |  |
| 1.6636   | 6                | 0 0 4 | 55.165                     |  |
| 1.5509   | 1L               | 1 0 3 | 59.561                     |  |
| 1.3198   | 2                | 1 0 4 | 71.412                     |  |
| 1.2521   | 5                | 1 1 0 | 75.934                     |  |
| 1.1720   | 5                | 1 1 2 | 82.177                     |  |
| 1.1346   | 1L               | 1 0 5 | 85.521                     |  |
| 1.1095   | 1L               | 0 0 6 | 87.943                     |  |
| 1.0843   | 1L               | 2 0 0 | 90.535                     |  |
| 1.0311   | 1                | 2 0 2 | 96.667                     |  |
| 1.0005   | 3                | 1 1 4 | 100.690                    |  |
| .9877  | 1L               | 1 0 6 | 102.501                    |  |
| .9086  | 1L               | 2 0 4 | 115.941                    |  |
| .8319  | 1L               | 0 0 8 | 135.641                    |  |
| .8304  | 1                | 1 1 6 | 136.150                    |  |
| .8197  | 1L               | 2 1 0 | 140.003                    |  |
| .7960  | 1L               | 2 1 2 | 150.810                    |  |

Boron Phosphate,  $\text{BPO}_4$

Synonym

Boron orthophosphate

Sample

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

Color

Colorless

Structure

Tetragonal,  $1\bar{4}$  (82). The structure was determined by Schulze (1934).

Crystallographic constants of this sample

$$a = 4.34253(15) \text{ \AA}$$

$$c = 6.6415(4)$$

$$c/a = 1.5294$$

$$Z = 2$$

$$V = 125.24 \text{ \AA}^3$$

$$\text{Density (calc)} = 2.805 \text{ g/cm}^3$$

Figure of merit

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

Polymorphism

Three other forms of  $\text{BPO}_4$  are reported. A quartz-like hexagonal (Shafer et al., 1956) and two high pressure hexagonal forms (Mackenzie et al., 1959, and Dachille and Dent-Glasser, 1959).

Additional pattern

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

References

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

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

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ mean } T = 26 \pm 1 \text{ }^\circ\text{C}$<br>Internal standard Ag, $a = 4.08651 \text{ \AA}$ |                  |       |                    |  |
|---|------------------|-------|--------------------|--|
| $d(\text{\AA})$   | $I^{\text{rel}}$ | $hkl$ | $2\theta (^\circ)$ |  |
| $\sigma = \pm 1$  |                  |       |                    |  |
| 3.635   | 100              | 1 0 1 | 24.468             |  |
| 3.321   | 3                | 0 0 2 | 26.826             |  |
| 3.070   | 4                | 1 1 0 | 29.064             |  |
| 2.2546  | 34               | 1 1 2 | 39.956             |  |
| 1.9719  | 2                | 1 0 3 | 45.988             |  |
| 1.8641  | 10               | 2 1 1 | 48.815             |  |
| 1.8175  | 5                | 2 0 2 | 50.152             |  |
| 1.6604  | 1L               | 0 0 4 | 55.282             |  |
| 1.5354  | 1                | 2 2 0 | 60.222             |  |
| 1.4597  | 10               | 2 1 3 | 63.700             |  |
| 1.4146  | 1L               | 3 0 1 | 65.987             |  |
| 1.3936  | 1L               | 2 2 2 | 67.109             |  |
| 1.3732  | 2                | 3 1 0 | 68.244             |  |
| 1.3192  | 5                | 2 0 4 | 71.454             |  |
| 1.2689  | 4                | 3 1 2 | 74.753             |  |
| 1.2114  | 2                | 3 0 3 | 78.970             |  |
| 1.1851  | 4                | 3 2 1 | 81.084             |  |
| 1.1272  | 1                | 2 2 4 | 86.218             |  |
| 1.1069  | 1L               | 0 0 6 | 88.198             |  |
| 1.0964  | 2                | 2 1 5 | 89.265             |  |
| 1.0859  | 1L               | 4 0 0 | 90.370             |  |
| 1.0580M   | 1                | 3 1 4 | 93.450             |  |
| 1.0580M   |                  | 3 2 3 | 93.450             |  |
| 1.0402  | 3                | 4 1 1 | 95.558             |  |
| 1.0319  | 1L               | 4 0 2 | 96.569             |  |
| .9861   | 1L               | 2 0 6 | 102.726            |  |
| .9781   | 1                | 3 3 2 | 103.915            |  |
| .9511   | 1L               | 4 1 3 | 108.181            |  |
| .9319   | 1L               | 4 2 2 | 111.497            |  |

Cadmium Aluminum Oxide, CdAl<sub>2</sub>O<sub>4</sub>

Synonyms

Cadmium aluminate  
Cadmium metaaluminate

CAS registry no.  
12252-16-3

Sample

The sample was prepared by heating CdO and γ-Al<sub>2</sub>O<sub>3</sub> in a sealed platinum tube for 18 hours at 975 °C, followed by 20 hours at 1200 °C.

Structure

Rhombohedral, R̄3 (148). Phenakite type (Colin and Théry, 1966).

Crystallographic constants of this sample

(Hexagonal axes)

a = 14.2146(3) Å  
c = 9.5698(3)

c/a = 0.6732

Z = 18

V = 1674.57 Å<sup>3</sup>

Density (calc) = 4.112 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 228.6(0.0031,43)

Polymerism

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

Additional pattern

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

References

Colin, F. and Théry, J. (1966). C. R. Séances Acad. Sci. Ser. C, 263, 1220.  
Hahn, H., Günter, F., Klingler, W., Störger, D., and Störger, G. (1955). Z. Anorg. Allg. Chem. 279, 241.

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 26.1 °C |                  |     |   |   |        |
|--|------------------|-----|---|---|--------|
| Internal standard Si, SRM 640a                     |                  |     |   |   |        |
| d(Å)   | I <sup>rel</sup> | hkℓ |   |   | 2θ(°)  |
| $\sigma = \pm 2$                                   |                  |     |   |   |        |
| 7.107  | 9                | 1   | 1 | 0 | 12.444 |
| 5.177  | 7                | 0   | 2 | 1 | 17.115 |
| 4.460  | 31               | 0   | 1 | 2 | 19.889 |
| 4.185  | 78               | 2   | 1 | 1 | 21.211 |
| 4.104  | 39               | 3   | 0 | 0 | 21.639 |
| 3.5527   | 86               | 2   | 2 | 0 | 25.045 |
| 3.3355   | 19               | 1   | 2 | 2 | 26.705 |
| 3.2157   | 28               | 1   | 3 | 1 | 27.719 |
| 2.9105   | 91               | 1   | 1 | 3 | 30.694 |
| 2.7794   | 6                | 3   | 1 | 2 | 32.180 |
| 2.6868   | 100              | 4   | 1 | 0 | 33.321 |
| 2.5889   | 5                | 0   | 4 | 2 | 34.620 |
| 2.4318   | 8                | 2   | 3 | 2 | 36.934 |
| 2.3737   | 58               | 2   | 2 | 3 | 37.873 |
| 2.3483   | 19               | 1   | 0 | 4 | 38.297 |
| 2.2605   | 11               | 2   | 4 | 1 | 39.847 |
| 2.1892   | 23               | 5   | 0 | 2 | 41.202 |
| 2.1541   | 3                | 5   | 1 | 1 | 41.905 |
| 2.1276   | 13               | 2   | 1 | 4 | 42.452 |
| 2.0923   | 8                | 4   | 2 | 2 | 43.205 |
| 2.0516   | 17               | 6   | 0 | 0 | 44.107 |
| 2.0071   | 18               | 1   | 5 | 2 | 45.136 |
| 1.9799   | 12               | 4   | 3 | 1 | 45.791 |
| 1.9711   | 13               | 5   | 2 | 0 | 46.008 |
| 1.9594   | 3                | 1   | 3 | 4 | 46.299 |
| 1.9021   | 37               | 3   | 3 | 3 | 47.780 |
| 1.8641   | 8                | 3   | 4 | 2 | 48.817 |
| 1.8425   | 2                | 1   | 6 | 1 | 49.425 |
| 1.8251   | 9                | 3   | 2 | 4 | 49.930 |
| 1.7768   | 2                | 4   | 4 | 0 | 51.384 |
| 1.7700   | 9                | 1   | 2 | 5 | 51.597 |
| 1.7474   | 2                | 6   | 1 | 2 | 52.313 |
| 1.7296   | 5                | 3   | 5 | 1 | 52.892 |
| 1.7254   | 7                | 6   | 0 | 3 | 53.032 |
| 1.7157   | 6                | 0   | 5 | 4 | 53.354 |
| 1.6805   | 13               | 6   | 2 | 1 | 54.565 |
| 1.6767   | 7                | 5   | 2 | 3 | 54.697 |
| 1.6684M  | 8                | 3   | 1 | 5 | 54.992 |
| 1.6684M  |                  | 2   | 4 | 4 | 54.992 |
| 1.6504   | 1                | 0   | 7 | 2 | 55.645 |
| 1.6303   | 13               | 7   | 1 | 0 | 56.391 |
| 1.6237   | 10               | 5   | 1 | 4 | 56.641 |
| 1.6079   | 1                | 2   | 6 | 2 | 57.248 |
| 1.5949   | 13               | 0   | 0 | 6 | 57.759 |
| 1.5510   | 10               | 6   | 3 | 0 | 59.558 |

Cadmium Aluminum Oxide, CdAl<sub>2</sub>O<sub>4</sub> - (continued)

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

Cadmium Zinc Phosphate,  $\text{Cd}_{0.9}\text{Zn}_{2.1}(\text{PO}_4)_2$

Sample

The sample was made by heating a mixture of  $\text{CdCO}_3$ ,  $\text{ZnO}$ , and  $(\text{NH}_4)_2\text{HPO}_4$  for 19 hours at 800 °C, followed by regrinding and heating for 2 days at 800 °C.

Color

Colorless

Structure

Monoclinic,  $P2_1/c$  (14). The structure was determined by Calvo and Stephens (1968). The structure of this phase is related to graftonite  $(\text{Fe}, \text{Mn}, \text{Ca})_3(\text{PO}_4)_2$  and  $\text{Cd}_2\text{Zn}(\text{PO}_4)_2$ . This phase called "Bss" has a range of composition from 20% to 35%  $\text{Cd}_3(\text{PO}_4)_2$  in the system  $\text{Cd}_3(\text{PO}_4)_2 - \text{Zn}_3(\text{PO}_4)_2$  (Brown and Hummel, 1963).

Crystallographic constants of this sample

$$a = 9.0594(14) \text{ \AA}$$

$$b = 11.5369(14)$$

$$c = 5.9197(8)$$

$$\beta = 98.556(14)^\circ$$

$$a/b = 0.7853$$

$$c/b = 0.5131$$

$$Z = 4$$

$$V = 611.83 \text{ \AA}^3$$

$$\text{Density (calc)} = 4.651 \text{ g/cm}^3$$

Figure of merit

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

Additional patterns

Brown and Hummel (1963)

Majling et al. (1979) Calculated pattern

References

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

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

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

| CuK $\alpha$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 25.1 °C<br>Internal standards Si, SRM 640a<br>Fluorophlogopite, SRM 675 |                                      |        |        |  |
|--|--------------------------------------|--------|--------|--|
| d( $\text{\AA}$ )  | I <sup>rel</sup><br>$\sigma = \pm 4$ | h k l  | 2θ(°)  |  |
| 8.96   | 10                                   | 1 0 0  | 9.868  |  |
| 7.06   | 1L                                   | 1 1 0  | 12.523 |  |
| 5.760  | 1L                                   | 0 2 0  | 15.370 |  |
| 5.212  | 1L                                   | 0 1 1  | 16.997 |  |
| 4.800  | 2                                    | -1 1 1 | 18.471 |  |
| 4.480  | 8                                    | 2 0 0  | 19.803 |  |
| 4.274  | 4                                    | 1 1 1  | 20.765 |  |
| 4.177  | 13                                   | 2 1 0  | 21.253 |  |
| 4.112  | 6                                    | 0 2 1  | 21.594 |  |
| 3.889  | 13                                   | -1 2 1 | 22.850 |  |
| 3.648  | 33                                   | -2 1 1 | 24.383 |  |
| 3.592  | 22                                   | 1 2 1  | 24.768 |  |
| 3.532  | 53                                   | 1 3 0  | 25.196 |  |
| 3.213  | 10                                   | 0 3 1  | 27.744 |  |
| 3.107  | 9                                    | -1 3 1 | 28.713 |  |
| 2.988  | 35                                   | 3 0 0  | 29.880 |  |
| 2.950  | 47                                   | 1 3 1  | 30.277 |  |
| 2.926  | 47                                   | 0 0 2  | 30.522 |  |
| 2.916  | 49                                   | 2 3 0  | 30.633 |  |
| 2.883M   | 100                                  | 0 4 0  | 30.989 |  |
| 2.883M   |                                      | 2 2 1  | 30.989 |  |
| 2.838  | 32                                   | 0 1 2  | 31.496 |  |
| 2.824  | 31                                   | -1 1 2 | 31.655 |  |
| 2.756  | 67                                   | -3 1 1 | 32.462 |  |
| 2.745  | 66                                   | 1 4 0  | 32.590 |  |
| 2.668  | 8                                    | 1 0 2  | 33.558 |  |
| 2.635  | 8                                    | -2 0 2 | 33.989 |  |
| 2.611  | 13                                   | 0 2 2  | 34.320 |  |
| 2.600M   | 17                                   | -1 2 2 | 34.473 |  |
| 2.600M   |                                      | 1 1 2  | 34.473 |  |
| 2.569  | 8                                    | -2 1 2 | 34.892 |  |
| 2.546  | 2                                    | -3 2 1 | 35.228 |  |
| 2.455  | 19                                   | 3 1 1  | 36.574 |  |
| 2.424  | 9                                    | 2 4 0  | 37.054 |  |
| 2.398  | 2                                    | -2 2 2 | 37.467 |  |
| 2.329  | 15                                   | 0 3 2  | 38.623 |  |
| 2.308  | 5                                    | -2 4 1 | 39.002 |  |
| 2.284  | 12                                   | -3 3 1 | 39.424 |  |
| 2.266  | 4                                    | -3 0 2 | 39.744 |  |
| 2.240  | 1                                    | 4 0 0  | 40.222 |  |
| 2.198  | 12                                   | 4 1 0  | 41.039 |  |
| 2.135  | 2                                    | 2 2 2  | 42.302 |  |
| 2.114  | 5                                    | -1 5 1 | 42.732 |  |
| 2.109  | 8                                    | -3 2 2 | 42.851 |  |
| 2.103  | 2                                    | 3 3 1  | 42.971 |  |
| 2.063  | 3                                    | 1 5 1  | 43.860 |  |
| 2.051  | 10                                   | 2 5 0  | 44.109 |  |
| 1.9786   | 8                                    | -2 5 1 | 45.825 |  |
| 1.9734   | 1                                    | 2 3 2  | 45.951 |  |
| 1.9517   | 25                                   | -3 3 2 | 46.492 |  |

Cadmium Zinc Phosphate, Cd<sub>0.9</sub>Zn<sub>2.1</sub>(PO<sub>4</sub>)<sub>2</sub> - (continued)

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

# Calcium Iron Silicate (Kirschsteinite), CaFeSiO<sub>4</sub>

## Sample

The sample was prepared from CaCO<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, and SiO<sub>2</sub>. The components, in stoichiometric proportions, were blended with a mortar and pestle in acetone. After drying, the sample was heated in an iron crucible in three eight hour stages; 1075 °C, 1110 °C, and 1140 °C in a controlled atmosphere with the partial pressure of oxygen less than or equal to 10<sup>-18</sup> atm.

## Color

Yellowish gray

## Structure

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

## Crystallographic constants of this sample

$$a = 6.4413(7) \text{ } \overset{\circ}{\text{Å}}$$

$$b = 11.1586(12)$$

$$c = 4.8753(3)$$

$$a/b = 0.5772$$

$$c/b = 0.4369$$

$$Z = 4$$

$$V = 350.42 \text{ } \overset{\circ}{\text{Å}}{}^3$$

$$\text{Density (calc)} = 3.564 \text{ g/cm}^3$$

## Figure of merit

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

## Additional pattern

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

## References

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

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

| CuKα <sub>1</sub> λ = 1.540598 $\overset{\circ}{\text{Å}}$ ; mean T = 26.0 °C<br>Internal standard Si, SRM 640a |                                      |       |   |   |        |
|---|--------------------------------------|-------|---|---|--------|
| d(A)  | $I^{\text{rel}}$<br>$\sigma = \pm 5$ | $hkl$ |   |   | 2θ(°)  |
| 5.579   | 31                                   | 0     | 2 | 0 | 15.872 |
| 4.466   | 13                                   | 0     | 1 | 1 | 19.865 |
| 4.217   | 16                                   | 1     | 2 | 0 | 21.049 |
| 3.886   | 11                                   | 1     | 0 | 1 | 22.864 |
| 3.672M  | 39                                   | 0     | 2 | 1 | 24.221 |
| 3.672M  |                                      | 1     | 1 | 1 | 24.221 |
| 3.222   | 9                                    | 2     | 0 | 0 | 27.662 |
| 3.190   | 8                                    | 1     | 2 | 1 | 27.946 |
| 2.955   | 74                                   | 0     | 3 | 1 | 30.217 |
| 2.789M  | 34                                   | 0     | 4 | 0 | 32.062 |
| 2.789M  |                                      | 2     | 2 | 0 | 32.062 |
| 2.687   | 67                                   | 1     | 3 | 1 | 33.315 |
| 2.612   | 100                                  | 2     | 1 | 1 | 34.298 |
| 2.5604  | 16                                   | 1     | 4 | 0 | 35.018 |
| 2.4375  | 12                                   | 0     | 0 | 2 | 36.845 |
| 2.4208M   | 27                                   | 0     | 4 | 1 | 37.108 |
| 2.4208M   |                                      | 2     | 2 | 1 | 37.108 |
| 2.3809  | 7                                    | 0     | 1 | 2 | 37.753 |
| 2.2328M   | 8                                    | 0     | 2 | 2 | 40.362 |
| 2.2328M   |                                      | 1     | 1 | 2 | 40.362 |
| 2.1779  | 15                                   | 2     | 3 | 1 | 41.426 |
| 2.1097M   | 3                                    | 1     | 2 | 2 | 42.831 |
| 2.1097M   |                                      | 2     | 4 | 0 | 42.831 |
| 2.0381  | 5                                    | 0     | 3 | 2 | 44.414 |
| 2.0294  | 9                                    | 0     | 5 | 1 | 44.613 |
| 1.9644  | 1L                                   | 3     | 0 | 1 | 46.174 |
| 1.9351+   | 10                                   | 2     | 4 | 1 | 46.914 |
| 1.9351+   |                                      | 3     | 1 | 1 | 46.914 |
| 1.9150  | 2                                    | 2     | 1 | 2 | 47.437 |
| 1.8534  | 5                                    | 3     | 2 | 1 | 49.116 |
| 1.8353M   | 85                                   | 0     | 4 | 2 | 49.634 |
| 1.8353M   |                                      | 2     | 2 | 2 | 49.634 |
| 1.7870  | 8                                    | 1     | 6 | 0 | 51.071 |
| 1.7649  | 9                                    | 1     | 4 | 2 | 51.757 |
| 1.7375M   | 17                                   | 0     | 6 | 1 | 52.635 |
| 1.7375M   |                                      | 3     | 3 | 1 | 52.635 |
| 1.7167  | 18                                   | 2     | 5 | 1 | 53.322 |
| 1.7015  | 10                                   | 3     | 4 | 0 | 53.835 |
| 1.6105M   | 51                                   | 2     | 6 | 0 | 57.150 |
| 1.6105M   |                                      | 4     | 0 | 0 | 57.150 |
| 1.5949M   | 12                                   | 1     | 5 | 2 | 57.760 |
| 1.5949M   |                                      | 2     | 4 | 2 | 57.760 |
| 1.5603M   | 7                                    | 0     | 2 | 3 | 59.167 |
| 1.5603M   |                                      | 1     | 1 | 3 | 59.167 |
| 1.5475M   | 4                                    | 3     | 2 | 2 | 59.703 |

Calcium Iron Silicate (Kirschsteinite), CaFeSiO<sub>4</sub> - (continued)

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

Calcium Magnesium Silicate (Monticellite), CaMgSiO<sub>4</sub>

Synonym

Calcium magnesium orthosilicate

CAS registry no.

14567-83-0

Sample

The sample was made by heating a mixture of CaCO<sub>3</sub>, basic magnesium carbonate and SiO<sub>2</sub> at 900 °C, followed by heating at 1350-1380 °C for 420 hours with periodic grindings.

Color

Colorless

Optical data

N<sub>α</sub> = 1.641, N<sub>β</sub> = 1.649, N<sub>γ</sub> = 1.655 (-) 2V = 80° (Sahama and Hytönen, 1958).

Structure

Orthorhombic, Pmn<sub>b</sub> (62). Olivine type (Brown and West, 1927). The structure was determined by Brown and West (1927) and refined by Onken (1964).

Crystallographic constants of this sample

a = 6.3666(6) Å

b = 11.0741(11)

c = 4.8224(6)

a/b = 0.5749

c/b = 0.4355

Z = 4

V = 340.00 Å<sup>3</sup>

Density (calc) = 3.057 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 76.4(0.010,39)

Additional patterns

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

Sahama and Hytönen (1958)

References

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

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

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

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

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

Calcium Magnesium Silicate (Monticellite), CaMgSiO<sub>4</sub> - (continued)

| d(A)<br>σ = ±4 | I <sup>rel</sup> | h k l | 2θ(°)  |
|----------------|------------------|-------|--------|
| 1.5796M        |                  | 2 4 2 | 58.372 |
| 1.5433         | 9                | 1 1 3 | 59.883 |
| 1.5311         | 3                | 3 2 2 | 60.409 |
| 1.5032         | 12               | 0 7 1 | 61.653 |
| 1.4736         | 1L               | 0 3 3 | 63.029 |
| 1.4578         | 1                | 4 2 1 | 63.796 |
| 1.4514         | 1                | 2 5 2 | 64.110 |
| 1.4357         | 1                | 1 3 3 | 64.897 |
| 1.4229         | 2                | 2 1 3 | 65.552 |
| 1.3987         | 6                | 4 3 1 | 66.833 |
| 1.3891         | 12               | 2 2 3 | 67.355 |
| 1.3804         | 3                | 3 4 2 | 67.837 |
| 1.3592         | 4                | 2 7 1 | 69.047 |
| 1.3312         | 1                | 2 6 2 | 70.708 |
| 1.3280         | 2                | 4 0 2 | 70.907 |
| 1.3188         | 1L               | 4 1 2 | 71.477 |
| 1.2932         | 1                | 3 5 2 | 73.118 |
| 1.2731         | 4                | 3 1 3 | 74.466 |
| 1.2692         | 4                | 2 8 0 | 74.733 |

Calcium Magnesium Silicate (Akermanite),  $\text{Ca}_2\text{MgSi}_2\text{O}_7$

**Sample**

The sample was prepared from basic magnesium carbonate,  $\text{CaCO}_3$  and  $\text{SiO}_2$ . The product was calcined at 850 °C then heated for 6 days between 1300-1380 °C with periodic grinding. To adjust the composition, 2%  $\text{SiO}_2$  was added before the final heating at 1380 °C for 48 hours.

**Color**

Colorless

**Structure**

Tetragonal,  $P\bar{4}2_1m$  (113), isostructural with  $\text{Ca}_2\text{ZnSi}_2\text{O}_7$  (Andrews, 1948). The structure of  $\text{Ca}_2\text{ZnSi}_2\text{O}_7$  was determined by Warren and Trautz (1930).

**Crystallographic constants of this sample**

$a = 7.8332(2)$  Å

$c = 5.0069(2)$

$c/a = 0.6392$

$Z = 2$

$V = 307.22$  Å<sup>3</sup>

Density (calc) = 2.947 g/cm<sup>3</sup>

**Figure of merit**

$F_{30} = 93.3(0.011, 30)$

**Additional patterns**

PDF card 10-391 (Ervin and Osborn, 1949)

Andrews (1948)

O'Daniel and Tscheischwili (1945-48)

**References**

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

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

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

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

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

Calcium Magnesium Silicate (Akermanite),  $\text{Ca}_2\text{MgSi}_2\text{O}_7$  - (continued)

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

Calcium Magnesium Silicate (Merwinite),  $\text{Ca}_3\text{Mg}(\text{SiO}_4)_2$

Synonym

Tricalcium magnesium orthosilicate

CAS registry no.

13596-18-4

Sample

The sample was made by heating  $\text{CaCO}_3$ , basic magnesium carbonate and  $\text{SiO}_2$  overnight at 900 °C, followed by heating at 1380 °C for 39 hours, and 1350 °C for 240 hours with intermediate grindings.

Color

Colorless

Structure

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

Crystallographic constants of this sample

$$a = 13.298(3) \text{ \AA}$$

$$b = 5.3046(12)$$

$$c = 9.352(3)$$

$$\beta = 92.09(2)^\circ$$

$$a/b = 2.5069$$

$$c/b = 1.7630$$

$$Z = 4$$

$$V = 659.26 \text{ \AA}^3$$

$$\text{Density (calc)} 3.312 \text{ g/cm}^3$$

Figure of merit

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

Additional patterns

PDF card 4-728 (Phemister et al., 1942)

PDF card 25-161 (Moore and Araki, 1972)

Yamaguchi and Suzuki (1967)

References

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

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

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

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

# Calcium Manganese Phosphate Fluoride, $\text{Ca}_8\text{Mn}_2(\text{PO}_4)_6\text{F}_2$

## Synonym

Calcium manganese orthophosphate fluoride

## Sample

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

## Color

Pink white

## Structure

Hexagonal,  $\text{P}6_3/\text{m}$  (176) (Schroeder, 1982).

## Crystallographic constants of this sample

$a = 9.3286(4)$  Å

$c = 6.7678(9)$

$c/a = 0.7255$

$Z = 1$

$V = 510.05$  Å<sup>3</sup>

Density (calc) = 3.380 g/cm<sup>3</sup>

## Figure of merit

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

## Reference

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

| CuK $\alpha_1$ $\lambda = 1.540598$ Å; temp. $26 \pm 1$ °C |                  |       |        |  |
|--|------------------|-------|--------|--|
| Internal standard Ag, $a = 4.08651$ Å                      |                  |       |        |  |
| d(Å)   | I <sup>rel</sup> | hkl   | 2θ(°)  |  |
| $\sigma = \pm 2$   |                  |       |        |  |
| 8.08   | 7                | 1 0 0 | 10.947 |  |
| 5.187  | 3                | 1 0 1 | 17.082 |  |
| 4.040  | 10               | 2 0 0 | 21.985 |  |
| 3.843  | 7                | 1 1 1 | 23.128 |  |
| 3.470  | 5                | 2 0 1 | 25.655 |  |
| 3.386  | 26               | 0 0 2 | 26.300 |  |
| 3.122  | 14               | 1 0 2 | 28.570 |  |
| 3.054  | 18               | 2 1 0 | 29.219 |  |
| 2.784  | 100              | 2 1 1 | 32.123 |  |
| 2.740  | 37               | 1 1 2 | 32.657 |  |
| 2.694  | 64               | 3 0 0 | 33.233 |  |
| 2.595  | 22               | 2 0 2 | 34.542 |  |
| 2.5018   | 18               | 3 0 1 | 35.865 |  |
| 2.3318   | 1                | 2 2 0 | 38.580 |  |
| 2.2664   | 6                | 2 1 2 | 39.738 |  |
| 2.2410   | 20               | 3 1 0 | 40.209 |  |
| 2.2061   | 3                | 2 2 1 | 40.873 |  |
| 2.1271   | 6                | 3 1 1 | 42.462 |  |
| 2.1073   | 2                | 3 0 2 | 42.882 |  |
| 2.0312   | 3                | 1 1 3 | 44.573 |  |

| d(Å)             | I <sup>rel</sup> | hkl   | 2θ(°)  |
|------------------|------------------|-------|--------|
| $\sigma = \pm 2$ |                  |       |        |
| 2.0200           | 2                | 4 0 0 | 44.834 |
| 1.9701           | 2                | 2 0 3 | 46.032 |
| 1.9358           | 3                | 4 0 1 | 46.897 |
| 1.9203           | 25               | 2 2 2 | 47.299 |
| 1.8680           | 12               | 3 1 2 | 48.707 |
| 1.8532           | 5                | 3 2 0 | 49.122 |
| 1.8143           | 23               | 2 1 3 | 50.246 |
| 1.7874           | 15               | 3 2 1 | 51.056 |
| 1.7628           | 15               | 4 1 0 | 51.821 |
| 1.7346           | 11               | 4 0 2 | 52.730 |
| 1.7060           | 2                | 4 1 1 | 53.684 |
| 1.6917           | 7                | 0 0 4 | 54.175 |
| 1.6256           | 7                | 3 2 2 | 56.569 |
| 1.6159           | 1                | 5 0 0 | 56.941 |
| 1.5900M          | 2                | 1 1 4 | 57.954 |
| 1.5900M          |                  | 3 1 3 | 57.954 |
| 1.5715           | 2                | 5 0 1 | 58.705 |
| 1.5637           | 1                | 4 1 2 | 59.026 |
| 1.5550           | 1                | 3 3 0 | 59.388 |
| 1.5266           | 5                | 4 2 0 | 60.606 |
| 1.5157           | 4                | 3 3 1 | 61.090 |
| 1.4893           | 2                | 4 2 1 | 62.292 |
| 1.4800           | 2                | 2 1 4 | 62.727 |
| 1.4580           | 9                | 5 0 2 | 63.785 |
| 1.4512           | 3                | 5 1 0 | 64.118 |
| 1.4324M          | 9                | 3 0 4 | 65.065 |
| 1.4324M          |                  | 3 2 3 | 65.065 |
| 1.4187           | 6                | 5 1 1 | 65.772 |
| 1.4123           | 2                | 3 3 2 | 66.105 |
| 1.3890           | 2                | 4 1 3 | 67.361 |
| 1.3468           | 1                | 6 0 0 | 69.771 |
| 1.3339           | 2                | 5 1 2 | 70.546 |
| 1.3285           | 1                | 4 3 0 | 70.879 |
| 1.3032           | 3                | 4 3 1 | 72.466 |
| 1.2936           | 3                | 5 2 0 | 73.094 |
| 1.2705           | 2                | 5 2 1 | 74.641 |
| 1.2640           | 2                | 4 2 3 | 75.094 |
| 1.2507           | 1                | 6 0 2 | 76.037 |
| 1.2366           | 5                | 4 3 2 | 77.061 |
| 1.2320           | 4                | 6 1 0 | 77.400 |
| 1.2202M          | 6                | 4 1 4 | 78.290 |
| 1.2202M          |                  | 5 1 3 | 78.290 |
| 1.2119           | 1                | 6 1 1 | 78.931 |
| 1.2084           | 4                | 5 2 2 | 79.204 |
| 1.1658           | 3                | 4 4 0 | 82.712 |
| 1.1542           | 1                | 5 3 0 | 83.729 |
| 1.1493           | 1                | 4 4 1 | 84.167 |
| 1.1446M          | 2                | 3 3 4 | 84.593 |
| 1.1446M          |                  | 4 3 3 | 84.593 |
| 1.1334           | 2                | 4 2 4 | 85.632 |
| 1.1223           | 1L               | 5 2 3 | 86.685 |
| 1.1015           | 1                | 5 1 4 | 88.745 |
| 1.0921           | 5                | 5 3 2 | 89.713 |

# Calcium Zirconium Phosphate, $\text{CaZr}_4(\text{PO}_4)_6$

## Synonym

Calcium zirconium orthophosphate

## CAS registry no.

67972-87-6

## Sample

The sample was made by heating a 1:4:6 molar mixture of  $\text{CaCO}_3$ ,  $\text{ZrO}_2$  and  $(\text{NH}_4)_2\text{HPO}_4$  up to 500 °C. It was then reground and heated at 1300 °C overnight.

## Color

Colorless

## Structure

Rhombohedral,  $R\ddot{\text{3}}m$ . The structure is similar to that of  $\text{NaZr}_2(\text{PO}_4)_3$  (Chernorukov et al., 1978).

## Crystallographic constants of this sample (Hexagonal axes)

$$a = 8.7852(4) \text{ \AA}$$

$$c = 22.682(2)$$

$$c/a = 2.5819$$

$$Z = 3$$

$$V = 1516.06 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.203 \text{ g/cm}^3$$

## Figure of merit

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

## Reference

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $26 \pm 1$ °C<br>Internal standards Si, SRM 640a<br>Fluorophlogopite, SRM 675 |                                      |         |   |                      |
|---|--------------------------------------|---------|---|----------------------|
| $d(\text{\AA})$   | $I^{\text{rel}}$<br>$\sigma = \pm 5$ | $h k l$ |   | $2\theta (\text{°})$ |
| 7.556   | 3                                    | 0       | 0 | 3                    |
| 7.208   | 4                                    | 1       | 0 | 1                    |
| 6.316   | 22                                   | 0       | 1 | 2                    |
| 4.546   | 69                                   | 1       | 0 | 4                    |
| 4.392   | 82                                   | 1       | 1 | 0                    |
| 3.896   | 6                                    | 0       | 1 | 5                    |
| 3.798   | 100                                  | 1       | 1 | 3                    |
| 3.607   | 1                                    | 2       | 0 | 2                    |
| 3.1594  | 63                                   | 0       | 2 | 4                    |
| 2.9140  | 3                                    | 2       | 0 | 5                    |
| 2.8651  | 95                                   | 1       | 1 | 6                    |
| 2.6559  | 5                                    | 0       | 1 | 8                    |
| 2.5643  | 26                                   | 2       | 1 | 4                    |
| 2.5355  | 44                                   | 3       | 0 | 0                    |
| 2.4286  | 3                                    | 1       | 2 | 5                    |
| 2.4040  | 2                                    | 3       | 0 | 3                    |
| 2.2735  | 8                                    | 2       | 0 | 8                    |
| 2.1965  | 6                                    | 2       | 2 | 0                    |
| 2.1860  | 7                                    | 1       | 1 | 9                    |
| 2.1734  | 4                                    | 1       | 0 | 10                   |
| 2.1507  | 4                                    | 2       | 1 | 7                    |
| 2.1062  | 12                                   | 3       | 0 | 6                    |
| 2.0745  | 2                                    | 3       | 1 | 2                    |
| 2.0191  | 25                                   | 1       | 2 | 8                    |
| 1.9777  | 15                                   | 1       | 3 | 4                    |
| 1.9483  | 8                                    | 0       | 2 | 10                   |
| 1.9134  | 2                                    | 3       | 1 | 5                    |
| 1.8989  | 32                                   | 2       | 2 | 6                    |
| 1.8895  | 2                                    | 0       | 0 | 12                   |
| 1.8760  | 5                                    | 0       | 4 | 2                    |
| 1.8130  | 1                                    | 2       | 0 | 11                   |
| 1.8033  | 1                                    | 4       | 0 | 4                    |
| 1.7807  | 23                                   | 2       | 1 | 10                   |
| 1.7679  | 5                                    | 1       | 3 | 7                    |
| 1.7538  | 1                                    | 0       | 4 | 5                    |
| 1.7358  | 1                                    | 1       | 1 | 12                   |
| 1.7004  | 2                                    | 1       | 0 | 13                   |
| 1.6924  | 12                                   | 3       | 1 | 8                    |
| 1.6759  | 2                                    | 1       | 2 | 11                   |
| 1.6679  | 16                                   | 3       | 2 | 4                    |
| 1.6597  | 28                                   | 4       | 1 | 0                    |
| 1.6286  | 2                                    | 2       | 3 | 5                    |
| 1.6212  | 2                                    | 4       | 1 | 3                    |
| 1.5840  | 7                                    | 0       | 1 | 14                   |
| 1.5793  | 7                                    | 0       | 4 | 8                    |

Calcium Zirconium Phosphate,  $\text{CaZr}_4(\text{PO}_4)_6$  - (continued)

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

Cerium Oxide (Cerianite), CeO<sub>2</sub>\*

CAS registry no.  
1306-38-3

Sample

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

Color

Light gray yellowish brown

Structure

Cubic, Fm3m (225). Isostructural with fluorite, CaF<sub>2</sub>. The structure of fluorite was determined by Bragg (1914).

Crystallographic constants of this sample

$$a = 5.41134(12) \text{ \AA}$$

$$Z = 4$$

$$V = 158.46 \text{ \AA}^3$$

$$\text{Density (calc)} = 7.215 \text{ g/cm}^3$$

Figure of merit

$$F_{16} = 134.1(0.0075, 16)$$

\*Comment

The true formula for this yttria-stabilized phase is Ce<sub>0.914</sub>Y<sub>0.086</sub>O<sub>1.957</sub>. This sample was prepared to produce a high density ceramic.

References

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

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

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 26.1 °C<br>Internal standard Ag, a = 4.08651 Å |                            |       |         |  |
|---|----------------------------|-------|---------|--|
| d(Å)  | I <sup>rel</sup><br>σ = ±1 | hkl   | 2θ(°)   |  |
| 3.123   | 100                        | 1 1 1 | 28.555  |  |
| 2.706   | 30                         | 2 0 0 | 33.082  |  |
| 1.9134  | 52                         | 2 2 0 | 47.479  |  |
| 1.6318  | 42                         | 3 1 1 | 56.335  |  |
| 1.5622  | 8                          | 2 2 2 | 59.087  |  |
| 1.3531  | 8                          | 4 0 0 | 69.402  |  |
| 1.2415  | 14                         | 3 3 1 | 76.700  |  |
| 1.2101  | 8                          | 4 2 0 | 79.070  |  |
| 1.1048  | 14                         | 4 2 2 | 88.412  |  |
| 1.0415  | 11                         | 5 1 1 | 95.397  |  |
| .9566   | 4                          | 4 4 0 | 107.265 |  |
| .9147   | 13                         | 5 3 1 | 114.730 |  |
| .9019   | 6                          | 6 0 0 | 117.317 |  |
| .8556   | 9                          | 6 2 0 | 128.393 |  |
| .8252   | 6                          | 5 3 3 | 137.969 |  |
| .8158   | 5                          | 6 2 2 | 141.566 |  |

Cesium Hydrogen Phosphate,  $\text{CsH}_5(\text{PO}_4)_2$

Synonym

Cesium pentahydrogen diphosphate

Sample

The sample was prepared by mixing an 85% solution of  $\text{H}_3\text{PO}_4$  with  $\text{Cs}_2\text{CO}_3$ . The precipitate was washed with alcohol and dried in air one week.

Color

Colorless

Structure

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

Crystallographic constants of this sample

$$a = 10.8814(11) \text{ \AA}$$

$$b = 7.7717(8)$$

$$c = 9.5320(9)$$

$$\beta = 96.586(10)^\circ$$

$$a/b = 1.4001$$

$$c/b = 1.2265$$

$$Z = 4$$

$$V = 800.77 \text{ \AA}^3$$

$$\text{Density (calc)} = 2.720 \text{ g/cm}^3$$

Figure of merit

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

Additional pattern

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

References

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ mean } T = 25.6^\circ \text{ C}$ |                  |        |                     |  |
|---|------------------|--------|---------------------|--|
| Internal standards Si, SRM 640a   |                  |        |                     |  |
| Fluorophlogopite, SRM 675   |                  |        |                     |  |
| $d(\text{\AA})$   | $I^{\text{rel}}$ | $hkl$  | $2\theta(\text{°})$ |  |
| $\sigma = \pm 3$  |                  |        |                     |  |
| 6.311   | 22               | 1 1 0  | 14.022              |  |
| 6.005   | 7                | 0 1 1  | 14.741              |  |
| 5.403   | 8                | 2 0 0  | 16.394              |  |
| 4.531   | 13               | -1 0 2 | 19.577              |  |
| 4.166M  | 39               | -2 1 1 | 21.311              |  |
| 4.166M  |                  | 1 0 2  | 21.311              |  |
| 3.918   | 37               | -1 1 2 | 22.678              |  |
| 3.879   | 40               | 2 1 1  | 22.909              |  |
| 3.785   | 37               | -2 0 2 | 23.485              |  |
| 3.672   | 52               | 1 1 2  | 24.217              |  |

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

Cesium Hydrogen Phosphate,  $\text{CsH}_5(\text{PO}_4)_2$  - (continued)

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

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

Cesium Zirconium Phosphate,  $\text{CsZr}_2(\text{PO}_4)_3$

**Synonyms**

Cesium zirconium orthophosphate  
Cesium dizirconium tris(phosphate)

**CAS registry no.**  
19527-88-9

**Sample**

The sample was prepared from a mixture of  $(\text{NH}_4)_2\text{HPO}_4$ ,  $\text{Cs}_2\text{CO}_3$  and  $\text{ZrO}_2$  in molar ratios of 6:1:4. The mixture was heated for 2 hours at 500 °C, reground, and heated for 2 hours at 1000 °C. It was reground; a small amount of  $\text{Cs}_2\text{CO}_3$  was added, and the mixture was heated at 900 °C for 16 hours.

**Color**

Colorless

**Structure**

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

**Crystallographic constants of this sample**  
(Hexagonal axes)

$$a = 8.5807(3) \text{ \AA}$$

$$c = 24.9654(13)$$

$$c/a = 2.9095$$

$$Z = 6$$

$$V = 1591.90 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.757 \text{ g/cm}^3$$

**Figure of merit**

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

**Additional pattern**

Roy et al. (1982)

**References**

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

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

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

Cesium Zirconium Phosphate, CsZr<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> - (continued)

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

# Chromium Tungsten Oxide, CrW<sub>0</sub><sub>4</sub>

## Synonym

Chromium tungstate

CAS registry no.  
56729-81-8

## Sample

The sample was prepared from Cr<sub>2</sub>O<sub>3</sub> and WO<sub>3</sub>. The constituent oxides in a 1:2 molar ratio were blended by grinding in an agate mortar under acetone. The powders were heated in a tungsten metal tray in a controlled atmosphere furnace. Temperatures and partial pressures of oxygen were chosen from the work of Trumm (1979). The following heat treatments were satisfactory:

800 °C for 8 hours, at partial oxygen pressure 10<sup>-20</sup> atm;  
1000 °C for 8 hours, at partial oxygen pressure 10<sup>-20</sup> atm;  
1300 °C for 8 hours, at partial oxygen pressure 10<sup>-17</sup> atm.

Traces of Cr<sub>2</sub>O<sub>3</sub> and W metal were present as extra phases.

## Color

Very dark greenish blue

## Structure

Monoclinic, C2/m (12), distorted rutile type, isostructural with AlWO<sub>4</sub>. The structure was determined by Vlasse et al. (1976).

## Crystallographic constants of this sample

a = 9.2708(6) Å  
b = 5.8282(3)  
c = 4.6445(3)  
β = 91.926(5)°

a/b = 1.5907

c/b = 0.7969

Z = 4

V = 250.81 Å<sup>3</sup>

Density (calc) = 7.941 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 78.9(0.0093, 41)

## Additional patterns

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

## References

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

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

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

| CuKα <sub>1</sub> λ = 1.540598 Å; temp. 26±1 °C<br>Internal standard Si, SRM 640a |                  |     |   |       |
|---|------------------|-----|---|-------|
| d(Å)  | I <sup>rel</sup> | hkl |   | 2θ(°) |
| σ = ±3  |                  |     |   |       |
| 4.934   | 2                | 1   | 1 | 0     |
| 4.637M  | 64               | 0   | 0 | 1     |
| 4.637M  |                  | 2   | 0 | 0     |
| 3.412   | 3                | -1  | 1 | 1     |
| 3.336   | 72               | -2  | 0 | 1     |
| 3.225   | 66               | 2   | 0 | 1     |
| 2.915   | 12               | 0   | 2 | 0     |
| 2.730   | 2                | 3   | 1 | 0     |
| 2.467M  | 100              | 0   | 2 | 1     |
| 2.467M  |                  | 2   | 2 | 0     |
| 2.321   | 26               | 0   | 0 | 2     |
| 2.316   | 24               | 4   | 0 | 0     |
| 2.1949  | 26               | -2  | 2 | 1     |
| 2.1623  | 2                | 2   | 2 | 1     |
| 2.1029  | 5                | -2  | 0 | 2     |
| 2.1014  | 3                | -4  | 0 | 1     |
| 2.0856  | 1L               | 1   | 1 | 2     |
| 2.0468  | 15               | 2   | 0 | 2     |
| 1.9018  | 3                | 1   | 3 | 0     |
| 1.8151  | 11               | 0   | 2 | 2     |
| 1.8140  | 10               | 4   | 2 | 0     |
| 1.7945  | 1                | -3  | 1 | 2     |
| 1.7638  | 2                | -1  | 3 | 1     |
| 1.7552  | 1                | 1   | 3 | 1     |
| 1.7425  | 1L               | 3   | 1 | 2     |
| 1.7052  | 38               | -2  | 2 | 2     |
| 1.6749M   | 39               | 2   | 2 | 2     |
| 1.6749M   |                  | 4   | 2 | 1     |
| 1.6679M   | 26               | -5  | 1 | 1     |
| 1.6679M   |                  | -4  | 0 | 2     |
| 1.6445  | 1                | 3   | 3 | 0     |
| 1.6332  | 1L               | 5   | 1 | 1     |
| 1.6125  | 12               | 4   | 0 | 2     |
| 1.5591  | 2                | -3  | 3 | 1     |
| 1.5474  | 3                | 0   | 0 | 3     |
| 1.5441  | 3                | 6   | 0 | 0     |
| 1.5414  | 2                | 3   | 3 | 1     |
| 1.4828  | 7                | -2  | 0 | 3     |
| 1.4801  | 7                | -6  | 0 | 1     |
| 1.4759  | 3                | -1  | 3 | 2     |
| 1.4657  | 1                | 1   | 3 | 2     |
| 1.4570  | 8                | 0   | 4 | 0     |
| 1.4532  | 10               | 2   | 0 | 3     |
| 1.4506  | 8                | 6   | 0 | 1     |
| 1.4475  | 6                | -4  | 2 | 2     |

Chromium Tungsten Oxide, CrW<sub>4</sub> - (continued)

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

# Cobalt Telluride, CoTe

CAS registry no.  
12017-13-9

## Sample

The sample was donated by CERAC/PURE, Inc.,  
Butler, Wisc. The sample contained less  
than 5% CoTe<sub>2</sub> as a second phase.

## Color

Very dark gray

## Structure

Hexagonal, P6<sub>3</sub>/mmc (194). Isostructural with  
NiAs (Oftedal, 1927).

## Crystallographic constants of this sample

a = 3.89276(15) Å  
c = 5.3746(3)

Z = 2

V = 70.533 Å<sup>3</sup>

Density (calc) = 8.783 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 75.5(0.011,36)

## Additional pattern

Oftedal (1927)

## Reference

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

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 26.4 °C |                  |       |  |         |
|--|------------------|-------|--|---------|
| Internal standard Si, SRM 640a                     |                  |       |  |         |
| d(A)   | I <sub>rel</sub> | hkl   |  | 2θ(°)   |
| $\sigma = \pm 3$                                   |                  |       |  |         |
| 3.369  | 2                | 1 0 0 |  | 26.436  |
| 2.856  | 100              | 1 0 1 |  | 31.295  |
| 2.688  | 10               | 0 0 2 |  | 33.310  |
| 2.101  | 45               | 1 0 2 |  | 43.007  |
| 1.9470   | 37               | 1 1 0 |  | 46.612  |
| 1.6082   | 16               | 2 0 1 |  | 57.239  |
| 1.5819   | 20               | 1 0 3 |  | 58.282  |
| 1.5768   | 18               | 1 1 2 |  | 58.486  |
| 1.4280   | 11               | 2 0 2 |  | 65.290  |
| 1.3433   | 4                | 0 0 4 |  | 69.981  |
| 1.2744   | 1L               | 2 1 0 |  | 74.376  |
| 1.2484   | 1L               | 1 0 4 |  | 76.197  |
| 1.2400   | 13               | 2 1 1 |  | 76.809  |
| 1.2278   | 7                | 2 0 3 |  | 77.718  |
| 1.1514   | 10               | 2 1 2 |  | 83.979  |
| 1.1236   | 6                | 3 0 0 |  | 86.561  |
| 1.1058   | 11               | 1 1 4 |  | 88.310  |
| 1.0384   | 5                | 2 1 3 |  | 95.775  |
| 1.0368   | 3                | 3 0 2 |  | 95.974  |
| 1.0240   | 3                | 1 0 5 |  | 97.564  |
| .9730  | 4                | 2 2 0 |  | 104.680 |
| .9246  | 2                | 2 1 4 |  | 112.841 |
| .9211  | 6                | 3 1 1 |  | 113.497 |
| .9149  | 2                | 2 2 2 |  | 114.692 |
| .9063  | 2                | 2 0 5 |  | 116.402 |
| .8957  | 2                | 0 0 6 |  | 118.624 |
| .8830  | 4                | 3 1 2 |  | 121.470 |
| .8657  | 4                | 1 0 6 |  | 125.699 |
| .8621  | 7                | 3 0 4 |  | 126.634 |
| .8327  | 2                | 4 0 1 |  | 135.370 |
| .8290  | 4                | 3 1 3 |  | 136.631 |

Copper Chromium Oxide, CuCr<sub>2</sub>O<sub>4</sub>

Synonym

Copper chromite

CAS registry no.  
12018-10-9

Sample

The sample was prepared by blending stoichiometric amounts of CuO and Cr<sub>2</sub>O<sub>3</sub> and heating in a platinum boat in pure oxygen for extended periods at temperatures as high as 975 °C, with periodic grinding.

Color

Black

Structure

Tetragonal, I<sub>4</sub>2d (122). Distorted normal spinel. The structure was determined by Prince (1957).

Crystallographic constants of this sample

$a = 6.0336(3)$  Å

$c = 7.7824(6)$

$c/a = 1.2898$

$Z = 4$

$V = 283.31$  Å<sup>3</sup>

Density (calc) = 5.428 g/cm<sup>3</sup>

Figure of merit

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

Polymorphism

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

Additional pattern

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

References

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

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

| CuK $\alpha_1$ $\lambda = 1.540598$ Å; mean T = 24.8 °C<br>Internal standard W, a = 3.16524 Å |                  |     |   |         |
|---|------------------|-----|---|---------|
| d(Å)  | I <sup>rel</sup> | hkl |   | 2θ(°)   |
| $\sigma = \pm 2$  |                  |     |   |         |
| 4.765   | 11               | 1   | 0 | 1       |
| 3.018   | 23               | 2   | 0 | 0       |
| 2.877   | 34               | 1   | 1 | 2       |
| 2.550   | 100              | 2   | 1 | 1       |
| 2.385M  | 67               | 2   | 0 | 2       |
|   |                  |     |   | 37.693  |
| 2.385M  |                  | 1   | 0 | 3       |
| 2.134   | 20               | 2   | 2 | 0       |
| 1.9463M   | 8                | 3   | 0 | 1       |
| 1.9463M   |                  | 0   | 0 | 4       |
| 1.8701  | 1                | 2   | 1 | 3       |
|   |                  |     |   | 48.650  |
| 1.7135  | 13               | 3   | 1 | 2       |
| 1.6361  | 39               | 3   | 2 | 1       |
| 1.5897  | 9                | 3   | 0 | 3       |
| 1.5083  | 28               | 4   | 0 | 0       |
| 1.4376M   | 35               | 4   | 1 | 1       |
|   |                  |     |   | 64.797  |
| 1.4376M   |                  | 2   | 2 | 4       |
| 1.4066M   | 2                | 4   | 0 | 2       |
| 1.4066M   |                  | 3   | 2 | 3       |
| 1.3491  | 3                | 4   | 2 | 0       |
| 1.3360  | 3                | 3   | 3 | 2       |
|   |                  |     |   | 70.422  |
| 1.2745M   | 14               | 4   | 2 | 2       |
| 1.2745M   |                  | 4   | 1 | 3       |
| 1.2407  | 3                | 1   | 1 | 6       |
| 1.2310  | 4                | 3   | 0 | 5       |
| 1.1920  | 5                | 4   | 0 | 4       |
|   |                  |     |   | 80.515  |
| 1.1320  | 2                | 5   | 1 | 2       |
| 1.1087  | 6                | 4   | 2 | 4       |
| 1.0941  | 7                | 4   | 3 | 3       |
| 1.0726  | 1                | 3   | 1 | 6       |
| 1.0662  | 7                | 4   | 1 | 5       |
|   |                  |     |   | 92.514  |
| 1.0280  | 3                | 2   | 1 | 7       |
| 1.0056  | 1                | 6   | 0 | 0       |
| 1.0001  | 2                | 5   | 3 | 2       |
| .9840   | 3                | 6   | 1 | 1       |
| .9731   | 2                | 3   | 0 | 7       |
|   |                  |     |   | 104.665 |
| .9536   | 4                | 4   | 3 | 5       |
| .9351   | 2                | 4   | 2 | 6       |
| .9260M  | 3                | 3   | 2 | 7       |
| .9260M  |                  | 2   | 0 | 8       |
| .8933   | 2                | 6   | 0 | 4       |
|   |                  |     |   | 119.145 |
| .8856   | 4                | 5   | 4 | 3       |
| .8741   | 1                | 5   | 1 | 6       |
|   |                  |     |   | 123.588 |

Copper Iron Oxide, CuFe<sub>2</sub>O<sub>4</sub>

Synonym

Copper ferrite

CAS registry no.  
12018-79-0

Sample

The sample was prepared by blending stoichiometric amounts of CuO and Fe<sub>2</sub>O<sub>3</sub> and heating in a flowing atmosphere of pure oxygen for extended periods at temperatures as high as 975 °C, with periodic grinding. The sample contained traces of CuO and an unidentified phase.

Color

Olive black

Structure

Tetragonal, I4<sub>1</sub>/amd (141). It is a tetragonally distorted inverse spinel. The structure was determined by Prince and Treuting (1956). The "a" dimension given by Prince and Treuting was divided by  $\sqrt{2}$  to make it conform to the body-centered space group.

Crystallographic constants of this sample

a = 5.8444(4) Å  
c = 8.6304(10)

c/a = 1.4767

Z = 4  
V = 294.79 Å<sup>3</sup>

Density (calc) = 5.390 g/cm<sup>3</sup>

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

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 26.1 °C<br>Internal standard Ag, a = 4.08651 Å |                  |     |   |   |        |
|---|------------------|-----|---|---|--------|
| d(Å)  | I <sub>rel</sub> | hkℓ |   |   | 2θ(°)  |
| $\sigma = \pm 2$  |                  |     |   |   |        |
| 4.839   | 17               | 1   | 0 | 1 | 18.319 |
| 2.985   | 32               | 1   | 1 | 2 | 29.908 |
| 2.923   | 13               | 2   | 0 | 0 | 30.559 |
| 2.582   | 53               | 1   | 0 | 3 | 34.719 |
| 2.502   | 100              | 2   | 1 | 1 | 35.862 |
| 2.420   | 14               | 2   | 0 | 2 | 37.122 |
| 2.1580  | 11               | 0   | 0 | 4 | 41.826 |
| 2.0667  | 22               | 2   | 2 | 0 | 43.768 |
| 1.9345  | 1                | 2   | 1 | 3 | 46.930 |
| 1.7360  | 5                | 2   | 0 | 4 | 52.683 |
| 1.6990  | 10               | 3   | 1 | 2 | 53.923 |
| 1.6550  | 12               | 1   | 0 | 5 | 55.477 |
| 1.6134  | 11               | 3   | 0 | 3 | 57.035 |
| 1.5932  | 24               | 3   | 2 | 1 | 57.829 |
| 1.4922  | 40               | 2   | 2 | 4 | 62.158 |
| 1.4611  | 16               | 4   | 0 | 0 | 63.632 |
| 1.4119  | 1                | 3   | 2 | 3 | 66.127 |
| 1.3583  | 2                | 1   | 1 | 6 | 69.099 |
| 1.3118  | 2                | 3   | 3 | 2 | 71.920 |
| 1.3067  | 2                | 4   | 2 | 0 | 72.241 |
| 1.2922  | 5                | 3   | 0 | 5 | 73.184 |
| 1.2900  | 4                | 2   | 0 | 6 | 73.331 |
| 1.2713  | 9                | 4   | 1 | 3 | 74.586 |
| 1.2507  | 4                | 4   | 2 | 2 | 76.037 |
| 1.2098  | 5                | 4   | 0 | 4 | 79.094 |

Polymorphism

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

Additional pattern

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

References

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

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

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

Copper Mercury Iodide,  $\beta$ -Cu<sub>2</sub>HgI<sub>4</sub>

Synonym

Cuprous mercuric tetraiodide

CAS registry no.

55945-38-5

Sample

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

Color

Vivid red

Structure

Tetragonal, I<sub>4</sub>2m (121). Pseudocubic, isostructural with Ag<sub>2</sub>HgI<sub>4</sub> (Ketelaar, 1931). The structure of Cu<sub>2</sub>HgI<sub>4</sub> was determined by Hahn et al. (1955).

Crystallographic constants of this sample

$$a = 6.07802(15) \text{ \AA}$$

$$c = 12.2540(4)$$

$$c/a = 2.0161$$

$$Z = 2$$

$$V = 452.69 \text{ \AA}^3$$

$$\text{Density (calc)} = 6.128 \text{ g/cm}^3$$

Figure of merit

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

Polymorphism

$\beta$ -Cu<sub>2</sub>HgI<sub>4</sub> transforms to a cubic form above 90 °C (Ketelaar, 1934).

Additional patterns

PDF card 18-450 (Hahn et al., 1955)

Ketelaar (1931)

References

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

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

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

| d(\text{\AA}) | $I^{\text{rel}}$<br>$\sigma = \pm 2$ | CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = $26 \pm 2 \text{ }^\circ\text{C}$ |   |    | $2\theta ({}^\circ)$ |
|---------------|--------------------------------------|--|---|----|----------------------|
|               |                                      | Internal standard Si, SRM 640a   |   |    |                      |
| 6.118         | 1L                                   | 0  | 0 | 2  | 14.466               |
| 5.446         | 12                                   | 1  | 0 | 1  | 16.263               |
| 4.299         | 2                                    | 1  | 1 | 0  | 20.645               |
| 3.517         | 100                                  | 1  | 1 | 2  | 25.302               |
| 3.389         | 14                                   | 1  | 0 | 3  | 26.275               |
| 3.063         | 3                                    | 0  | 0 | 4  | 29.133               |
| 3.038         | 4                                    | 2  | 0 | 0  | 29.375               |
| 2.722         | 1L                                   | 2  | 0 | 2  | 32.876               |
| 2.654         | 17                                   | 2  | 1 | 1  | 33.751               |
| 2.4945        | 1                                    | 1  | 1 | 4  | 35.974               |
| 2.2725        | 7                                    | 1  | 0 | 5  | 39.628               |
| 2.2623        | 7                                    | 2  | 1 | 3  | 39.813               |
| 2.1572        | 62                                   | 2  | 0 | 4  | 41.842               |
| 2.0418        | 1L                                   | 0  | 0 | 6  | 44.328               |
| 2.0274        | 1L                                   | 2  | 2 | 2  | 44.661               |
| 1.9985        | 6                                    | 3  | 0 | 1  | 45.341               |
| 1.8445        | 18                                   | 1  | 1 | 6  | 49.369               |
| 1.8338        | 30                                   | 3  | 1 | 2  | 49.675               |
| 1.8200        | 4                                    | 2  | 1 | 5  | 50.079               |
| 1.7591        | 2                                    | 2  | 2 | 4  | 51.939               |
| 1.6820        | 1L                                   | 1  | 0 | 7  | 54.513               |
| 1.6698        | 1L                                   | 3  | 2 | 1  | 54.945               |
| 1.6280        | 1L                                   | 3  | 1 | 4  | 56.478               |
| 1.5580        | 5                                    | 3  | 2 | 3  | 59.261               |
| 1.5317        | 3                                    | 0  | 0 | 8  | 60.387               |
| 1.5194        | 5                                    | 4  | 0 | 0  | 60.924               |
| 1.4801        | 2                                    | 2  | 2 | 6  | 62.725               |
| 1.4716        | 2                                    | 2  | 1 | 7  | 63.125               |
| 1.4635        | 1L                                   | 4  | 1 | 1  | 63.516               |
| 1.3996        | 10                                   | 3  | 1 | 6  | 66.783               |
| 1.3889        | 8                                    | 3  | 2 | 5  | 67.370               |
| 1.3863        | 3                                    | 4  | 1 | 3  | 67.512               |
| 1.3681        | 1                                    | 2  | 0 | 8  | 68.530               |
| 1.3610        | 1L                                   | 4  | 0 | 4  | 68.942               |
| 1.3286        | 1L                                   | 1  | 0 | 9  | 70.868               |
| 1.3245        | 2                                    | 3  | 0 | 7  | 71.121               |
| 1.2630        | 2                                    | 4  | 1 | 5  | 75.165               |
| 1.2472        | 6                                    | 2  | 2 | 8  | 76.287               |
| 1.2422        | 9                                    | 4  | 2 | 4  | 76.650               |
| 1.2173        | 1                                    | 2  | 1 | 9  | 78.513               |
| 1.2141        | 1                                    | 3  | 2 | 7  | 78.758               |
| 1.2096        | 1                                    | 4  | 3 | 1  | 79.107               |
| 1.1783        | 2                                    | 1  | 1 | 10 | 81.646               |
| 1.1728        | 3                                    | 3  | 3 | 6  | 82.112               |
| 1.1700        | 5                                    | 5  | 1 | 2  | 82.352               |

Copper Mercury Iodide,  $\beta\text{-Cu}_2\text{HgI}_4$  - (continued)

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

Europium Oxide, Eu<sub>2</sub>O<sub>3</sub>

Synonym

Europium sesquioxide

CAS registry no.  
1308-96-9

Sample

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

Color

Colorless

Structure

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

Crystallographic constants of this sample

$a = 10.8683(2)$  Å

$Z = 16$

$V = 1283.76$  Å<sup>3</sup>

Density (calc) = 7.283 g/cm<sup>3</sup>

Figure of merit

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

Polymorphism

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

Additional patterns

PDF card 12-393 (General Electric, ANP Dept., Cincinnati, OH)

PDF card 32-380 (Ferguson, I. and Hughes, UK Atomic Energy Authority. See UKAEA Report ND-R-150 (S). Gives  $a$  as 1/2 of value used here.)

References

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

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

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

| CuKα <sub>1</sub> λ = 1.540598 Å; temp. 26±1 °C<br>Internal standard W, a = 3.16524 Å |                  |     |   |   |        |
|---|------------------|-----|---|---|--------|
| d(Å)  | I <sup>rel</sup> | hkl |   |   | 2θ(°)  |
| $\sigma = \pm 1$  |                  |     |   |   |        |
| 4.436   | 8                | 2   | 1 | 1 | 19.998 |
| 3.138   | 100              | 2   | 2 | 2 | 28.422 |
| 2.904   | 2                | 3   | 2 | 1 | 30.760 |
| 2.718   | 34               | 4   | 0 | 0 | 32.927 |
| 2.5624  | 6                | 4   | 1 | 1 | 34.990 |
| 2.4314  | 1                | 4   | 2 | 0 | 36.940 |
| 2.3174  | 5                | 3   | 3 | 2 | 38.829 |
| 2.2193  | 1L               | 4   | 2 | 2 | 40.619 |
| 2.1319  | 8                | 4   | 3 | 1 | 42.363 |
| 1.9844  | 3                | 5   | 2 | 1 | 45.683 |
| 1.9215  | 43               | 4   | 4 | 0 | 47.267 |
| 1.8641  | 2                | 4   | 3 | 3 | 48.815 |
| 1.8116  | 1L               | 6   | 0 | 0 | 50.326 |
| 1.7632  | 6                | 6   | 1 | 1 | 51.809 |
| 1.7186  | 1                | 6   | 2 | 0 | 53.257 |
| 1.6772  | 4                | 5   | 4 | 1 | 54.682 |
| 1.6387  | 31               | 6   | 2 | 2 | 56.078 |
| 1.6027  | 6                | 6   | 3 | 1 | 57.453 |
| 1.5688  | 6                | 4   | 4 | 4 | 58.813 |
| 1.5372  | 2                | 5   | 4 | 3 | 60.144 |
| 1.5072  | 1                | 6   | 4 | 0 | 61.473 |
| 1.4794  | 3                | 7   | 2 | 1 | 62.756 |
| 1.4527  | 1                | 6   | 4 | 2 | 64.045 |
| 1.3803  | 2                | 6   | 5 | 1 | 67.844 |
| 1.3586  | 4                | 8   | 0 | 0 | 69.081 |
| 1.3379  | 3                | 7   | 4 | 1 | 70.303 |
| 1.3181  | 2                | 8   | 2 | 0 | 71.521 |
| 1.2990  | 2                | 6   | 5 | 3 | 72.737 |
| 1.2809  | 1                | 6   | 6 | 0 | 73.939 |
| 1.2636  | 3                | 8   | 3 | 1 | 75.124 |
| 1.2468  | 8                | 6   | 6 | 2 | 76.312 |
| 1.2152  | 6                | 8   | 4 | 0 | 78.678 |
| 1.2002  | 1L               | 8   | 3 | 3 | 79.855 |
| 1.1860  | 1L               | 8   | 4 | 2 | 81.010 |
| 1.1722  | 2                | 7   | 6 | 1 | 82.164 |
| 1.1457  | 2                | 8   | 5 | 1 | 84.498 |
| 1.1211  | 2                | 9   | 3 | 2 | 86.801 |
| 1.1093  | 5                | 8   | 4 | 4 | 87.963 |
| 1.0981  | 2                | 9   | 4 | 1 | 89.095 |
| 1.0870  | 1                | 8   | 6 | 0 | 90.255 |

Europium Oxide, Eu<sub>2</sub>O<sub>3</sub> - (continued)

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

Europium Oxide, Eu<sub>2</sub>O<sub>3</sub>

Synonym

Europium sesquioxide

CAS registry no.

1308-96-9

Sample

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

Color

Colorless

Structure

Monoclinic, Roth and Schneider (1960). Its aspect C\*/\* was assumed to be the same as that of Sm<sub>2</sub>O<sub>3</sub> determined by Douglass and Staritzky (1956).

Crystallographic constants of this sample

a = 14.1126(12) Å

b = 3.6025(3)

c = 8.8089(4)

β = 100.050(6)°

a/b = 3.9174

c/b = 2.4452

Z = 6

V = 440.98 Å<sup>3</sup>

Density (calc) = 7.951 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 62.1(0.0070, 69)

Polymorphism

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

Additional pattern

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

References

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

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

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

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 25.3 °C<br>Internal standard W, a = 3.16524 Å |                  |     |   |   |        |
|--|------------------|-----|---|---|--------|
| d(Å)   | I <sup>rel</sup> | hkℓ |   |   | 2θ(°)  |
| σ = ±3   |                  |     |   |   |        |
| 5.953  | 4                | -2  | 0 | 1 | 14.869 |
| 5.014  | 1L               | 2   | 0 | 1 | 17.676 |
| 4.003  | 8                | -2  | 0 | 2 | 22.192 |
| 3.419  | 18               | 2   | 0 | 2 | 26.042 |
| 3.187  | 83               | 1   | 1 | 1 | 27.971 |
| 3.046  | 85               | 4   | 0 | 1 | 29.297 |
| 2.977  | 87               | -4  | 0 | 2 | 29.996 |
| 2.891  | 58               | 0   | 0 | 3 | 30.906 |
| 2.844  | 89               | 3   | 1 | 0 | 31.432 |
| 2.778  | 100              | -1  | 1 | 2 | 32.196 |
| 2.662  | 4                | 1   | 1 | 2 | 33.642 |
| 2.5179   | 2                | 2   | 0 | 3 | 35.628 |
| 2.3162   | 16               | 6   | 0 | 0 | 38.850 |
| 2.2756   | 6                | -1  | 1 | 3 | 39.571 |
| 2.2072   | 26               | -5  | 1 | 1 | 40.852 |
| 2.1800M  | 9                | -2  | 0 | 4 | 41.385 |
| 2.1800M  |                  | 1   | 1 | 3 | 41.385 |
| 2.1459M  | 56               | 6   | 0 | 1 | 42.072 |
| 2.1459M  |                  | -3  | 1 | 3 | 42.072 |
| 2.0662   | 1                | 5   | 1 | 1 | 43.778 |
| 2.0534   | 1L               | 4   | 0 | 3 | 44.064 |
| 1.9739   | 2                | 2   | 0 | 4 | 45.940 |
| 1.9267   | 56               | 3   | 1 | 3 | 47.132 |
| 1.8804   | 4                | -5  | 1 | 3 | 48.366 |
| 1.8614   | 4                | 5   | 1 | 2 | 48.892 |
| 1.8213   | 3                | -3  | 1 | 4 | 50.042 |
| 1.8014   | 32               | 0   | 2 | 0 | 50.632 |
| 1.7635M  | 17               | 0   | 2 | 1 | 51.799 |
| 1.7635M  |                  | -8  | 0 | 1 | 51.799 |
| 1.7425   | 1L               | -6  | 0 | 4 | 52.472 |
| 1.7061   | 39               | -7  | 1 | 2 | 53.679 |
| 1.6729   | 19               | -4  | 0 | 5 | 54.834 |
| 1.6635M  | 17               | -5  | 1 | 4 | 55.168 |
| 1.6635M  |                  | 0   | 2 | 2 | 55.168 |
| 1.6563   | 34               | 7   | 1 | 1 | 55.429 |
| 1.6443   | 7                | 5   | 1 | 3 | 55.868 |
| 1.6410   | 7                | 3   | 1 | 4 | 55.993 |
| 1.6178   | 4                | 2   | 0 | 5 | 56.866 |
| 1.5939   | 4                | 2   | 2 | 2 | 57.801 |
| 1.5809   | 18               | -1  | 1 | 5 | 58.322 |
| 1.5569   | 6                | -3  | 1 | 5 | 59.308 |
| 1.5504   | 23               | 4   | 2 | 1 | 59.580 |
| 1.5412   | 24               | -4  | 2 | 2 | 59.975 |
| 1.5289   | 18               | 0   | 2 | 3 | 60.507 |
| 1.5232M  | 14               | 8   | 0 | 2 | 60.758 |

Europium Oxide, Eu<sub>2</sub>O<sub>3</sub> - (continued)

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

# Hafnium Oxide, $\text{HfO}_2$

CAS registry no.  
12055-23-1

### Sample

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

Color  
Colorless

### Structure

Monoclinic,  $P2_1/a$  (14), isostructural with  $\text{ZrO}_2$  (Geller and Corenzwit, 1953). The structure of  $\text{ZrO}_2$  was redetermined by McCullough and Trueblood (1959) and Adams and Rogers (1959).

### Crystallographic constants of this sample

$a = 5.2851(2)$  Å  
 $b = 5.1819(2)$   
 $c = 5.1157(2)$   
 $\beta = 99.259(3)^\circ$

$a/b = 1.0199$

$c/b = 0.9872$

$Z = 4$

$V = 138.28$  Å<sup>3</sup>

Density (calc) = 10.111 g/cm<sup>3</sup>

### Figure of merit

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

### Polymorphism

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

### Additional pattern

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

### References

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

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

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

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

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

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

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

| CuK $\alpha_1$ $\lambda = 1.540598$ Å; mean T = 25.4 °C |                  |       |   |       |        |
|---|------------------|-------|---|-------|--------|
| Internal standards Ag, a = 4.08651 Å                    |                  |       |   |       |        |
| Fluorophlogopite, SRM 675                               |                  |       |   |       |        |
| d(Å)  | I <sup>rel</sup> | $hkl$ |   | 2θ(°) |        |
| $\sigma = \pm 1$  |                  |       |   |       |        |
| 5.051   | 6                | 0     | 0 | 1     | 17.544 |
| 3.677   | 16               | 1     | 1 | 0     | 24.185 |
| 3.616   | 12               | 0     | 1 | 1     | 24.597 |
| 3.147   | 100              | -1    | 1 | 1     | 28.336 |
| 2.823   | 78               | 1     | 1 | 1     | 31.665 |
| 2.6080  | 25               | 2     | 0 | 0     | 34.358 |
| 2.5907  | 20               | 0     | 2 | 0     | 34.595 |
| 2.5244  | 23               | 0     | 0 | 2     | 35.534 |
| 2.4870  | 7                | -2    | 0 | 1     | 36.086 |
| 2.3204  | 9                | 1     | 2 | 0     | 38.776 |
| 2.3050  | 1                | 0     | 2 | 1     | 39.046 |
| 2.2690  | 1L               | 0     | 1 | 2     | 39.691 |
| 2.2423  | 2                | -2    | 1 | 1     | 40.185 |
| 2.2010  | 15               | -1    | 1 | 2     | 40.971 |
| 2.1792  | 5                | 2     | 0 | 1     | 41.401 |
| 2.1678  | 5                | -1    | 2 | 1     | 41.628 |
| 2.0088  | 5                | 2     | 1 | 1     | 45.096 |
| 1.9803  | 7                | -2    | 0 | 2     | 45.783 |
| 1.8494  | 3                | -2    | 1 | 2     | 49.230 |
| 1.8379  | 18               | 2     | 2 | 0     | 49.559 |
| 1.8079  | 23               | 0     | 2 | 2     | 50.436 |
| 1.7936  | 12               | -2    | 2 | 1     | 50.868 |
| 1.7727  | 6                | -1    | 2 | 2     | 51.513 |
| 1.6834M   | 12               | 2     | 0 | 2     | 54.461 |
| 1.6834M   |                  | 0     | 0 | 3     | 54.461 |
| 1.6673  | 1                | 2     | 2 | 1     | 55.032 |
| 1.6483  | 13               | 3     | 1 | 0     | 55.722 |
| 1.6431  | 10               | -3    | 1 | 1     | 55.914 |
| 1.6342  | 9                | 0     | 3 | 1     | 56.246 |
| 1.6006+   | 9                | 0     | 1 | 3     | 57.535 |
| 1.6006+   |                  | -1    | 1 | 3     | 57.535 |
| 1.5833  | 7                | -1    | 3 | 1     | 58.225 |
| 1.5732  | 5                | -2    | 2 | 2     | 58.635 |
| 1.5370  | 9                | 1     | 3 | 1     | 60.155 |
| 1.5306  | 9                | -2    | 0 | 3     | 60.433 |
| 1.5009  | 6                | 3     | 1 | 1     | 61.759 |
| 1.4881  | 8                | -3    | 1 | 2     | 62.350 |
| 1.4687  | 11               | 1     | 1 | 3     | 63.265 |
| 1.4439  | 2                | 3     | 2 | 0     | 64.484 |
| 1.4401M   | 3                | 2     | 3 | 0     | 64.676 |
| 1.4401M   |                  | -3    | 2 | 1     | 64.676 |
| 1.4252  | 1                | 0     | 3 | 2     | 65.433 |
| 1.4184  | 3                | -2    | 3 | 1     | 65.784 |
| 1.4118M   | 9                | 2     | 2 | 2     | 66.133 |
| 1.4118M   |                  | 0     | 2 | 3     | 66.133 |
| 1.4083  | 4                | -1    | 3 | 2     | 66.318 |
| 1.3537  | 3                | 2     | 3 | 1     | 69.367 |
| 1.3414  | 1                | 3     | 2 | 1     | 70.094 |
| 1.3325  | 1                | -3    | 2 | 2     | 70.634 |
| 1.3181M   | 4                | 1     | 2 | 3     | 71.520 |

Hafnium Oxide, HfO<sub>2</sub> - (continued)

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

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

# Iron Niobium Oxide, $\text{Fe}(\text{NbO}_3)_2$

## Synonyms

Iron niobate  
Ferrous niobate

CAS registry no.  
12022-59-2

## Sample

The sample was prepared according to the paper by Turnock (1966). Stoichiometric amounts of  $\text{Fe}_2\text{O}_3$  and  $\text{Nb}_2\text{O}_5$  were mixed and heated in a platinum boat (presaturated with Fe by heating a sample of  $\text{FeNb}_2\text{O}_6$  under the same conditions as in the synthesis). Two heatings in the 1130-1160 °C range in a controlled atmosphere with the partial pressure of oxygen less than or equal to  $10^{-14}$  atm. The sample contains a trace of  $\text{NbO}_2$ .

## Color

Black

## Structure

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

## Crystallographic constants of this sample

$a = 5.7350(3)$  Å

$b = 14.2688(7)$

$c = 5.0504(3)$

$a/b = 0.4019$

$c/b = 0.3539$

$Z = 4$

$V = 413.29$  Å<sup>3</sup>

Density (calc) = 5.427 g/cm<sup>3</sup>

## Figure of merit

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

## Additional pattern

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

## References

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

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

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

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

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 26.8 °C |                  |     |    |   |        |
|--|------------------|-----|----|---|--------|
| Internal standard Si, SRM 640a                     |                  |     |    |   |        |
| d(Å)   | I <sup>rel</sup> | hkl |    |   | 2θ(°)  |
| $\sigma = \pm 2$                                   |                  |     |    |   |        |
| 7.14   | 4                | 0   | 2  | 0 | 12.394 |
| 5.319  | 1                | 1   | 1  | 0 | 16.655 |
| 3.661M   | 38               | 1   | 1  | 1 | 24.290 |
| 3.661M   |                  | 1   | 3  | 0 | 24.290 |
| 3.567  | 5                | 0   | 4  | 0 | 24.944 |
| 2.965  | 100              | 1   | 3  | 1 | 30.118 |
| 2.868  | 11               | 2   | 0  | 0 | 31.164 |
| 2.662  | 1                | 2   | 2  | 0 | 33.642 |
| 2.526  | 14               | 0   | 0  | 2 | 35.510 |
| 2.495  | 14               | 2   | 0  | 1 | 35.972 |
| 2.379M   | 7                | 0   | 2  | 2 | 37.790 |
| 2.379M   |                  | 0   | 6  | 0 | 37.790 |
| 2.354  | 1L               | 2   | 2  | 1 | 38.196 |
| 2.2302   | 4                | 0   | 3  | 2 | 40.411 |
| 2.2088   | 8                | 2   | 3  | 1 | 40.820 |
| 2.0790   | 10               | 1   | 3  | 2 | 43.495 |
| 2.0613   | 2                | 0   | 4  | 2 | 43.887 |
| 2.0438   | 2                | 2   | 4  | 1 | 44.283 |
| 1.9212   | 1L               | 1   | 7  | 0 | 47.274 |
| 1.8952M  | 8                | 2   | 0  | 2 | 47.964 |
| 1.8952M  |                  | 3   | 1  | 0 | 47.964 |
| 1.8307M  | 8                | 2   | 2  | 2 | 49.765 |
| 1.8307M  |                  | 2   | 6  | 0 | 49.765 |
| 1.7957M  | 2                | 1   | 5  | 2 | 50.805 |
| 1.7957M  |                  | 1   | 7  | 1 | 50.805 |
| 1.7740M  | 14               | 3   | 1  | 1 | 51.471 |
| 1.7740M  |                  | 3   | 3  | 0 | 51.471 |
| 1.7315   | 17               | 0   | 6  | 2 | 52.829 |
| 1.7211   | 22               | 2   | 6  | 1 | 53.175 |
| 1.6738M  | 2                | 2   | 4  | 2 | 54.801 |
| 1.6738M  |                  | 3   | 3  | 1 | 54.801 |
| 1.6052   | 1L               | 1   | 1  | 3 | 57.355 |
| 1.5294M  | 14               | 1   | 3  | 3 | 60.485 |
| 1.5294M  |                  | 1   | 7  | 2 | 60.485 |
| 1.5155M  | 1L               | 3   | 1  | 2 | 61.101 |
| 1.5155M  |                  | 3   | 5  | 1 | 61.101 |
| 1.4821   | 5                | 2   | 6  | 2 | 62.631 |
| 1.4625   | 12               | 1   | 9  | 1 | 63.563 |
| 1.4517M  | 18               | 2   | 0  | 3 | 64.094 |
| 1.4517M  |                  | 3   | 3  | 2 | 64.094 |
| 1.4338   | 2                | 4   | 0  | 0 | 64.995 |
| 1.4271   | 1L               | 0   | 10 | 0 | 65.337 |
| 1.4231   | 1L               | 2   | 2  | 3 | 65.544 |
| 1.3946   | 1                | 3   | 7  | 0 | 67.056 |
| 1.3792   | 5                | 4   | 0  | 1 | 67.905 |

Iron Niobium Oxide,  $\text{Fe}(\text{NbO}_3)_2$ - (continued)

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

# Iron Niobium Oxide, $\text{Fe}_4\text{Nb}_2\text{O}_9$

## Synonym

Iron niobate

## Sample

The sample was prepared by blending  $\text{Fe}^2\text{Nb}_2\text{O}_6$  with  $\text{Fe}_2\text{O}_3$  in the appropriate molar ratio. The mixture was heated in an iron boat at 1160 °C for 8 hours, in a controlled atmosphere with the partial pressure of oxygen less than or equal to  $10^{-16}$  atm. The product was essentially single phase and contained only a trace of  $\text{Fe}^2\text{Nb}_2\text{O}_6$  as a second phase.

## Color

Colorless

## Structure

Hexagonal,  $P6/***$ ,  $Z = 2$ , isostructural with  $\text{Co}_4\text{Nb}_2\text{O}_9$  (Bertaut et al., 1960).

## Crystallographic constants of this sample

$$a = 5.2253(2) \text{ \AA}$$

$$c = 14.2070(8)$$

$$c/a = 2.7189$$

$$Z = 2$$

$$V = 335.94 \text{ \AA}^3$$

$$\text{Density (calc)} = 5.469 \text{ g/cm}^3$$

## Figure of merit

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

## Reference

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 27.6 °C |     |                  |       |                      |
|--|-----|------------------|-------|----------------------|
| Internal standards W, $a = 3.16524 \text{ \AA}$                    |     |                  |       |                      |
| Fluorophlogopite, SRM 675  |     |                  |       |                      |
| $d(\text{\AA})$  |     | $I^{\text{rel}}$ | $hkl$ | $2\theta (\text{°})$ |
| $\sigma = \pm 2$   |     |                  |       |                      |
| 7.12   | 1   | 0 0 2            |       | 12.428               |
| 4.524  | 20  | 1 0 0            |       | 19.605               |
| 3.818  | 23  | 1 0 2            |       | 23.282               |
| 3.553  | 2   | 0 0 4            |       | 25.040               |
| 2.793  | 100 | 1 0 4            |       | 32.019               |
| 2.611  | 72  | 1 1 0            |       | 34.314               |
| 2.368  | 3   | 0 0 6            |       | 37.961               |
| 2.287  | 12  | 1 1 3            |       | 39.369               |
| 2.263  | 2   | 2 0 0            |       | 39.801               |
| 2.1557   | 2   | 2 0 2            |       | 41.873               |
| 2.1045   | 2   | 1 1 4            |       | 42.941               |
| 2.0979   | 2   | 1 0 6            |       | 43.083               |
| 1.9084   | 29  | 2 0 4            |       | 47.612               |
| 1.7753   | 4   | 0 0 8            |       | 51.432               |
| 1.7540   | 31  | 1 1 6            |       | 52.101               |

| $d(\text{\AA})$ | $I^{\text{rel}}$ | $hkl$            |   |    | $2\theta (\text{°})$ |
|-----------------|------------------|------------------|---|----|----------------------|
|                 |                  | $\sigma = \pm 2$ |   |    |                      |
| 1.7108          | 2                | 2                | 1 | 0  | 53.520               |
| 1.6630          | 3                | 2                | 1 | 2  | 55.187               |
| 1.6530          | 7                | 1                | 0 | 8  | 55.552               |
| 1.6362          | 1                | 2                | 0 | 6  | 56.172               |
| 1.5413          | 23               | 2                | 1 | 4  | 59.972               |
| 1.5087          | 21               | 3                | 0 | 0  | 61.405               |
| 1.4684          | 2                | 1                | 1 | 8  | 63.279               |
| 1.3973          | 3                | 2                | 0 | 8  | 66.911               |
| 1.3886          | 3                | 3                | 0 | 4  | 67.385               |
| 1.3555          | 8                | 1                | 0 | 10 | 69.261               |
| 1.3065          | 4                | 2                | 2 | 0  | 72.255               |
| 1.2721          | 2                | 3                | 0 | 6  | 74.531               |
| 1.2594          | 1                | 2                | 2 | 3  | 75.419               |
| 1.2553          | 1L               | 3                | 1 | 0  | 75.704               |
| 1.2360          | 2                | 3                | 1 | 2  | 77.103               |
| 1.2322          | 3                | 2                | 1 | 8  | 77.388               |
| 1.2032          | 4                | 2                | 0 | 10 | 79.617               |
| 1.1835          | 6                | 3                | 1 | 4  | 81.216               |
| 1.1496          | 1                | 3                | 0 | 8  | 84.143               |
| 1.1440          | 4                | 2                | 2 | 6  | 84.655               |
| 1.1316          | 1L               | 4                | 0 | 0  | 85.800               |
| 1.0929M         | 4                | 2                | 1 | 10 | 89.626               |
| 1.0929M         |                  | 0                | 0 | 13 | 89.626               |
| 1.0781          | 2                | 4                | 0 | 4  | 91.206               |
| 1.0522          | 1L               | 2                | 2 | 8  | 94.120               |
| 1.0270          | 1L               | 3                | 2 | 2  | 97.185               |
| 1.0251          | 1                | 3                | 1 | 8  | 97.426               |
| .9965           | 3                | 3                | 2 | 4  | 101.247              |
| .9903           | 2                | 1                | 0 | 14 | 102.129              |
| .9875           | 4                | 4                | 1 | 0  | 102.524              |
| .9541           | 1                | 4                | 0 | 8  | 107.679              |
| .9508           | 1                | 3                | 2 | 6  | 108.215              |
| .9460           | 1                | 1                | 1 | 14 | 109.033              |
| .9407           | 3                | 3                | 1 | 10 | 109.944              |
| .9260           | 2                | 2                | 0 | 14 | 112.582              |
| .9114           | 3                | 4                | 1 | 6  | 115.386              |
| .8962           | 1L               | 3                | 2 | 8  | 118.532              |
| .8849M          | 1L               | 4                | 0 | 10 | 121.021              |
| .8849M          |                  | 3                | 0 | 13 | 121.021              |
| .8770           | 1L               | 5                | 0 | 4  | 122.887              |
| .8727           | 2                | 2                | 1 | 14 | 123.940              |
| .8709           | 3                | 3                | 3 | 0  | 124.382              |
| .8629           | 1L               | 4                | 1 | 8  | 126.414              |

# Iron Silicate (Fayalite), $\text{Fe}_2\text{SiO}_4$

## Synonym

Ferrous orthosilicate

## Sample

The sample was prepared by grinding together equimolar parts of  $\text{Fe}_2\text{O}_3$  and  $\text{SiO}_2$  under acetone. After drying, the specimen was transferred to a high purity iron boat. It was heated twice for 8 hours each time in a controlled atmosphere with the partial pressure of oxygen less than or equal to  $10^{-20}$  atm, first at  $1110^\circ\text{C}$  and then at  $1150^\circ\text{C}$ .

## Color

Grayish olive

## Structure

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

## Crystallographic constants of this sample

$$a = 6.0902(5) \text{ \AA}$$

$$b = 10.4805(8)$$

$$c = 4.8215(5)$$

$$a/b = 0.5811$$

$$c/b = 0.4600$$

$$Z = 4$$

$$V = 307.75 \text{ \AA}^3$$

$$\text{Density (calc)} = 4.398 \text{ g/cm}^3$$

## Figure of merit

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

## Polymorphism

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

## Additional patterns

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

## References

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

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$ ; temp. $26 \pm 1^\circ\text{C}$<br>Internal standard W, $a = 3.16524 \text{ \AA}$ |                                      |       |   |   |                           |
|--|--------------------------------------|-------|---|---|---------------------------|
| $d(\text{\AA})$  | $I^{\text{rel}}$<br>$\sigma = \pm 3$ | $hkl$ |   |   | $2\theta (\text{)}^\circ$ |
|  |                                      | 0     | 2 | 0 |                           |
| 5.242  | 6                                    | 0     | 2 | 0 | 16.901                    |
| 4.380  | 9                                    | 0     | 1 | 1 | 20.257                    |
| 3.974  | 11                                   | 1     | 2 | 0 | 22.353                    |
| 3.783  | 7                                    | 1     | 0 | 1 | 23.496                    |
| 3.556  | 55                                   | 1     | 1 | 1 | 25.019                    |
| 3.064  | 6                                    | 1     | 2 | 1 | 29.123                    |
| 3.046  | 7                                    | 2     | 0 | 0 | 29.295                    |
| 2.829  | 86                                   | 0     | 3 | 1 | 31.599                    |
| 2.633  | 32                                   | 2     | 2 | 0 | 34.020                    |
| 2.619  | 23                                   | 0     | 4 | 0 | 34.205                    |
| 2.565  | 45                                   | 1     | 3 | 1 | 34.952                    |
| 2.500  | 100                                  | 2     | 1 | 1 | 35.893                    |
| 2.407  | 25                                   | 1     | 4 | 0 | 37.331                    |
| 2.351  | 10                                   | 0     | 1 | 2 | 38.259                    |
| 2.311  | 23                                   | 2     | 2 | 1 | 38.949                    |
| 2.303  | 21                                   | 0     | 4 | 1 | 39.073                    |
| 2.193  | 9                                    | 1     | 1 | 2 | 41.134                    |
| 2.1532   | 7                                    | 1     | 4 | 1 | 41.923                    |
| 2.0723   | 8                                    | 2     | 3 | 1 | 43.643                    |
| 1.9855M  | 5                                    | 2     | 4 | 0 | 45.655                    |
| 1.9855M  |                                      | 0     | 3 | 2 | 45.655                    |
| 1.9220   | 5                                    | 0     | 5 | 1 | 47.253                    |
| 1.8418   | 12                                   | 3     | 1 | 1 | 49.446                    |
| 1.8327   | 10                                   | 1     | 5 | 1 | 49.709                    |
| 1.7781   | 79                                   | 2     | 2 | 2 | 51.343                    |
| 1.7735   | 65                                   | 0     | 4 | 2 | 51.486                    |
| 1.7624   | 6                                    | 3     | 2 | 1 | 51.834                    |
| 1.7032   | 13                                   | 1     | 4 | 2 | 53.779                    |
| 1.6789   | 15                                   | 1     | 6 | 0 | 54.621                    |
| 1.6496   | 17                                   | 3     | 3 | 1 | 55.674                    |
| 1.6253   | 17                                   | 2     | 5 | 1 | 56.581                    |
| 1.6044   | 9                                    | 3     | 4 | 0 | 57.386                    |
| 1.5885   | 6                                    | 0     | 1 | 3 | 58.014                    |
| 1.5367M  | 11                                   | 0     | 2 | 3 | 60.166                    |
| 1.5367M  |                                      | 1     | 1 | 3 | 60.166                    |
| 1.5331   | 10                                   | 2     | 4 | 2 | 60.326                    |
| 1.5225M  | 26                                   | 4     | 0 | 0 | 60.789                    |
| 1.5225M  |                                      | 3     | 4 | 1 | 60.789                    |
| 1.5151   | 31                                   | 2     | 6 | 0 | 61.115                    |
| 1.4896M  | 3                                    | 1     | 2 | 3 | 62.276                    |

Iron Silicate (Fayalite), Fe<sub>2</sub>SiO<sub>4</sub> - (continued)

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

# Iron Titanium Oxide (Ulvöspinel), $\text{Fe}_2\text{TiO}_4$

**Synonym**

Iron titanate

**CAS registry no.**

12434-86-5

**Sample**

The sample was prepared from stoichiometric amounts of  $\text{Fe}_2\text{O}_3$  and  $\text{TiO}_2$ , blended in an agate mortar. The mixture was dried and transferred to a high-purity iron boat for heat treatments. All heatings were done in a controlled atmosphere at an oxygen partial pressure of  $10^{-18}$  atmosphere or lower. Three heatings, 1140 °C for 8 hours, 1150 °C for 8 hours, and 1200 °C for 8 hours were sufficient to yield a single phase, well crystallized product.

**Color**

Dark gray

**Structure**

Cubic,  $\text{Fd}3m$  (227), isostructural with spinel,  $\text{MgAl}_2\text{O}_4$  (Barth and Posnjak, 1932). The structure was refined by Forster and Hall (1965) by neutron diffraction methods.

**Crystallographic constants of this sample**

$a = 8.53520(12)$  Å

$Z = 8$

$V = 621.786 \text{ } \text{\AA}^3$

Density (calc) = 4.777 g/cm<sup>3</sup>

**Figure of merit**

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

**Additional patterns**

PDF card 24-537 (Ashworth, Dept. of Geology, Univ. of Durham, U.K.)

Forster and Hall (1965)  
Pouillard (1950)

**References**

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

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $26 \pm 1$ °C<br>Internal standards W, a = 3.16524 $\text{\AA}$<br>Fluorophlogopite, SRM 675 |                                      |       |   |   |                      |
|--|--------------------------------------|-------|---|---|----------------------|
| $d(\text{\AA})$  | $I^{\text{rel}}$<br>$\sigma = \pm 2$ | $hkl$ |   |   | $2\theta (\text{°})$ |
| 4.924  | 8                                    | 1     | 1 | 1 | 18.002               |
| 3.018  | 33                                   | 2     | 2 | 0 | 29.573               |
| 2.573  | 100                                  | 3     | 1 | 1 | 34.837               |
| 2.4640   | 6                                    | 2     | 2 | 2 | 36.434               |
| 2.1339   | 19                                   | 4     | 0 | 0 | 42.321               |
| 1.7419   | 10                                   | 4     | 2 | 2 | 52.490               |
| 1.6426   | 33                                   | 5     | 1 | 1 | 55.932               |
| 1.5089   | 39                                   | 4     | 4 | 0 | 61.395               |
| 1.4427   | 1                                    | 5     | 3 | 1 | 64.545               |
| 1.3495   | 3                                    | 6     | 2 | 0 | 69.615               |
| 1.3016   | 7                                    | 5     | 3 | 3 | 72.572               |
| 1.2867   | 3                                    | 6     | 2 | 2 | 73.551               |
| 1.2318   | 2                                    | 4     | 4 | 4 | 77.413               |
| 1.1952   | 1L                                   | 7     | 1 | 1 | 80.255               |
| 1.1406   | 3                                    | 6     | 4 | 2 | 84.960               |
| 1.1111   | 8                                    | 7     | 3 | 1 | 87.782               |
| 1.0669   | 2                                    | 8     | 0 | 0 | 92.435               |
| 1.0059   | 1                                    | 6     | 6 | 0 | 99.948               |
| .9856  | 5                                    | 7     | 5 | 1 | 102.805              |
| .9792  | 2                                    | 6     | 6 | 2 | 103.754              |
| .9543  | 2                                    | 8     | 4 | 0 | 107.649              |
| .9369  | 1L                                   | 7     | 5 | 3 | 110.606              |
| .9099  | 1L                                   | 6     | 6 | 4 | 115.689              |
| .8947  | 4                                    | 9     | 3 | 1 | 118.843              |
| .8711  | 10                                   | 8     | 4 | 4 | 124.332              |
| .8578  | 1L                                   | 7     | 7 | 1 | 127.778              |
| .8370  | 2                                    | 10    | 2 | 0 | 133.953              |
| .8251  | 4                                    | 7     | 7 | 3 | 138.003              |
| .8212  | 2                                    | 10    | 2 | 2 | 139.428              |
| .7959  | 1L                                   | 9     | 5 | 3 | 150.838              |

Lanthanum Boride, LaB<sub>6</sub>

CAS registry no.  
12008-21-8

Sample

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

Color

Purplish black

Structure

Cubic, Pm3m (221), isostructural with CaB<sub>6</sub>. The structure was determined by von Stackelburg and Neumann (1932).

Crystallographic constants of this sample

$a = 4.15690(5)$  Å

Z = 1

V = 71.830 Å<sup>3</sup>

Density (calc) = 4.711 g/cm<sup>3</sup>

Figure of merit

F<sub>24</sub> = 180.5(0.0055, 24)

Additional pattern

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

Reference

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

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 25.9 °C<br>Internal standards Ag, a = 4.08651 Å<br>Fluorophlogopite, SRM 675 |                                      |       |         |  |
|---|--------------------------------------|-------|---------|--|
| d(Å)  | I <sup>rel</sup><br>$\sigma = \pm 5$ | hkl   | 2θ(°)   |  |
| 4.158   | 54                                   | 1 0 0 | 21.354  |  |
| 2.939   | 100                                  | 1 1 0 | 30.387  |  |
| 2.3998  | 41                                   | 1 1 1 | 37.445  |  |
| 2.0780  | 22                                   | 2 0 0 | 43.517  |  |
| 1.8586  | 46                                   | 2 1 0 | 48.969  |  |
| 1.6969  | 24                                   | 2 1 1 | 53.995  |  |
| 1.4697  | 8                                    | 2 2 0 | 63.218  |  |
| 1.3853  | 23                                   | 3 0 0 | 67.564  |  |
| 1.3143  | 16                                   | 3 1 0 | 71.757  |  |
| 1.2533  | 10                                   | 3 1 1 | 75.849  |  |
| 1.2000  | 2                                    | 2 2 2 | 79.869  |  |
| 1.1529  | 6                                    | 3 2 0 | 83.849  |  |
| 1.1110  | 13                                   | 3 2 1 | 87.793  |  |
| 1.0393  | 2                                    | 4 0 0 | 95.665  |  |
| 1.0082  | 8                                    | 4 1 0 | 99.640  |  |
| .9798   | 7                                    | 4 1 1 | 103.656 |  |
| .9536   | 3                                    | 3 3 1 | 107.755 |  |
| .9295   | 4                                    | 4 2 0 | 111.940 |  |
| .9071   | 9                                    | 4 2 1 | 116.250 |  |
| .8862   | 3                                    | 3 3 2 | 120.725 |  |
| .8485   | 3                                    | 4 2 2 | 130.416 |  |
| .8314   | 3                                    | 5 0 0 | 135.794 |  |
| .8152   | 10                                   | 5 1 0 | 141.773 |  |
| .8000   | 6                                    | 5 1 1 | 148.670 |  |

# Lithium Thorium Molybdenum Oxide, $\text{Li}_4\text{Th}_7(\text{MoO}_4)_{16}$

## Synonym

Lithium thorium molybdate

## Sample

One mole of  $\text{Li}_2\text{MoO}_4$ , 3.5 moles of  $\text{ThO}_2$  and 7 moles of  $\text{MoO}_3$  were heated at 700 °C for 21 hours.

## Color

Colorless

## Structure

Cubic,  $I\bar{3}3\bar{3}$  Martel and Roth (1981). Apparently isostructural with cubic phase in the system lithium thorium tungsten oxide, Finch and Clark (1965).

## Crystallographic constants of this sample

$a = 14.4504(3)$  Å

$Z = 2$

$V = 3017.5$  Å<sup>3</sup>

Density (calc) = 4.635 g/cm<sup>3</sup>

## Figure of merit

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

## References

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

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

| CuK $\alpha_1$ λ = 1.540598 Å; temp. 26±1 °C |                  |       |  |        |
|--|------------------|-------|--|--------|
| Internal standard W, a = 3.16524 Å           |                  |       |  |        |
| d(Å)   | I <sup>rel</sup> | hkl   |  | 2θ(°)  |
| $\sigma = \pm 2$                             |                  |       |  |        |
| 5.894  | 15               | 2 1 1 |  | 15.018 |
| 5.104  | 59               | 2 2 0 |  | 17.361 |
| 4.571  | 1L               | 3 1 0 |  | 19.402 |
| 3.862  | 68               | 3 2 1 |  | 23.010 |
| 3.611  | 94               | 4 0 0 |  | 24.635 |
| 3.231  | 37               | 4 2 0 |  | 27.582 |
| 3.081  | 100              | 3 3 2 |  | 28.954 |
| 2.950  | 75               | 4 2 2 |  | 30.269 |
| 2.834  | 10               | 5 1 0 |  | 31.544 |
| 2.638  | 26               | 5 2 1 |  | 33.954 |
| 2.5561                                       | 34               | 4 4 0 |  | 35.079 |
| 2.4786                                       | 5                | 5 3 0 |  | 36.213 |
| 2.3433                                       | 8                | 6 1 1 |  | 38.383 |
| 2.2851                                       | 23               | 6 2 0 |  | 39.401 |
| 2.2306                                       | 19               | 5 4 1 |  | 40.404 |
| 2.1304                                       | 20               | 6 3 1 |  | 42.393 |
| 2.0862                                       | 5                | 4 4 4 |  | 43.336 |
| 2.0435                                       | 22               | 5 5 0 |  | 44.290 |
| 2.0037                                       | 6                | 6 4 0 |  | 45.218 |
| 1.9661                                       | 56               | 7 2 1 |  | 46.131 |

| d(Å)             | I <sup>rel</sup> | hkl    |  |  | 2θ(°)  |
|------------------|------------------|--------|--|--|--------|
| $\sigma = \pm 2$ |                  |        |  |  |        |
| 1.9308           | 43               | 6 4 2  |  |  | 47.025 |
| 1.8972           | 17               | 7 3 0  |  |  | 47.911 |
| 1.8350           | 67               | 7 3 2  |  |  | 49.642 |
| 1.8061           | 16               | 8 0 0  |  |  | 50.492 |
| 1.7787           | 20               | 7 4 1  |  |  | 51.325 |
| 1.7524           | 7                | 8 2 0  |  |  | 52.152 |
| 1.7270           | 15               | 6 5 3  |  |  | 52.979 |
| 1.7031           | 14               | 6 6 0  |  |  | 53.782 |
| 1.6797           | 30               | 7 5 0  |  |  | 54.592 |
| 1.6151           | 11               | 8 4 0  |  |  | 56.972 |
| 1.5956           | 3                | 9 1 0  |  |  | 57.732 |
| 1.5583           | 40               | 7 6 1  |  |  | 59.249 |
| 1.5407           | 8                | 6 6 4  |  |  | 59.997 |
| 1.5231           | 20               | 9 3 0  |  |  | 60.761 |
| 1.4905           | 15               | 9 3 2  |  |  | 62.237 |
| 1.4750           | 2                | 8 4 4  |  |  | 62.963 |
| 1.4598           | 10               | 7 7 0  |  |  | 63.696 |
| 1.4450           | 5                | 8 6 0  |  |  | 64.428 |
| 1.4312           | 2                | 10 1 1 |  |  | 65.123 |
| 1.4169           | 11               | 10 2 0 |  |  | 65.865 |
| 1.4036           | 3                | 9 4 3  |  |  | 66.571 |
| 1.3774           | 25               | 10 3 1 |  |  | 68.006 |
| 1.3533           | 7                | 8 7 1  |  |  | 69.386 |
| 1.3415           | 4                | 10 4 0 |  |  | 70.091 |
| 1.3299           | 26               | 10 3 3 |  |  | 70.791 |
| 1.3192           | 4                | 10 4 2 |  |  | 71.455 |
| 1.3082           | 11               | 11 1 0 |  |  | 72.149 |
| 1.2872           | 16               | 10 5 1 |  |  | 73.517 |
| 1.2771           | 3                | 8 8 0  |  |  | 74.196 |
| 1.2673           | 10               | 11 3 0 |  |  | 74.864 |
| 1.2482           | 15               | 11 3 2 |  |  | 76.215 |
| 1.2390           | 5                | 10 6 0 |  |  | 76.879 |
| 1.2299           | 14               | 11 4 1 |  |  | 77.555 |
| 1.2126           | 14               | 9 6 5  |  |  | 78.873 |
| 1.2041           | 3                | 12 0 0 |  |  | 79.543 |
| 1.1960           | 21               | 11 5 0 |  |  | 80.195 |
| 1.1878           | 5                | 12 2 0 |  |  | 80.856 |
| 1.1797           | 9                | 11 5 2 |  |  | 81.528 |
| 1.1723           | 4                | 12 2 2 |  |  | 82.158 |
| 1.1643           | 8                | 12 3 1 |  |  | 82.846 |
| 1.1497           | 11               | 11 6 1 |  |  | 84.131 |
| 1.1354           | 6                | 9 9 0  |  |  | 85.445 |
| 1.1283           | 2                | 10 8 0 |  |  | 86.107 |
| 1.1216           | 15               | 11 6 3 |  |  | 86.756 |
| 1.1150           | 2                | 10 8 2 |  |  | 87.396 |
| 1.1083           | 8                | 11 7 0 |  |  | 88.055 |
| 1.0956           | 5                | 11 7 2 |  |  | 89.350 |
| 1.0893           | 1                | 12 4 4 |  |  | 90.010 |
| 1.0832           | 5                | 13 3 0 |  |  | 90.658 |
| 1.0772           | 4                | 12 6 0 |  |  | 91.302 |
| 1.0712           | 4                | 11 6 5 |  |  | 91.959 |
| 1.0655           | 1                | 12 6 2 |  |  | 92.601 |
| 1.0597           | 12               | 11 8 1 |  |  | 93.260 |

Lithium Thorium Tungsten Oxide,  $\text{Li}_4\text{Th}_7(\text{WO}_4)_{16}$

Synonym

Lithium thorium tungstate

Sample

$\text{Li}_2\text{WO}_4$  was prepared by reacting  $\text{Li}_2\text{CO}_3$  and  $\text{WO}_3$  in equimolar proportions at 700 °C for 24 hours to form  $\text{Li}_2\text{WO}_4$ . Then  $\text{Li}_2\text{WO}_4$ ,  $\text{ThO}_2$ , and  $\text{WO}_3$  in the molar ratios of 1:3.5:7 were ground together under acetone, heated in gold to 700 °C for 48 hours with regrinding every 24 hours, then heated a further 16 hours at 700 °C, reground and heated at 750 °C for 21 hours.

Color

Colorless

Structure

Cubic,  $I\bar{3}3\bar{m}$ . Finch and Clark (1965) referred to a body-centered cubic phase of this approximate composition.

Crystallographic constants of this sample

$a = 14.4969(4)$  Å

$Z = 2$

$V = 3046.7$  Å<sup>3</sup>

Density (calc) = 6.124 g/cm<sup>3</sup>

Figure of merit

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

Reference

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

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

Lithium Thorium Tungsten Oxide,  $\text{Li}_4\text{Th}_7(\text{WO}_4)_{16}$  - (continued)

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

9

# Lithium Titanium Oxide, $\text{Li}_2\text{Ti}_3\text{O}_7$

**Synonym**

Lithium titanate

**Sample**

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

**Color**

Colorless

**Structure**

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

**Crystallographic constants of this sample**

$$a = 5.0182(4) \text{ \AA}$$

$$b = 9.5523(8)$$

$$c = 2.9455(3)$$

$$a/b = 0.5253$$

$$c/b = 0.3084$$

$$Z = 1$$

$$V = 141.19 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.170 \text{ g/cm}^3$$

**Figure of merit**

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

**Reference**

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $26 \pm 1^\circ \text{C}$ |                  |         |                       |  |
|---|------------------|---------|-----------------------|--|
| Internal standard W, $a = 3.16524 \text{ \AA}$                                    |                  |         |                       |  |
| $d(\text{\AA})$   | $I^{\text{rel}}$ | $h k l$ | $2\theta (\text{\\})$ |  |
| $\sigma = \pm 4$  |                  |         |                       |  |
| 4.777   | 3                | 0 2 0   | 18.561                |  |
| 4.440   | 100              | 1 1 0   | 19.982                |  |
| 3.461   | 9                | 1 2 0   | 25.721                |  |
| 2.688   | 46               | 1 3 0   | 33.303                |  |
| 2.541   | 3                | 1 0 1   | 35.291                |  |
| 2.507M  | 24               | 2 0 0   | 35.790                |  |
| 2.507M  |                  | 0 2 1   | 35.790                |  |
| 2.457   | 23               | 1 1 1   | 36.543                |  |
| 2.388   | 2                | 0 4 0   | 37.637                |  |
| 2.243   | 32               | 1 2 1   | 40.179                |  |
| 2.222   | 3                | 2 2 0   | 40.569                |  |
| 2.156   | 6                | 1 4 0   | 41.861                |  |
| 1.9857  | 13               | 1 3 1   | 45.651                |  |
| 1.9707  | 12               | 2 3 0   | 46.017                |  |
| 1.8554  | 3                | 0 4 1   | 49.060                |  |
| 1.7733  | 32               | 2 2 1   | 51.494                |  |
| 1.7301  | 21               | 2 4 0   | 52.878                |  |
| 1.6382  | 9                | 2 3 1   | 56.095                |  |
| 1.5923  | 1L               | 0 6 0   | 57.863                |  |
| 1.5792  | 3                | 3 2 0   | 58.389                |  |

| $d(\text{\AA})$  | $I^{\text{rel}}$ | $h k l$ | $2\theta (\text{\\})$ |
|------------------|------------------|---------|-----------------------|
| $\sigma = \pm 4$ |                  |         |                       |
| 1.5265           | 17               | 1 5 1   | 60.612                |
| 1.4917           | 2                | 2 4 1   | 62.179                |
| 1.4814           | 7                | 3 3 0   | 62.663                |
| 1.4729           | 7                | 0 0 2   | 63.067                |
| 1.4540           | 5                | 3 0 1   | 63.981                |
| 1.4380           | 14               | 3 1 1   | 64.782                |
| 1.4001           | 10               | 0 6 1   | 66.760                |
| 1.3976           | 9                | 1 1 2   | 66.895                |
| 1.3913           | 2                | 3 2 1   | 67.236                |
| 1.3697           | 2                | 3 4 0   | 68.444                |
| 1.3444           | 2                | 2 6 0   | 69.916                |
| 1.3233           | 1                | 3 3 1   | 71.198                |
| 1.3168           | 4                | 1 7 0   | 71.605                |
| 1.2914           | 6                | 1 3 2   | 73.235                |
| 1.2703           | 1                | 2 0 2   | 74.658                |
| 1.2589M          | 3                | 2 1 2   | 75.451                |
| 1.2589M          |                  | 3 5 0   | 75.451                |
| 1.2440           | 3                | 4 1 0   | 76.519                |
| 1.2418           | 3                | 3 4 1   | 76.678                |
| 1.2230           | 1                | 2 6 1   | 78.078                |
| 1.2162           | 1L               | 1 4 2   | 78.601                |
| 1.1940           | 1                | 0 8 0   | 80.354                |
| 1.1798           | 2                | 2 3 2   | 81.523                |
| 1.1617           | 1                | 1 8 0   | 83.074                |
| 1.1573           | 1                | 3 5 1   | 83.457                |
| 1.1530           | 2                | 3 6 0   | 83.837                |
| 1.1458           | 2                | 4 1 1   | 84.485                |
| 1.1216M          | 6                | 4 2 1   | 86.750                |
| 1.1216M          |                  | 2 4 2   | 86.750                |
| 1.1103M          | 1                | 4 4 0   | 87.861                |
| 1.1103M          |                  | 2 7 1   | 87.861                |
| 1.1069           | 2                | 0 8 1   | 88.200                |
| 1.0979           | 1L               | 3 1 2   | 89.108                |
| 1.0849           | 1                | 4 3 1   | 90.469                |
| 1.0781           | 2                | 2 8 0   | 91.201                |
| 1.0769           | 2                | 3 2 2   | 91.332                |
| 1.0740           | 2                | 3 6 1   | 91.648                |
| 1.0575M          | 3                | 2 5 2   | 93.511                |
| 1.0575M          |                  | 3 7 0   | 93.511                |
| 1.0488           | 1                | 4 5 0   | 94.522                |
| 1.0444           | 2                | 3 3 2   | 95.051                |
| 1.0392           | 1L               | 4 4 1   | 95.673                |
| 1.0124           | 2                | 2 8 1   | 99.082                |
| .9982            | 1                | 5 1 0   | 101.013               |

Magnesium Manganese Zinc Iron Sulfate Hydroxide Hydrate, Zincobotryogen,  
 $(\text{Zn},\text{Mg},\text{Mn})\text{Fe}(\text{SO}_4)_2(\text{OH}) \cdot 7\text{H}_2\text{O}$

**Sample**

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

**Chemical analysis**

$\text{SO}_3$ -36.03,  $\text{Fe}_2\text{O}_3$ -18.34,  $\text{MgO}$ -2.50,  $\text{FeO}$ -0.85,  $\text{MnO}$ -1.75,  $\text{ZnO}$ -11.77,  $\text{H}_2\text{O}$ +29.13, minor  $\text{H}_2\text{O}$ - $\text{Na}_2\text{O}$ ; this corresponds to the formula  $(\text{Zn}_{0.59}\text{Mg}_{0.26}\text{Mn}_{0.10}\text{Fe}_{0.05})\text{Fe}^3(\text{SO}_4)_2(\text{OH}) \cdot 7\text{H}_2\text{O}$  (Kwanchih et al., 1964).

**Color**

Deep orange

**Optical data**

Biaxial(+).  $N_{\alpha} = 1.542$ ,  $N_{\beta} = 1.551$ ,  $N_{\gamma} = 1.587$ .  $2V = 54^\circ$  (calc.). Ibid.

**Structure**

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

**Crystallographic constants of this sample**

$$a = 10.523(2) \text{ \AA}$$

$$b = 17.841(3)$$

$$c = 7.137(2)$$

$$\beta = 100.11(2)^\circ$$

$$a/b = 0.5898$$

$$c/b = 0.4000$$

$$Z = 4$$

$$V = 1310.10 \text{ \AA}^3$$

$$\text{Density (calc)} = 2.237 \text{ g/cm}^3$$

**Figure of merit**

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

**Additional pattern**

Kwanchih et al. (1964)

**References**

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

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

| $d(\text{\AA})$ | $I^{\text{rel}}$<br>$\sigma = \pm 4$ | $\frac{\text{CuK}\alpha_1}{\lambda} = 1.540598 \text{ \AA}; \text{ mean } T = 25.7^\circ \text{ C}$ |   |   | $2\theta (\text{)}^\circ$ |
|-----------------|--------------------------------------|---|---|---|---------------------------|
|                 |                                      | Internal standards Si, SRM 640a   |   |   |                           |
| 8.96            | 100                                  | 1   | 1 | 0 | 9.860                     |
| 6.76            | 8                                    | 1   | 2 | 0 | 13.090                    |
| 6.354           | 58                                   | -1  | 0 | 1 | 13.926                    |
| 5.990           | 8                                    | -1  | 1 | 1 | 14.778                    |
| 5.525           | 36                                   | 0   | 2 | 1 | 16.030                    |
| 5.395           | 28                                   | 1   | 0 | 1 | 16.419                    |
| 5.163M          | 75                                   | 1   | 1 | 1 | 17.162                    |
| 5.163M          |                                      | 1   | 3 | 0 | 17.162                    |
| 4.613           | 17                                   | 1   | 2 | 1 | 19.226                    |
| 4.538           | 29                                   | 0   | 3 | 1 | 19.544                    |
| 4.480           | 23                                   | 2   | 2 | 0 | 19.800                    |
| 4.456           | 26                                   | 0   | 4 | 0 | 19.910                    |
| 4.425           | 29                                   | -2  | 1 | 1 | 20.049                    |
| 4.340           | 40                                   | -1  | 3 | 1 | 20.447                    |
| 4.095           | 53                                   | 1   | 4 | 0 | 21.684                    |
| 3.905           | 27                                   | 2   | 3 | 0 | 22.753                    |
| 3.766           | 41                                   | 0   | 4 | 1 | 23.603                    |
| 3.655           | 9                                    | -1  | 4 | 1 | 24.333                    |
| 3.541           | 41                                   | 2   | 2 | 1 | 25.128                    |
| 3.451           | 25                                   | -1  | 1 | 2 | 25.792                    |
| 3.389           | 32                                   | 3   | 1 | 0 | 26.278                    |
| 3.343           | 19                                   | -3  | 0 | 1 | 26.640                    |
| 3.267           | 26                                   | 0   | 2 | 2 | 27.277                    |
| 3.219           | 51                                   | 3   | 2 | 0 | 27.689                    |
| 3.181M          | 17                                   | 0   | 5 | 1 | 28.030                    |
| 3.181M          |                                      | -2  | 0 | 2 | 28.030                    |
| 3.112M          | 14                                   | 1   | 1 | 2 | 28.664                    |
| 3.112M          |                                      | -1  | 5 | 1 | 28.664                    |
| 3.027M          | 61                                   | -1  | 3 | 2 | 29.485                    |
| 3.027M          |                                      | 0   | 3 | 2 | 29.485                    |
| 2.987           | 16                                   | 3   | 3 | 0 | 29.894                    |
| 2.905           | 12                                   | 3   | 0 | 1 | 30.750                    |
| 2.867           | 7                                    | 3   | 1 | 1 | 31.172                    |
| 2.858           | 6                                    | 1   | 6 | 0 | 31.269                    |
| 2.813           | 24                                   | -2  | 5 | 1 | 31.787                    |
| 2.803           | 31                                   | -2  | 3 | 2 | 31.907                    |
| 2.762M          | 52                                   | -1  | 4 | 2 | 32.384                    |
| 2.762M          |                                      | 3   | 2 | 1 | 32.384                    |
| 2.732           | 13                                   | 3   | 4 | 0 | 32.752                    |
| 2.695M          | 13                                   | 2   | 0 | 2 | 33.210                    |
| 2.695M          |                                      | -1  | 6 | 1 | 33.210                    |
| 2.673           | 15                                   | -3  | 4 | 1 | 33.502                    |
| 2.609           | 8                                    | 3   | 3 | 1 | 34.349                    |
| 2.594           | 11                                   | -3  | 2 | 2 | 34.554                    |
| 2.580M          | 14                                   | 2   | 2 | 2 | 34.747                    |
| 2.580M          |                                      | 1   | 4 | 2 | 34.747                    |
| 2.563           | 12                                   | 4   | 1 | 0 | 34.987                    |
| 2.555           | 12                                   | -4  | 1 | 1 | 35.090                    |
| 2.487           | 28                                   | 4   | 2 | 0 | 36.080                    |
| 2.480M          | 28                                   | 3   | 5 | 0 | 36.190                    |

Magnesium Manganese Zinc Iron Sulfate Hydroxide Hydrate, Zincobotryogen,  
 $(\text{Zn},\text{Mg},\text{Mn})\text{Fe}(\text{SO}_4)_2(\text{OH}) \cdot 7\text{H}_2\text{O}$  - (continued)

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

Magnesium Silicate (Clinoenstatite),  $\text{MgSiO}_3$

Synonym

Magnesium metasilicate

CAS registry no.

13776-74-4

Sample

The sample was prepared by solid state reaction of basic magnesium carbonate and  $\text{SiO}_2$ . After an overnight calcine at 850 °C, the sample was heated at temperatures in the 1450 °C to 1500 °C range for about 4 days with daily regrindings.

Color

Colorless

Structure

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

Crystallographic constants of this sample

$$a = 9.6061(10) \text{\AA}$$

$$b = 8.8185(8)$$

$$c = 5.1710(5)$$

$$\beta = 108.289(10)^\circ$$

$$a/b = 1.0893$$

$$c/b = 0.5864$$

$$Z = 8$$

$$V = 415.92 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.206 \text{ g/cm}^3$$

Figure of merit

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

Polymorphism

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

Additional patterns

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

References

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

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

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

| $d(\text{\AA})$ | $I^{\text{rel}}$<br>$\sigma = \pm 4$ | $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ mean } T = 26 \pm 2 \text{ }^\circ\text{C}$ |     |     |                    |
|-----------------|--------------------------------------|--|-----|-----|--------------------|
|                 |                                      | Internal standard Ag, $a = 4.08651 \text{ \AA}$  |     |     |                    |
|                 |                                      | $h$  | $k$ | $l$ | $2\theta (^\circ)$ |
| 6.341           | 1                                    | 1  | 1   | 0   | 13.955             |
| 4.410           | 9                                    | 0  | 2   | 0   | 20.119             |
| 4.372           | 3                                    | -1   | 1   | 1   | 20.296             |
| 4.293           | 8                                    | 0  | 1   | 1   | 20.673             |
| 4.048           | 1L                                   | 2  | 1   | 0   | 21.937             |
| 3.530           | 4                                    | 1  | 1   | 1   | 25.206             |
| 3.316           | 8                                    | -1   | 2   | 1   | 26.863             |
| 3.280           | 30                                   | 0  | 2   | 1   | 27.162             |
| 3.170           | 47                                   | 2  | 2   | 0   | 28.125             |
| 3.041           | 4                                    | 3  | 0   | 0   | 29.350             |
| 2.976           | 69                                   | -2   | 2   | 1   | 30.000             |
| 2.874           | 100                                  | 3  | 1   | 0   | 31.094             |
| 2.798           | 3                                    | 1  | 3   | 0   | 31.956             |
| 2.769           | 2                                    | 2  | 1   | 1   | 32.308             |
| 2.582           | 2                                    | -1   | 0   | 2   | 34.716             |
| 2.539           | 23                                   | -1   | 3   | 1   | 35.323             |
| 2.523           | 19                                   | 0  | 3   | 1   | 35.555             |
| 2.516           | 17                                   | -2   | 0   | 2   | 35.659             |
| 2.472           | 13                                   | 2  | 3   | 0   | 36.319             |
| 2.455           | 35                                   | 0  | 0   | 2   | 36.570             |
| 2.433           | 14                                   | 2  | 2   | 1   | 36.916             |
| 2.375           | 11                                   | -2   | 3   | 1   | 37.847             |
| 2.280           | 4                                    | 4  | 0   | 0   | 39.483             |
| 2.209           | 9                                    | 4  | 1   | 0   | 40.815             |
| 2.204M          | 9                                    | 0  | 4   | 0   | 40.921             |
| 2.204M          |                                      | 1  | 0   | 2   | 40.921             |
| 2.1443M         | 6                                    | 0  | 2   | 2   | 42.107             |
| 2.1443M         |                                      | 1  | 4   | 0   | 42.107             |
| 2.1380          | 5                                    | 1  | 1   | 2   | 42.237             |
| 2.1166          | 26                                   | -3   | 3   | 1   | 42.684             |
| 2.0901          | 5                                    | -4   | 2   | 1   | 43.253             |
| 2.0359          | 3                                    | -3   | 2   | 2   | 44.465             |
| 2.0247          | 6                                    | 4  | 2   | 0   | 44.722             |
| 2.0193          | 10                                   | -1   | 4   | 1   | 44.849             |
| 2.0114          | 9                                    | 0  | 4   | 1   | 45.035             |
| 1.9862          | 6                                    | 2  | 4   | 0   | 45.639             |
| 1.9655          | 4                                    | -4   | 1   | 2   | 46.148             |
| 1.9349          | 8                                    | -2   | 4   | 1   | 46.921             |
| 1.9238          | 5                                    | 2  | 0   | 2   | 47.206             |
| 1.9135          | 2                                    | 1  | 4   | 1   | 47.476             |
| 1.8847          | 2                                    | 0  | 3   | 2   | 48.249             |
| 1.8737          | 2                                    | -5   | 1   | 1   | 48.549             |
| 1.8455          | 3                                    | -4   | 3   | 1   | 49.339             |
| 1.8085          | 2                                    | -3   | 3   | 2   | 50.420             |
| 1.8038          | 1                                    | 3  | 3   | 1   | 50.560             |
| 1.7862M         | 9                                    | -3   | 4   | 1   | 51.095             |
| 1.7862M         |                                      | 5  | 1   | 0   | 51.095             |
| 1.7640M         | 7                                    | 2  | 2   | 2   | 51.784             |
| 1.7640M         |                                      | 1  | 3   | 2   | 51.784             |
| 1.7586M         | 8                                    | 2  | 4   | 1   | 51.955             |

Magnesium Silicate (Clinoenstatite), MgSiO<sub>3</sub> - (continued)

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

Magnesium Silicate (Forsterite),  $\text{Mg}_2\text{SiO}_4$

Synonym

Magnesium orthosilicate

CAS registry no.  
10034-94-3

Sample

$\text{MgCO}_3$  and  $\text{SiO}_2$  were mixed in a 2:1 molar ratio and heated at 800 °C overnight, 1300 °C for 21 hours, 1500 °C for 25 hours, and 1525 °C for 24 hours with intermittent grinding. There was a trace of  $\text{MgO}$  in the sample.

Color

Colorless

Structure

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

Crystallographic constants of this sample

$$a = 5.9817(5) \text{ \AA}$$

$$b = 10.1978(8)$$

$$c = 4.7553(3)$$

$$a/b = 0.5866$$

$$c/b = 0.4663$$

$$Z = 4$$

$$V = 290.07 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.222 \text{ g/cm}^3$$

Figure of merit

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

Additional patterns

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

Swanson and Tatge (1951)

References

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

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = $26 \pm 2$ °C<br>Internal standard Si, SRM 640a |                  |     |   |       |
|--|------------------|-----|---|-------|
| d( $\text{\AA}$ )  | I <sup>rel</sup> | hkl |   | 2θ(°) |
| $\sigma = \pm 4$   |                  |     |   |       |
| 5.102  | 22               | 0   | 2 | 0     |
| 4.307  | 4                | 0   | 1 | 1     |
| 3.881  | 76               | 1   | 2 | 0     |
| 3.722  | 25               | 1   | 0 | 1     |
| 3.496  | 26               | 1   | 1 | 1     |
| 3.477  | 22               | 0   | 2 | 1     |
| 3.006  | 14               | 1   | 2 | 1     |
| 2.991  | 18               | 2   | 0 | 0     |
| 2.765  | 66               | 0   | 3 | 1     |
| 2.5097   | 83               | 1   | 3 | 1     |
| 2.4567   | 100              | 2   | 1 | 1     |
| 2.3456   | 13               | 1   | 4 | 0     |
| 2.3150   | 13               | 0   | 1 | 2     |
| 2.2673   | 57               | 2   | 2 | 1     |
| 2.2470   | 37               | 0   | 4 | 1     |
| 2.1589   | 23               | 1   | 1 | 2     |
| 2.0303   | 7                | 2   | 3 | 1     |
| 1.9479   | 6                | 0   | 3 | 2     |
| 1.9407   | 5                | 2   | 4 | 0     |
| 1.8744   | 8                | 0   | 5 | 1     |
| 1.8608   | 3                | 2   | 0 | 2     |
| 1.8569   | 2                | 3   | 2 | 0     |
| 1.8388   | 1L               | 3   | 0 | 1     |
| 1.8299   | 1                | 2   | 1 | 2     |
| 1.8090   | 4                | 3   | 1 | 1     |
| 1.7886   | 5                | 1   | 5 | 1     |
| 1.7483   | 73               | 2   | 2 | 2     |
| 1.7386   | 24               | 0   | 4 | 2     |
| 1.7294   | 6                | 3   | 2 | 1     |
| 1.6698   | 16               | 1   | 4 | 2     |
| 1.6347   | 15               | 1   | 6 | 0     |
| 1.6173   | 17               | 3   | 3 | 1     |
| 1.6008   | 2                | 0   | 6 | 1     |
| 1.5884   | 4                | 2   | 5 | 1     |
| 1.5708   | 11               | 3   | 4 | 0     |
| 1.5666   | 8                | 0   | 1 | 3     |
| 1.5323   | 2                | 1   | 0 | 3     |
| 1.5144   | 10               | 1   | 1 | 3     |
| 1.5111   | 9                | 3   | 1 | 2     |
| 1.5032   | 11               | 2   | 4 | 2     |

Magnesium Silicate (Forsterite),  $\text{Mg}_2\text{SiO}_4$  - (continued)

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

Potassium Barium Niobium Oxide,  $\text{KBa}_2(\text{NbO}_3)_5$

Synonym

Potassium barium niobate

CAS registry no.

12400-06-5

Sample

The sample was made by heating a mixture of  $\text{KNbO}_3$ ,  $\text{BaCO}_3$ , and  $\text{Nb}_2\text{O}_5$  at temperatures up to 1340 °C for 56 hours with intermediate grindings.

Color

Colorless

Structure

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

Crystallographic constants of this sample

$$a = 12.5407(5) \text{ \AA}$$

$$c = 4.0210(3)$$

$$c/a = 0.3206$$

$$Z = 2$$

$$V = 632.38 \text{ \AA}^3$$

$$\text{Density (calc)} = 5.348 \text{ g/cm}^3$$

Figure of merit

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

Additional pattern

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

Reference

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

|  |  |  |  |
|--|--|--|--|
| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = $26 \pm 2$ °C |  |  |  |
| Internal standards W, $a = 3.16524 \text{ \AA}$                          |  |  |  |
| Fluorophlogopite, SRM 675  |  |  |  |

| d( $\text{\AA}$ ) | I <sup>rel</sup> | hkl   | 2θ(°)  |
|-------------------|------------------|-------|--------|
| $\sigma = \pm 4$  |                  |       |        |
| 8.87              | 1                | 1 1 0 | 9.968  |
| 6.279             | 1L               | 2 0 0 | 14.093 |
| 5.609             | 1                | 2 1 0 | 15.787 |
| 4.433             | 1L               | 2 2 0 | 20.014 |
| 4.021             | 13               | 0 0 1 | 22.086 |
| 3.967             | 4                | 3 1 0 | 22.394 |
| 3.664             | 1                | 1 1 1 | 24.274 |
| 3.479             | 29               | 3 2 0 | 25.585 |
| 3.386             | 3                | 2 0 1 | 26.303 |
| 3.269             | 59               | 2 1 1 | 27.255 |
| 3.136             | 9                | 4 0 0 | 28.440 |
| 3.042             | 68               | 4 1 0 | 29.332 |
| 2.981             | 23               | 2 2 1 | 29.955 |
| 2.957             | 15               | 3 3 0 | 30.204 |
| 2.824             | 100              | 3 1 1 | 31.661 |

| d( $\text{\AA}$ ) | I <sup>rel</sup> | hkl   | 2θ(°)  |
|-------------------|------------------|-------|--------|
| $\sigma = \pm 4$  |                  |       |        |
| 2.804             | 36               | 4 2 0 | 31.889 |
| 2.631             | 16               | 3 2 1 | 34.052 |
| 2.474             | 4                | 4 0 1 | 36.280 |
| 2.427             | 1                | 4 1 1 | 37.013 |
| 2.3811            | 1                | 3 3 1 | 37.750 |
| 2.3291            | 9                | 5 2 0 | 38.626 |
| 2.3015            | 1                | 4 2 1 | 39.108 |
| 2.2167            | 2                | 4 4 0 | 40.669 |
| 2.1506            | 17               | 5 3 0 | 41.976 |
| 2.0981            | 2                | 5 1 1 | 43.079 |
| 2.0901            | 3                | 6 0 0 | 43.252 |
| 2.0616            | 1                | 6 1 0 | 43.880 |
| 2.0100            | 25               | 0 0 2 | 45.069 |
| 1.9823            | 15               | 6 2 0 | 45.734 |
| 1.9581            | 1                | 5 4 0 | 46.332 |
| 1.9416            | 1                | 4 4 1 | 46.748 |
| 1.8963            | 4                | 5 3 1 | 47.934 |
| 1.8690            | 8                | 6 3 0 | 48.678 |
| 1.8544            | 14               | 6 0 1 | 49.088 |
| 1.7785            | 21               | 6 2 1 | 51.332 |
| 1.7733            | 27               | 5 5 0 | 51.492 |
| 1.7606            | 18               | 5 4 1 | 51.892 |
| 1.7404            | 7                | 3 2 2 | 52.540 |
| 1.7225            | 2                | 7 2 0 | 53.127 |
| 1.6951            | 9                | 6 3 1 | 54.056 |
| 1.6770            | 20               | 4 1 2 | 54.687 |
| 1.6622            | 4                | 3 3 2 | 55.217 |
| 1.6464            | 2                | 7 3 0 | 55.792 |
| 1.6339            | 11               | 4 2 2 | 56.256 |
| 1.6226            | 26               | 5 5 1 | 56.684 |
| 1.6058            | 1L               | 6 5 0 | 57.332 |
| 1.5837            | 4                | 7 2 1 | 58.209 |
| 1.5677            | 1                | 8 0 0 | 58.858 |
| 1.5553            | 3                | 7 4 0 | 59.375 |
| 1.5206            | 12               | 8 2 0 | 60.871 |
| 1.4912            | 1                | 6 5 1 | 62.202 |
| 1.4780            | 3                | 6 6 0 | 62.825 |
| 1.4680            | 12               | 8 3 0 | 63.300 |
| 1.4578            | 2                | 7 5 0 | 63.793 |
| 1.4509            | 3                | 7 4 1 | 64.134 |
| 1.4117            | 5                | 6 2 2 | 66.139 |
| 1.4018            | 1                | 8 4 0 | 66.665 |
| 1.3847            | 2                | 9 1 0 | 67.597 |
| 1.3787            | 3                | 8 3 1 | 67.931 |
| 1.3690            | 6                | 6 3 2 | 68.480 |
| 1.3298            | 7                | 5 5 2 | 70.795 |
| 1.3239            | 2                | 8 4 1 | 71.162 |
| 1.3095            | 1                | 9 1 1 | 72.067 |
| 1.3034            | 2                | 2 1 3 | 72.453 |
| 1.2886            | 1                | 7 6 1 | 73.421 |
| 1.2830            | 1                | 2 2 3 | 73.796 |
| 1.2735            | 2                | 9 4 0 | 74.442 |
| 1.2700            | 3                | 3 1 3 | 74.680 |
| 1.2668            | 2                | 7 7 0 | 74.900 |

Potassium Strontium Niobium Oxide,  $\text{K Sr}_2(\text{NbO}_3)_5$

Synonym

Potassium strontium niobate

CAS registry no.

12358-94-0

Sample

The sample was made by heating  $\text{KNbO}_3$ ,  $\text{SrCO}_3$ , and  $\text{Nb}_2\text{O}_5$  at 850 °C for 18 hours, at 1300 °C for 18 hours, and at 1340 °C for 20 hours.

Color

Colorless

Structure

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

Crystallographic constants of this sample

$$a = 12.461(1) \text{ \AA}$$

$$c = 3.9431(8)$$

$$c/a = 0.3164$$

$$Z = 2$$

$$V = 612.27 \text{ \AA}^3$$

$$\text{Density (calc)} = 4.984 \text{ g/cm}^3$$

Figure of merit

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

Reference

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 26±2 °C |                                      |     |   |        |
|--|--------------------------------------|-----|---|--------|
| Internal standards Si, SRM 640a                                    |                                      |     |   |        |
| Fluorophlogopite, SRM 675  |                                      |     |   |        |
| d( $\text{\AA}$ )  | I <sup>rel</sup><br>$\sigma = \pm 1$ | hkl |   | 2θ(°)  |
| 8.82   | 2                                    | 1   | 1 | 0      |
| 6.24   | 5                                    | 2   | 0 | 0      |
| 5.578  | 2                                    | 2   | 1 | 0      |
| 3.944M   | 34                                   | 0   | 0 | 1      |
| 3.944M   |                                      | 3   | 1 | 0      |
|  |                                      |     |   | 22.527 |
|  |                                      |     |   | 22.527 |
| 3.602  | 4                                    | 1   | 1 | 1      |
| 3.458  | 37                                   | 3   | 2 | 0      |
| 3.219  | 43                                   | 2   | 1 | 1      |
| 3.116  | 12                                   | 4   | 0 | 0      |
| 3.023  | 52                                   | 4   | 1 | 0      |
|  |                                      |     |   | 29.521 |
| 2.939M   | 25                                   | 2   | 2 | 1      |
| 2.939M   |                                      | 3   | 3 | 0      |
| 2.788M   | 100                                  | 3   | 1 | 1      |
| 2.788M   |                                      | 4   | 2 | 0      |
| 2.600  | 20                                   | 3   | 2 | 1      |
|  |                                      |     |   | 34.472 |
| 2.446M   | 2                                    | 4   | 0 | 1      |
| 2.446M   |                                      | 5   | 1 | 0      |
| 2.399  | 1                                    | 4   | 1 | 1      |
| 2.356  | 2                                    | 3   | 3 | 1      |
| 2.315  | 3                                    | 5   | 2 | 0      |
|  |                                      |     |   | 38.875 |
| 2.202  | 1                                    | 4   | 4 | 0      |
| 2.137  | 8                                    | 5   | 3 | 0      |
| 2.077M   | 3                                    | 5   | 1 | 1      |
| 2.077M   |                                      | 6   | 0 | 0      |
| 2.048  | 3                                    | 6   | 1 | 0      |
|  |                                      |     |   | 44.179 |
| 1.9709M  | 36                                   | 0   | 0 | 2      |
| 1.9709M  |                                      | 6   | 2 | 0      |
| 1.9468   | 6                                    | 5   | 4 | 0      |
| 1.9229M  | 1                                    | 1   | 1 | 2      |
| 1.9229M  |                                      | 4   | 4 | 1      |
|  |                                      |     |   | 47.231 |
| 1.8786M  | 1                                    | 2   | 0 | 2      |
| 1.8786M  |                                      | 5   | 3 | 1      |
| 1.8576M  | 12                                   | 2   | 1 | 2      |
| 1.8576M  |                                      | 6   | 3 | 0      |
| 1.8375   | 8                                    | 6   | 0 | 1      |
|  |                                      |     |   | 49.568 |
| 1.7625+  | 20                                   | 6   | 2 | 1      |
| 1.7625+  |                                      | 5   | 5 | 0      |
| 1.7452   | 10                                   | 5   | 4 | 1      |
| 1.7288   | 1L                                   | 6   | 4 | 0      |
| 1.7127   | 6                                    | 3   | 2 | 2      |
|  |                                      |     |   | 53.456 |
| 1.6805   | 7                                    | 6   | 3 | 1      |
| 1.6656   | 1                                    | 4   | 0 | 2      |
| 1.6513   | 12                                   | 4   | 1 | 2      |
| 1.6377   | 2                                    | 3   | 3 | 2      |
| 1.6090M  | 31                                   | 4   | 2 | 2      |
|  |                                      |     |   | 57.206 |

Potassium Strontium Niobium Oxide,  $\text{K Sr}_2(\text{NbO}_3)_5$  - (continued)

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

Potassium Titanium Phosphate,  $KTi_2(PO_4)_3$

Synonym

Potassium titanium orthophosphate

CAS registry no.

30622-41-4

Sample

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

Color

Colorless

Structure

Rhombohedral,  $R^{**}$ . Isostructural with many other similar double phosphates (Masse, 1970).

Crystallographic constants of this sample

(Hexagonal axes)

$a = 8.3582(5)$  Å

$c = 23.086(2)$

$c/a = 2.7621$

$Z = 6$

$V = 1396.71$  Å<sup>3</sup>

Density (calc) = 2.995 g/cm<sup>3</sup>

Figure of merit

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

Polymorphism

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

Additional pattern

PDF card 25-691 (Masse, 1970)

References

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

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

| CuK $\alpha$ $\lambda = 1.540598$ Å; mean T = $26 \pm 2$ °C<br>Internal standards Si, SRM 640a<br>Fluorophlogopite, SRM 675 |                                      |         |   |    |                      |
|---|--------------------------------------|---------|---|----|----------------------|
| $d(\text{\AA})$   | $I^{\text{rel}}$<br>$\sigma = \pm 2$ | $h k l$ |   |    | $2\theta (\text{°})$ |
| 6.131   | 8                                    | 0       | 1 | 2  | 14.435               |
| 4.514   | 9                                    | 1       | 0 | 4  | 19.653               |
| 4.178   | 42                                   | 1       | 1 | 0  | 21.248               |
| 3.846   | 1                                    | 0       | 0 | 6  | 23.109               |
| 3.672   | 100                                  | 1       | 1 | 3  | 24.218               |
| 3.452   | 5                                    | 2       | 0 | 2  | 25.790               |
| 3.065   | 24                                   | 0       | 2 | 4  | 29.110               |
| 2.830   | 80                                   | 1       | 1 | 6  | 31.587               |
| 2.716   | 11                                   | 2       | 1 | 1  | 32.951               |
| 2.681   | 5                                    | 0       | 1 | 8  | 33.398               |
| 2.662   | 6                                    | 1       | 2 | 2  | 33.643               |
| 2.4129  | 16                                   | 3       | 0 | 0  | 37.234               |
| 2.3541  | 2                                    | 1       | 2 | 5  | 38.200               |
| 2.2562  | 2                                    | 2       | 0 | 8  | 39.926               |
| 2.1986  | 4                                    | 1       | 0 | 10 | 41.019               |
| 2.1866  | 8                                    | 1       | 1 | 9  | 41.253               |
| 2.1050  | 2                                    | 2       | 1 | 7  | 42.931               |
| 2.0438  | 11                                   | 3       | 0 | 6  | 44.284               |
| 2.0166  | 3                                    | 2       | 2 | 3  | 44.912               |
| 1.9850  | 6                                    | 1       | 2 | 8  | 45.668               |
| 1.9468  | 2                                    | 0       | 2 | 10 | 46.616               |
| 1.9233  | 3                                    | 0       | 0 | 12 | 47.221               |
| 1.8964  | 2                                    | 1       | 3 | 4  | 47.931               |
| 1.8363  | 22                                   | 2       | 2 | 6  | 49.605               |
| 1.7880  | 1                                    | 0       | 4 | 2  | 51.038               |
| 1.7642  | 8                                    | 2       | 1 | 10 | 51.779               |
| 1.7266  | 2                                    | 4       | 0 | 4  | 52.992               |
| 1.7149  | 6                                    | 1       | 3 | 7  | 53.382               |
| 1.6651  | 1L                                   | 1       | 2 | 11 | 55.113               |
| 1.6481  | 6                                    | 3       | 1 | 8  | 55.728               |
| 1.6202  | 1                                    | 2       | 2 | 9  | 56.774               |
| 1.6081  | 1L                                   | 0       | 1 | 14 | 57.243               |
| 1.5955  | 1                                    | 3       | 2 | 4  | 57.737               |
| 1.5797  | 11                                   | 4       | 1 | 0  | 58.369               |
| 1.5627  | 1                                    | 2       | 3 | 5  | 59.065               |
| 1.5474  | 2                                    | 4       | 1 | 3  | 59.711               |
| 1.5332  | 4                                    | 0       | 4 | 8  | 60.319               |
| 1.5150  | 6                                    | 1       | 3 | 10 | 61.123               |
| 1.5043  | 10                                   | 3       | 0 | 12 | 61.602               |
| 1.5005  | 9                                    | 2       | 0 | 14 | 61.776               |
| 1.4832  | 1                                    | 3       | 2 | 7  | 62.577               |
| 1.4611  | 7                                    | 4       | 1 | 6  | 63.636               |
| 1.4511  | 2                                    | 3       | 1 | 11 | 64.124               |
| 1.4442  | 1                                    | 1       | 1 | 15 | 64.466               |
| 1.4244  | 2                                    | 4       | 0 | 10 | 65.476               |
| 1.4123  | 3                                    | 1       | 2 | 14 | 66.108               |
| 1.4044  | 1L                                   | 0       | 5 | 4  | 66.528               |
| 1.3928  | 2                                    | 3       | 3 | 0  | 67.154               |
| 1.3708  | 1L                                   | 3       | 3 | 3  | 68.377               |

Potassium Zinc Phosphate, KZnPO<sub>4</sub>

Synonym

Potassium zinc orthophosphate

CAS registry no.

13826-55-6

Sample

The sample was prepared by heating KH<sub>2</sub>PO<sub>4</sub> and ZnO at 800 °C for 2 days. After grinding and sieving, it was held at 800 °C overnight.

Color

Colorless

Structure

Hexagonal, P6<sub>3</sub>/<sup>1</sup> (Averbuch-Pouchot and Durif, 1973).

Crystallographic constants of this sample

a = 18.1626(12) Å

c = 8.5066(11)

c/a = 0.4684

Z = 24

V = 2430.20 Å<sup>3</sup>

Density (calc) = 3.2702 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 57.4(0.0093,56)

Additional patterns

PDF card 20-1447 (Salutsky and Steiger, 1964)

PDF card 20-1448 (Frazier et al., 1966)

PDF card 25-1342 (Averbuch-Pouchot and Durif, 1973)

Barbou des Courières and Simonot-Grange (1979)

Grins and Nygren (1982)

References

Averbuch-Pouchot, M. T. and Durif, A. (1973).

Mat. Res. Bull. 8, 353.

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

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

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

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

| CuKα <sub>1</sub> λ = 1.540598 Å; temp. 26±1 °C<br>Internal standard Ag, a = 4.08651 Å |                            |       |        |  |
|--|----------------------------|-------|--------|--|
| d(Å)   | f <sup>rel</sup><br>σ = ±3 | hkl   | 2θ(°)  |  |
| 9.08   | 1L                         | 1 1 0 | 9.738  |  |
| 6.203  | 13                         | 1 1 1 | 14.268 |  |
| 4.537  | 16                         | 2 2 0 | 19.549 |  |
| 4.252  | 34                         | 0 0 2 | 20.873 |  |
| 4.004  | 19                         | 2 2 1 | 22.183 |  |
| 3.884  | 1                          | 3 1 1 | 22.881 |  |
| 3.852  | 2                          | 1 1 2 | 23.072 |  |
| 3.609  | 1                          | 3 2 0 | 24.651 |  |
| 3.567  | 1                          | 4 0 1 | 24.941 |  |
| 3.436  | 1                          | 4 1 0 | 25.912 |  |
| 3.320  | 1                          | 3 2 1 | 26.834 |  |
| 3.302  | 3                          | 3 0 2 | 26.982 |  |
| 3.182  | 34                         | 4 1 1 | 28.020 |  |
| 3.103  | 100                        | 2 2 2 | 28.743 |  |
| 3.045  | 1L                         | 3 1 2 | 29.303 |  |
| 2.972  | 3                          | 4 2 0 | 30.040 |  |
| 2.851  | 2                          | 3 3 1 | 31.349 |  |
| 2.824  | 2                          | 5 1 0 | 31.660 |  |
| 2.750  | 1                          | 3 2 2 | 32.528 |  |
| 2.706  | 12                         | 1 1 3 | 33.073 |  |
| 2.671  | 1L                         | 4 1 2 | 33.522 |  |
| 2.621  | 60                         | 6 0 0 | 34.177 |  |
| 2.558  | 1                          | 2 1 3 | 35.047 |  |
| 2.518  | 2                          | 5 2 0 | 35.626 |  |
| 2.505  | 11                         | 6 0 1 | 35.823 |  |
| 2.465  | 3                          | 3 3 2 | 36.422 |  |
| 2.436  | 3                          | 4 2 2 | 36.869 |  |
| 2.416  | 8                          | 5 2 1 | 37.191 |  |
| 2.405  | 10                         | 2 2 3 | 37.368 |  |
| 2.377  | 2                          | 3 1 3 | 37.818 |  |
| 2.354  | 1                          | 5 1 2 | 38.202 |  |
| 2.309  | 1L                         | 6 1 1 | 38.972 |  |
| 2.299  | 1                          | 4 0 3 | 39.153 |  |
| 2.2313M  | 2                          | 6 0 2 | 40.391 |  |
| 2.2313M  |                            | 3 2 3 | 40.391 |  |
| 2.2095   | 1                          | 4 3 2 | 40.807 |  |
| 2.1932   | 9                          | 4 4 1 | 41.125 |  |
| 2.1868   | 10                         | 4 1 3 | 41.250 |  |
| 2.1665   | 2                          | 5 2 2 | 41.655 |  |
| 2.1259   | 6                          | 0 0 4 | 42.488 |  |
| 2.1144   | 1                          | 6 2 1 | 42.731 |  |
| 2.0696M  | 4                          | 1 1 4 | 43.702 |  |
| 2.0696M  |                            | 3 3 3 | 43.702 |  |
| 2.0028+  | 9                          | 4 4 2 | 45.238 |  |
| 2.0028+  |                            | 2 1 4 | 45.238 |  |
| 1.9815   | 1                          | 6 3 0 | 45.752 |  |
| 1.9705   | 2                          | 3 0 4 | 46.023 |  |
| 1.9251M  | 4                          | 2 2 4 | 47.173 |  |
| 1.9251M  |                            | 6 0 3 | 47.173 |  |
| 1.9112M  | 1                          | 3 1 4 | 47.537 |  |

Potassium Zinc Phosphate, KZnPO<sub>4</sub> - (continued)

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

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

# Rubidium Hydrogen Phosphate, $\text{RbH}_2\text{PO}_4$

**Synonym**

Rubidium dihydrogen orthophosphate

**CAS registry no.**

13774-16-8

**Sample**

The sample was made by adding  $\text{Rb}_2\text{CO}_3$  to an 85% solution of  $\text{H}_3\text{PO}_4$ . The precipitate was washed with alcohol.

**Color**

Colorless

**Structure**

Tetragonal,  $I\bar{4}2d$  (122). The structure was determined by Al-Karaghoubi et al. (1978). Isostructural with  $\text{KH}_2\text{PO}_4$ .

**Crystallographic constants of this sample**

$a = 7.6080(3) \text{ \AA}$   
 $c = 7.2979(6)$

$c/a = 0.9592$

$Z = 4$

$V = 422.42 \text{ \AA}^3$

Density (calc) =  $2.869 \text{ g/cm}^3$

**Figure of merit**

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

**Additional patterns**

PDF card 30-1064 (Smith et al., 1979)  
 (calculated pattern)

Nirsha et al. (1981)

**References**

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

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ mean } T = 25.7^\circ \text{ C}$ |                  |         |                           |  |
|---|------------------|---------|---------------------------|--|
| Internal standards Ag, $a = 4.08651 \text{ \AA}$  |                  |         |                           |  |
| Fluorophlogopite, SRM 675   |                  |         |                           |  |
| $d(\text{\AA})$   | $I^{\text{rel}}$ | $h k l$ | $2\theta (\text{)}^\circ$ |  |
| $\sigma = \pm 1$  |                  |         |                           |  |
| 5.262   | 2                | 1 0 1   | 16.837                    |  |
| 3.803   | 100              | 2 0 0   | 23.375                    |  |
| 3.083   | 15               | 2 1 1   | 28.934                    |  |
| 3.020   | 67               | 1 1 2   | 29.555                    |  |
| 2.689   | 24               | 2 2 0   | 33.292                    |  |

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

# Rubidium Phosphate, RbPO<sub>3</sub>

## Synonym

Rubidium metaphosphate

## Sample

The sample was prepared by heating RbH<sub>2</sub>PO<sub>4</sub> at 250 °C for 17 hours.

## Color

Colorless

## Structure

Monoclinic, P2<sub>1</sub>/n (14). The structure of RbPO<sub>3</sub> was determined by Corbridge (1956) and refined by Cruickshank (1964).

## Crystallographic constants of this sample

$$a = 12.1221(14) \text{ \AA}$$

$$b = 4.2307(5)$$

$$c = 6.4773(9)$$

$$\beta = 95.980(11)^\circ$$

$$a/b = 2.8652$$

$$c/b = 1.5310$$

$$Z = 4$$

$$V = 330.38 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.306 \text{ g/cm}^3$$

## Figure of merit

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

## Additional patterns

Majling et al. (1979) (calculated pattern)

Nirsha et al. (1981)

## References

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

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

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

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

CuKα<sub>1</sub> λ = 1.540598 Å; mean T = 25.6 °C

Internal standards W, a = 3.16524 Å

Fluorophlogopite, SRM 675

| d(Å)   | I <sup>rel</sup> | hkl    | 2θ(°)  |
|--------|------------------|--------|--------|
| σ = ±1 |                  |        |        |
| 6.025  | 1                | 2 0 0  | 14.690 |
| 5.944  | 1                | -1 0 1 | 14.891 |
| 3.994  | 8                | 1 1 0  | 22.241 |
| 3.582  | 31               | -3 0 1 | 24.839 |
| 3.536  | 19               | 0 1 1  | 25.164 |

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

Rubidium Strontium Niobium Oxide,  $\text{RbSr}_2(\text{NbO}_3)_5$

Synonym

Rubidium strontium niobate

Sample

The sample was prepared by heating  $\text{Rb}_2\text{CO}_3$ ,  $\text{SrCO}_3$ , and  $\text{Nb}_2\text{O}_5$  at 900 °C overnight, followed by heating at 1275 °C overnight with intermediate grindings.

Color

Colorless

Structure

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

Crystallographic constants of this sample

$a = 12.5127(7)$  Å  
 $c = 3.9600(4)$

$c/a = 0.3165$

$Z = 2$

$V = 620.01$  Å<sup>3</sup>

Density (calc) = 5.172 g/cm<sup>3</sup>

Figure of merit

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

Reference

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

| CuK $\alpha_1$ λ = 1.540598 Å; mean T = 26±2 °C |                  |       |        |  |
|---|------------------|-------|--------|--|
| Internal standards Ag, a = 4.08651 Å            |                  |       |        |  |
| Fluorophlogopite, SRM 675                       |                  |       |        |  |
| d(Å)  | I <sup>rel</sup> | hkl   | 2θ(°)  |  |
| $\sigma = \pm 1$                                |                  |       |        |  |
| 8.86  | 1                | 1 1 0 | 9.971  |  |
| 6.263   | 3                | 2 0 0 | 14.129 |  |
| 3.961M  | 22               | 0 0 1 | 22.428 |  |
| 3.961M  |                  | 3 1 0 | 22.428 |  |
| 3.616   | 3                | 1 1 1 | 24.601 |  |
| 3.472   | 29               | 3 2 0 | 25.638 |  |
| 3.346   | 1                | 2 0 1 | 26.620 |  |
| 3.233   | 51               | 2 1 1 | 27.564 |  |
| 3.129   | 8                | 4 0 0 | 28.506 |  |
| 3.036   | 54               | 4 1 0 | 29.400 |  |
| 2.951   | 26               | 2 2 1 | 30.260 |  |
| 2.799M  | 100              | 3 1 1 | 31.952 |  |
| 2.799M  |                  | 4 2 0 | 31.952 |  |
| 2.610   | 17               | 3 2 1 | 34.327 |  |
| 2.455   | 2                | 4 0 1 | 36.574 |  |

| d(Å)             | I <sup>rel</sup> | hkl   | 2θ(°)  |
|------------------|------------------|-------|--------|
| $\sigma = \pm 1$ |                  |       |        |
| 2.4097           | 1                | 4 1 1 | 37.285 |
| 2.3233           | 5                | 5 2 0 | 38.727 |
| 2.2846           | 1                | 4 2 1 | 39.409 |
| 2.2110           | 1                | 4 4 0 | 40.779 |
| 2.1461           | 10               | 5 3 0 | 42.069 |
| 2.0851           | 3                | 6 0 0 | 43.361 |
| 1.9796           | 33               | 0 0 2 | 45.799 |
| 1.9538           | 2                | 5 4 0 | 46.440 |
| 1.9314           | 2                | 4 4 1 | 47.009 |
| 1.8867           | 3                | 5 3 1 | 48.193 |
| 1.8653           | 10               | 6 3 0 | 48.781 |
| 1.8455           | 8                | 6 0 1 | 49.340 |
| 1.7696M          | 20               | 6 2 1 | 51.609 |
| 1.7696M          |                  | 5 5 0 | 51.609 |
| 1.7524           | 11               | 5 4 1 | 52.154 |
| 1.7197           | 6                | 3 2 2 | 53.223 |
| 1.6874           | 7                | 6 3 1 | 54.323 |
| 1.6729           | 2                | 4 0 2 | 54.834 |
| 1.6583           | 14               | 4 1 2 | 55.356 |
| 1.6433           | 3                | 7 3 0 | 55.906 |
| 1.6158           | 29               | 5 5 1 | 56.943 |
| 1.5766           | 2                | 7 2 1 | 58.495 |
| 1.5520           | 2                | 7 4 0 | 59.516 |
| 1.5415           | 1L               | 5 1 2 | 59.961 |
| 1.5173           | 6                | 8 2 0 | 61.018 |
| 1.5069           | 1                | 5 2 2 | 61.486 |
| 1.4849           | 1                | 6 5 1 | 62.500 |
| 1.4750M          | 3                | 4 4 2 | 62.967 |
| 1.4750M          |                  | 6 6 0 | 62.967 |
| 1.4646           | 5                | 8 3 0 | 63.465 |
| 1.4551           | 5                | 5 3 2 | 63.925 |
| 1.4452           | 1                | 7 4 1 | 64.420 |
| 1.4359           | 1L               | 6 0 2 | 64.883 |
| 1.3994M          | 5                | 6 2 2 | 66.797 |
| 1.3994M          |                  | 8 4 0 | 66.797 |
| 1.3907           | 1                | 5 4 2 | 67.272 |
| 1.3736           | 4                | 8 3 1 | 68.219 |
| 1.3654           | 2                | 7 5 1 | 68.685 |
| 1.3577           | 5                | 6 3 2 | 69.133 |
| 1.3263           | 1                | 8 5 0 | 71.015 |
| 1.3194M          | 7                | 7 1 2 | 71.441 |
| 1.3194M          |                  | 8 4 1 | 71.441 |
| 1.2846           | 2                | 2 1 3 | 73.689 |
| 1.2705           | 2                | 9 4 0 | 74.645 |
| 1.2646           | 3                | 7 3 2 | 75.051 |

Sodium Antimony Fluoride, NaSbF<sub>4</sub>

Synonyms

Sodium fluoantimonite  
Sodium antimony tetrafluoride

Sample

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

Color

Colorless

Optical data

Biaxial (-)  $N_{\alpha} = 1.475$ ,  $N_{\beta} = 1.521$ ,  $N_{\gamma} = 1.540$ .  $2V$  is about  $75^\circ$  (Byström et al., 1953)

Structure

Monoclinic, P<sub>2</sub><sub>1</sub> (4). The structure of NaSbF<sub>4</sub> was determined by Byström et al. (1953). The authors gave the space group as P<sub>2</sub><sub>1</sub> or P<sub>2</sub><sub>1</sub>/a. P<sub>2</sub><sub>1</sub> indexed our data more completely than P<sub>2</sub><sub>1</sub>/a.

Crystallographic constants of this sample

$$a = 8.5749(12) \text{ \AA}$$

$$b = 5.5299(10)$$

$$c = 8.0703(9)$$

$$\beta = 94.089(14)^\circ$$

$$Z = 4$$

$$V = 381.71 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.841 \text{ g/cm}^3$$

Figure of merit

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

Reference

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 26.5 °C |                  |     |   |       |        |
|--|------------------|-----|---|-------|--------|
| Internal standard Si, SRM 640a                                     |                  |     |   |       |        |
| d(Å)   | I <sup>rel</sup> | hkl |   | 2θ(°) |        |
| $\sigma = \pm 3$   |                  |     |   |       |        |
| 8.05   | 22               | 0   | 0 | 1     | 10.983 |
| 4.643  | 21               | 1   | 1 | 0     | 19.100 |
| 4.554  | 93               | 0   | 1 | 1     | 19.475 |
| 4.273  | 19               | 2   | 0 | 0     | 20.771 |
| 4.092  | 8                | -1  | 1 | 1     | 21.702 |
| 4.022  | 59               | 0   | 0 | 2     | 22.083 |
| 3.959  | 2                | 1   | 1 | 1     | 22.440 |
| 3.890  | 23               | -2  | 0 | 1     | 22.840 |
| 3.669  | 47               | 2   | 0 | 1     | 24.239 |
| 3.381  | 100              | 2   | 1 | 0     | 26.338 |
| 3.254  | 94               | 0   | 1 | 2     | 27.383 |
| 3.184  | 16               | -2  | 1 | 1     | 28.004 |
| 3.041  | 21               | -2  | 0 | 2     | 29.345 |
| 2.985  | 3                | 1   | 1 | 2     | 29.907 |
| 2.832  | 9                | 2   | 0 | 2     | 31.571 |
| 2.765  | 10               | 0   | 2 | 0     | 32.349 |
| 2.747  | 3                | -3  | 0 | 1     | 32.573 |
| 2.684  | 9                | 0   | 0 | 3     | 33.361 |
| 2.666  | 3                | -2  | 1 | 2     | 33.590 |
| 2.631M   | 6                | 1   | 2 | 0     | 34.049 |
| 2.631M   |                  | 3   | 0 | 1     | 34.049 |
| 2.520  | 18               | 2   | 1 | 2     | 35.595 |
| 2.415  | 2                | 0   | 1 | 3     | 37.201 |
| 2.375  | 10               | 3   | 1 | 1     | 37.856 |
| 2.363  | 8                | -1  | 1 | 3     | 38.052 |
| 2.349  | 5                | -2  | 0 | 3     | 38.280 |
| 2.285  | 5                | 1   | 1 | 3     | 39.398 |
| 2.2790   | 6                | 0   | 2 | 2     | 39.510 |
| 2.2545   | 17               | -2  | 2 | 1     | 39.957 |
| 2.2241   | 15               | -1  | 2 | 2     | 40.528 |
| 2.2095M  | 10               | -3  | 1 | 2     | 40.808 |
| 2.2095M  |                  | 2   | 2 | 1     | 40.808 |
| 2.1629   | 20               | -2  | 1 | 3     | 41.726 |
| 2.1388   | 20               | 4   | 0 | 0     | 42.219 |
| 2.0463M  | 44               | 2   | 1 | 3     | 44.227 |
| 2.0463M  |                  | -2  | 2 | 2     | 44.227 |
| 2.0123   | 13               | 0   | 0 | 4     | 45.015 |
| 1.9903   | 6                | -1  | 0 | 4     | 45.538 |
| 1.9779   | 15               | 2   | 2 | 2     | 45.841 |
| 1.9669   | 10               | -4  | 1 | 1     | 46.111 |
| 1.9256   | 9                | 0   | 2 | 3     | 47.161 |
| 1.9067   | 9                | 4   | 1 | 1     | 47.655 |
| 1.8916   | 22               | 0   | 1 | 4     | 48.062 |
| 1.8731M  | 5                | -1  | 1 | 4     | 48.565 |
| 1.8731M  |                  | -2  | 0 | 4     | 48.565 |
| 1.8585   | 3                | 1   | 2 | 3     | 48.973 |
| 1.8360   | 21               | -4  | 1 | 2     | 49.614 |
| 1.8164   | 3                | -3  | 2 | 2     | 50.184 |
| 1.7955   | 3                | 0   | 3 | 1     | 50.809 |
| 1.7741   | 17               | -2  | 1 | 4     | 51.466 |

Sodium Barium Niobium Oxide,  $\text{NaBa}_2(\text{NbO}_3)_5$

Synonym

B-S-N

Sample

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

Chemical analysis

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

Structure

Tetragonal. Bobb et al. (1969) reported this phase as orthorhombic ( $\text{Ccc}2$ ), with  $a$  and  $b$  very nearly equal. Our sample showed no definitive departure from tetragonal. It is a distorted tungsten bronze structure with the  $c$  axis doubled. Barns (1968) reported the phase as orthorhombic, with  $a$  and  $b$  equal.

Crystallographic constants of this sample

$$a = 17.609(2) \text{ \AA}$$

$$c = 7.987(2)$$

$$c/a = 0.4536$$

$$Z = 8$$

$$V = 2476.58 \text{ \AA}^3$$

$$\text{Density (calc)} = 5.376 \text{ g/cm}^3$$

Figure of merit

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

Polymorphism

Above  $\sim 290^\circ\text{C}$  this composition is truly tetragonal (Abell et al., 1973).

Additional patterns

PDF card 27-1408 (Abell et al., 1973)

PDF card 27-1409 (Cook, W., Priv. Com.)

PDF card 23-654 (Barns, 1968)

References

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

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

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

| $d(\text{\AA})$ | $I^{\text{rel}}$<br>$\sigma = \pm 2$ | CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean $T = 25.8^\circ\text{C}$ |   |   | $2\theta (\text{)}^\circ$ |
|-----------------|--------------------------------------|---|---|---|---------------------------|
|                 |                                      | Internal standards Si, SRM 640a   |   |   |                           |
| 8.81            | 1L                                   | 2   | 0 | 0 | 10.034                    |
| 6.229           | 2                                    | 2   | 2 | 0 | 14.208                    |
| 5.573           | 6                                    | 3   | 1 | 0 | 15.891                    |
| 3.994           | 19                                   | 0   | 0 | 2 | 22.241                    |
| 3.939           | 11                                   | 4   | 2 | 0 | 22.555                    |
| 3.454           | 32                                   | 5   | 1 | 0 | 25.775                    |
| 3.361           | 15                                   | 2   | 2 | 2 | 26.498                    |
| 3.245           | 89                                   | 3   | 1 | 2 | 27.466                    |
| 3.113           | 4                                    | 4   | 4 | 0 | 28.653                    |
| 3.020           | 100                                  | 5   | 3 | 0 | 29.556                    |
| 2.957           | 23                                   | 4   | 0 | 2 | 30.195                    |
| 2.933           | 26                                   | 6   | 0 | 0 | 30.452                    |
| 2.897           | 3                                    | 6   | 1 | 0 | 30.839                    |
| 2.804           | 87                                   | 4   | 2 | 2 | 31.894                    |
| 2.612           | 23                                   | 5   | 1 | 2 | 34.305                    |
| 2.455           | 9                                    | 4   | 4 | 2 | 36.566                    |
| 2.410           | 2                                    | 5   | 3 | 2 | 37.288                    |
| 2.363           | 4                                    | 6   | 0 | 2 | 38.052                    |
| 2.313           | 8                                    | 7   | 3 | 0 | 38.908                    |
| 2.1363          | 13                                   | 8   | 2 | 0 | 42.272                    |
| 2.0752          | 4                                    | 6   | 6 | 0 | 43.579                    |
| 2.0471          | 1L                                   | 7   | 5 | 0 | 44.208                    |
| 1.9955          | 2                                    | 8   | 3 | 1 | 45.414                    |
| 1.9687          | 27                                   | 8   | 4 | 0 | 46.068                    |
| 1.9451          | 1L                                   | 9   | 1 | 0 | 46.660                    |
| 1.8806          | 3                                    | 3   | 1 | 4 | 48.360                    |
| 1.8554          | 11                                   | 9   | 3 | 0 | 49.059                    |
| 1.8417          | 11                                   | 6   | 6 | 2 | 49.450                    |
| 1.7802          | 1                                    | 4   | 2 | 4 | 51.279                    |
| 1.7606          | 32                                   | 8   | 6 | 0 | 51.892                    |
| 1.7464          | 18                                   | 7   | 3 | 3 | 52.346                    |
| 1.7259          | 5                                    | 10  | 2 | 0 | 53.016                    |
| 1.7093          | 2                                    | 9   | 5 | 0 | 53.570                    |
| 1.6811          | 10                                   | 4   | 4 | 4 | 54.543                    |
| 1.6654M         | 21                                   | 8   | 2 | 3 | 55.100                    |
| 1.6654M         |                                      | 5   | 3 | 4 | 55.100                    |
| 1.6515          | 6                                    | 6   | 0 | 4 | 55.606                    |
| 1.6228M         | 7                                    | 7   | 5 | 3 | 56.675                    |
| 1.6228M         |                                      | 6   | 2 | 4 | 56.675                    |
| 1.6108          | 18                                   | 8   | 6 | 2 | 57.138                    |
| 1.5952          | 1L                                   | 9   | 6 | 1 | 57.746                    |
| 1.5833          | 1                                    | 8   | 4 | 3 | 58.224                    |
| 1.5724M         | 4                                    | 9   | 5 | 2 | 58.666                    |
| 1.5724M         |                                      | 2   | 0 | 5 | 58.666                    |
| 1.5565          | 2                                    | 8   | 8 | 0 | 59.324                    |

Sodium Germanium Phosphate,  $\text{NaGe}_2(\text{PO}_4)_3$

Synonym

Sodium germanium orthophosphate

CAS registry no.  
22239-25-4

Sample

The sample was made by heating a 1:4:6 molar mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{GeO}_2$ , and  $(\text{NH}_4)_2\text{HPO}_4$  up to 500 °C. Then it was reground and heated at 1050 °C overnight.

Color

Colorless

Structure

Rhombohedral, R<sup>\*\*</sup>. This phase was reported to be isostructural with  $\text{NaZr}_2(\text{PO}_4)_3$  in space group R3c (Hagman and Kierkegaard, 1968). However several lines could not be indexed on that space group.

Crystallographic constants of this sample  
(Hexagonal axes)

$a = 8.0894(6) \text{ \AA}$   
 $c = 21.522(3)$

$c/a = 2.6605$

$Z = 6$

$V = 1219.68 \text{ \AA}^3$

Density (calc) = 3.701 g/cm<sup>3</sup>

Figure of merit

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

Additional pattern

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

Reference

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $26 \pm 1 \text{ }^\circ\text{C}$<br>Internal standard Si, SRM 640a |                  |       |   |    |                      |
|---|------------------|-------|---|----|----------------------|
| $d(\text{\AA})$   | $I^{\text{rel}}$ | $hkl$ |   |    | $2\theta ({}^\circ)$ |
| $\sigma = \pm 1$  |                  |       |   |    |                      |
| 5.869   | 25               | 0     | 1 | 2  | 15.083               |
| 4.265   | 68               | 1     | 0 | 4  | 20.809               |
| 4.044   | 83               | 1     | 1 | 0  | 21.960               |
| 3.524   | 100              | 1     | 1 | 3  | 25.255               |
| 3.326   | 1                | 2     | 0 | 2  | 26.784               |
| 2.936   | 57               | 0     | 2 | 4  | 30.418               |
| 2.717   | 1L               | 2     | 0 | 5  | 32.946               |
| 2.684   | 88               | 1     | 1 | 6  | 33.357               |
| 2.629   | 15               | 2     | 1 | 1  | 34.082               |
| 2.570   | 2                | 1     | 2 | 2  | 34.882               |
| 2.511   | 4                | 0     | 1 | 8  | 35.732               |
| 2.375   | 11               | 2     | 1 | 4  | 37.844               |
| 2.336   | 29               | 3     | 0 | 0  | 38.508               |
| 2.311   | 1                | 0     | 2 | 7  | 38.938               |
| 2.221   | 7                | 3     | 0 | 3  | 40.590               |
| 2.1331  | 5                | 2     | 0 | 8  | 42.337               |
| 2.0587M   | 8                | 1     | 1 | 9  | 43.946               |
| 2.0587M   |                  | 1     | 0 | 10 | 43.946               |
| 2.0215  | 4                | 2     | 2 | 0  | 44.797               |
| 2.0073  | 3                | 2     | 1 | 7  | 45.133               |
| 1.9573  | 10               | 3     | 0 | 6  | 46.352               |
| 1.9133  | 3                | 3     | 1 | 2  | 47.483               |
| 1.8868  | 16               | 1     | 2 | 8  | 48.190               |
| 1.8335  | 9                | 0     | 2 | 10 | 49.685               |
| 1.8273  | 11               | 1     | 3 | 4  | 49.864               |
| 1.7941  | 3                | 0     | 0 | 12 | 50.854               |
| 1.7617  | 26               | 2     | 2 | 6  | 51.858               |
| 1.7286  | 3                | 0     | 4 | 2  | 52.925               |
| 1.6698  | 17               | 2     | 1 | 10 | 54.943               |
| 1.6424  | 4                | 1     | 3 | 7  | 55.941               |
| 1.6027  | 1                | 3     | 2 | 1  | 57.452               |
| 1.5749  | 10               | 3     | 1 | 8  | 58.562               |
| 1.5399  | 10               | 3     | 2 | 4  | 60.030               |
| 1.5287  | 16               | 4     | 1 | 0  | 60.515               |
| 1.5062  | 5                | 2     | 3 | 5  | 61.515               |
| 1.5018  | 4                | 0     | 1 | 14 | 61.716               |
| 1.4953  | 1                | 4     | 1 | 3  | 62.017               |
| 1.4674  | 5                | 0     | 4 | 8  | 63.327               |
| 1.4421  | 12               | 1     | 3 | 10 | 64.572               |
| 1.4240  | 4                | 3     | 2 | 7  | 65.496               |
| 1.4219  | 1                | 3     | 0 | 12 | 65.602               |
| 1.4063  | 15               | 4     | 1 | 6  | 66.427               |
| 1.3797  | 2                | 2     | 3 | 8  | 67.875               |
| 1.3586  | 6                | 4     | 0 | 10 | 69.081               |
| 1.3554  | 5                | 0     | 5 | 4  | 69.266               |

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

| $d(\text{\AA})$  | $I^{\text{rel}}$ | $h k \ell$ | $2\theta (\text{\\circ})$ |
|------------------|------------------|------------|---------------------------|
| $\sigma = \pm 1$ |                  |            |                           |
| 1.3525           | 5                | 1 1 15     | 69.436                    |
| 1.3480           | 8                | 3 3 0      | 69.699                    |
| 1.3293           | 6                | 1 2 14     | 70.826                    |
| 1.3213           | 1L               | 2 4 1      | 71.319                    |
| 1.2880           | 4                | 4 1 9      | 73.463                    |
| 1.2657           | 1L               | 4 2 5      | 74.975                    |

Sodium Iron Silicate (Acmite),  $\text{NaFe}(\text{SiO}_3)_2$

Synonyms

Sodium iron metasilicate  
Aegirine  
Aegirite

CAS registry no.  
14483-20-6

Sample

The sample was made by heating  $\text{Na}_2\text{CO}_3$ ,  $\text{Fe}_2\text{O}_3$ , and  $\text{SiO}_2$  for about 10 days at temperatures up to 950 °C. The sample contained a small amount of  $\text{Fe}_2\text{O}_3$ .

Color

Deep brown

Structure

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

Crystallographic constants of this sample

$$a = 9.5277(14) \text{ \AA}$$

$$b = 8.8067(14)$$

$$c = 5.287(1)$$

$$\beta = 104.686(13)^\circ$$

$$a/b = 1.0819$$

$$c/b = 0.6003$$

$$Z = 4$$

$$V = 429.13 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.576 \text{ g/cm}^3$$

Figure of merit

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

Additional patterns

PDF card 18-1222 (Frondel and Klein, 1965)

Nat. Min.

PDF card 31-1309 (Nickel and Mark, 1965)

Nat. Min.

Borg and Smith (1969)

Brown (1982)

References

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

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

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

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

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

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

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

Sodium Molybdenum Oxide Hydrate,  $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$

Synonym

Sodium molybdate hydrate

CAS registry no.  
10102-40-6

Sample

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

Color

Colorless

Structure

Orthorhombic, Pcab (61) (Pistorius, 1960). The structure of  $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$  was determined by Matsumoto et al. (1975).

Crystallographic constants of this sample

$a = 10.566(2)$  Å

$b = 13.842(2)$

$c = 8.4823(15)$

$a/b = 0.7633$

$c/b = 0.6128$

$Z = 8$

$V = 1240.65$  Å<sup>3</sup>

Density (calc) 2.591 g/cm<sup>3</sup>

Figure of merit

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

Additional pattern

PDF card 13-236 (Pistorius, 1960)

References

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

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

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

Sodium Molybdenum Oxide Hydrate,  $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$  - (continued)

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

Sodium Strontium Niobium Oxide,  $\text{NaSr}_2(\text{NbO}_3)_5$

Synonym

Sodium strontium niobate

Sample

The sample was made by heating  $\text{NaNbO}_3$ ,  $\text{SrCO}_3$ , and  $\text{Nb}_2\text{O}_5$  up to 1300 °C for about 48 hours, with intermediate grindings.

Color

Colorless

Structure

Tetragonal. Tungsten bronze structure (Morin, 1973). This phase has been reported as orthorhombic (Giess et al., 1969) but this work found no evidence for symmetry lower than tetragonal. This phase occurs in the region of the  $\text{NaNbO}_3$ - $\text{SrNb}_2\text{O}_6$  system from 65 to 79%  $\text{SrNb}_2\text{O}_6$  and changes cell size little over the region (Morin, 1973).

Crystallographic constants of this sample

$$a = 12.3562(9) \text{ \AA}$$

$$c = 3.8979(6)$$

$$c/a = 0.3155$$

$$Z = 2$$

$$V = 595.11 \text{ \AA}^3$$

$$\text{Density (calc)} = 5.038 \text{ g/cm}^3$$

Figure of merit

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

Polymorphism

Van Uitert (1968) reports that  $\text{NaSr}_2\text{Nb}_5\text{O}_{15}$  is stable as tetragonal only above 184 °C.

Additional pattern

PDF card 27-787 (Morin, Priv. Comm., 1974). The composition given was  $\text{Na}_{0.18}\text{Sr}_{0.41}\text{NbO}_3$ .

References

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

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

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

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ mean } T = 26.1 \text{ }^\circ\text{C}$<br>Internal standard Si, SRM 640a |                  |         |                      |  |
|--|------------------|---------|----------------------|--|
| $d(\text{\AA})$  | $I^{\text{rel}}$ | $h k l$ | $2\theta ({}^\circ)$ |  |
| $\sigma = \pm 4$   |                  |         |                      |  |
| 6.184  | 1                | 2 0 0   | 14.312               |  |
| 5.526  | 1                | 2 1 0   | 16.025               |  |
| 4.369  | 1                | 2 2 0   | 20.312               |  |
| 3.899  | 45               | 0 0 1   | 22.789               |  |
| 3.556  | 2                | 1 1 1   | 25.022               |  |
| 3.426  | 32               | 3 2 0   | 25.989               |  |
| 3.297  | 2                | 2 0 1   | 27.025               |  |
| 3.185  | 47               | 2 1 1   | 27.992               |  |
| 3.088  | 8                | 4 0 0   | 28.887               |  |
| 2.996  | 62               | 4 1 0   | 29.795               |  |
| 2.909  | 23               | 2 2 1   | 30.711               |  |
| 2.760  | 100              | 3 1 1   | 32.414               |  |
| 2.574  | 25               | 3 2 1   | 34.831               |  |
| 2.421  | 5                | 4 0 1   | 37.101               |  |
| 2.376  | 2                | 4 1 1   | 37.841               |  |
| 2.295  | 4                | 5 2 0   | 39.232               |  |
| 2.255  | 2                | 4 2 1   | 39.952               |  |
| 2.185  | 1L               | 4 4 0   | 41.287               |  |
| 2.1186   | 7                | 5 3 0   | 42.641               |  |
| 2.0591M  | 1                | 6 0 0   | 43.936               |  |
| 2.0591M  |                  | 5 1 1   | 43.936               |  |
| 2.0312   | 2                | 6 1 0   | 44.572               |  |
| 1.9774   | 1                | 5 2 1   | 45.854               |  |
| 1.9546   | 9                | 6 2 0   | 46.419               |  |
| 1.9491   | 23               | 0 0 2   | 46.558               |  |
| 1.9314   | 1                | 5 4 0   | 47.011               |  |
| 1.9064   | 1                | 4 4 1   | 47.664               |  |
| 1.8608   | 2                | 5 3 1   | 48.908               |  |
| 1.8421   | 12               | 6 3 0   | 49.437               |  |
| 1.8206   | 9                | 6 0 1   | 50.060               |  |
| 1.7606   | 4                | 3 0 2   | 51.890               |  |
| 1.7470M  | 33               | 5 5 0   | 52.326               |  |
| 1.7470M  |                  | 6 2 1   | 52.326               |  |
| 1.7295   | 12               | 5 4 1   | 52.896               |  |
| 1.6943   | 8                | 3 2 2   | 54.085               |  |
| 1.6656   | 9                | 6 3 1   | 55.095               |  |
| 1.6479   | 2                | 4 0 2   | 55.736               |  |
| 1.6336   | 17               | 4 1 2   | 56.268               |  |
| 1.6197   | 3                | 3 3 2   | 56.794               |  |
| 1.6080   | 4                | 7 0 1   | 57.246               |  |

Sodium Strontium Niobium Oxide,  $\text{NaSr}_2(\text{NbO}_3)_5$  - (continued)

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

# Strontium Aluminum Oxide, SrAl<sub>2</sub>O<sub>4</sub>

**Synonym**

Strontium aluminate

CAS registry no.  
12004-37-4

**Sample**

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

**Color**

Colorless

**Structure**

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

**Crystallographic constants of this sample**

$$a = 8.4424(8) \text{ \AA}$$

$$b = 8.8221(10)$$

$$c = 5.1607(6)$$

$$\beta = 93.415(6)^\circ$$

$$a/b = 0.9570$$

$$c/b = 0.5850$$

$$Z = 4$$

$$V = 383.68 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.559 \text{ g/cm}^3$$

**Figures of merit**

$$F_{30} = 83.1(0.0071, 51)$$

$$M_{20} = 47.6$$

**Polymorphism**

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

**Additional pattern**

PDF card 9-39 (Carlson, 1955)

**References**

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

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

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

Strontium Aluminum Oxide, SrAl<sub>2</sub>O<sub>4</sub> - (continued)

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

Strontium Silicate,  $\alpha$ -SrSiO<sub>3</sub>

Synonym

Strontium metasilicate

CAS registry no.  
12712-63-9

Sample

The sample was made by heating a mixture of SrCO<sub>3</sub> and amorphous SiO<sub>2</sub> for 21 hours at 1400 °C, followed by grinding and heating about 5 days at 1300 °C.

Color  
Colorless

Structure

Monoclinic, C2 (5). The structure of  $\alpha$ -SrSiO<sub>3</sub> was determined by Machida et al. (1982). This phase was earlier indexed as hexagonal.

Crystallographic constants of this sample

$$a = 12.340(3) \text{ \AA}$$

$$b = 7.136(2)$$

$$c = 10.880(3)$$

$$\beta = 111.51(3)^\circ$$

$$a/b = 1.7293$$

$$c/b = 1.5247$$

$$Z = 12$$

$$V = 891.35 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.660 \text{ g/cm}^3$$

Figure of merit

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

Polymorphism

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

Additional patterns

PDF card 30-1302 (Shimizu et al., 1970)

PDF card 32-1258 (Moir et al., 1975).

References

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

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 25.2 °C |                                      |     |   |       |        |
|--|--------------------------------------|-----|---|-------|--------|
| Internal standards Si, SRM 640a                                    |                                      |     |   |       |        |
| Fluorophlogopite, SRM 675  |                                      |     |   |       |        |
| d( $\text{\AA}$ )  | I <sup>rel</sup><br>$\sigma = \pm 2$ | hkl |   | 2θ(°) |        |
| 6.05   | 1L                                   | 1   | 1 | 0     | 14.624 |
| 5.73   | 1L                                   | 2   | 0 | 0     | 15.457 |
| 5.056  | 17                                   | 0   | 0 | 2     | 17.527 |
| 4.803  | 1L                                   | 1   | 1 | 1     | 18.456 |
| 4.755  | 1                                    | -2  | 0 | 2     | 18.647 |
| 4.320  | 1                                    | -1  | 1 | 2     | 20.541 |
| 3.566M   | 66                                   | 0   | 2 | 0     | 24.951 |
| 3.566M   |                                      | -3  | 1 | 1     | 24.951 |
| 3.365  | 30                                   | 0   | 2 | 1     | 26.466 |
| 3.254  | 1                                    | 2   | 0 | 2     | 27.389 |
| 3.225  | 1L                                   | -1  | 1 | 3     | 27.639 |
| 2.928  | 50                                   | 3   | 1 | 1     | 30.510 |
| 2.917  | 100                                  | 0   | 2 | 2     | 30.627 |
| 2.760  | 1                                    | 2   | 2 | 1     | 32.409 |
| 2.531+   | 21                                   | 2   | 0 | 3     | 35.437 |
| 2.531+   |                                      | 0   | 0 | 4     | 35.437 |
| 2.514  | 9                                    | -1  | 1 | 4     | 35.692 |
| 2.462  | 1                                    | 3   | 1 | 2     | 36.463 |
| 2.452  | 1                                    | 0   | 2 | 3     | 36.621 |
| 2.324  | 1                                    | -5  | 1 | 2     | 38.715 |
| 2.185  | 1L                                   | 5   | 1 | 0     | 41.287 |
| 2.073  | 27                                   | 3   | 1 | 3     | 43.629 |
| 2.060  | 75                                   | -3  | 3 | 1     | 43.906 |
| 1.914  | 18                                   | 6   | 0 | 0     | 47.453 |
| 1.909  | 22                                   | 3   | 3 | 1     | 47.593 |
| 1.897  | 3                                    | -6  | 0 | 4     | 47.913 |
| 1.854  | 1L                                   | 1   | 3 | 3     | 49.092 |
| 1.808  | 1L                                   | -2  | 0 | 6     | 50.430 |
| 1.7837   | 10                                   | 0   | 4 | 0     | 51.169 |
| 1.7579   | 2                                    | -6  | 2 | 1     | 51.976 |
| 1.7525+  | 2                                    | -3  | 3 | 4     | 52.151 |
| 1.7525+  |                                      | -3  | 1 | 6     | 52.151 |
| 1.6858M  | 9                                    | 0   | 0 | 6     | 54.378 |
| 1.6858M  |                                      | 6   | 2 | 0     | 54.378 |
| 1.6821   | 11                                   | 0   | 4 | 2     | 54.507 |
| 1.6767   | 7                                    | -6  | 2 | 4     | 54.699 |
| 1.6724   | 2                                    | -7  | 1 | 1     | 54.851 |
| 1.6023   | 4                                    | 3   | 3 | 3     | 57.470 |
| 1.5983   | 5                                    | 7   | 1 | 0     | 57.626 |
| 1.5967   | 4                                    | 5   | 1 | 3     | 57.689 |

Strontium Zirconium Phosphate,  $\text{SrZr}_4(\text{PO}_4)_6$

Synonym

Strontium zirconium orthophosphate

CAS registry no.

67972-88-7

Sample

The sample was made by heating a 1:4:6 molar mixture of  $\text{SrCO}_3$ ,  $\text{ZrO}_2$ , and  $(\text{NH}_4)_2\text{HPO}_4$  up to 500 °C. After regrinding it was heated to 1300 °C for 70 hours.

Color

Colorless

Structure

Rhombohedral, R\*\*. The structure is similar to that of  $\text{NaZr}_2(\text{PO}_4)_3$  (Chernorukov et al., 1978.)

Crystallographic constants of this sample  
(Hexagonal axes)

$$a = 8.6935(4) \text{ \AA}$$

$$c = 23.389(2)$$

$$c/a = 2.6904$$

$$Z = 3$$

$$V = 1530.85 \text{ \AA}^3$$

$$\text{Density (calc)} = 3.327 \text{ g/cm}^3$$

Figure of merit

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

Reference

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

| CuK $\alpha$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $26 \pm 1$ °C<br>Internal standards Si, SRM 640a<br>Fluorophlogopite, SRM 675 |                                      |         |   |    |                      |
|---|--------------------------------------|---------|---|----|----------------------|
| $d(\text{\AA})$   | $I^{\text{rel}}$<br>$\sigma = \pm 3$ | $h k l$ |   |    | $2\theta (\text{°})$ |
|   |                                      | 0       | 0 | 3  |                      |
| 7.796   | 4                                    | 0       | 0 | 3  | 11.341               |
| 7.170   | 9                                    | 1       | 0 | 1  | 12.334               |
| 6.333   | 10                                   | 0       | 1 | 2  | 13.972               |
| 4.619   | 35                                   | 1       | 0 | 4  | 19.198               |
| 4.348   | 75                                   | 1       | 1 | 0  | 20.407               |
| 3.972   | 5                                    | 0       | 1 | 5  | 22.366               |
| 3.795   | 74                                   | 1       | 1 | 3  | 23.420               |
| 3.716   | 2                                    | 0       | 2 | 1  | 23.926               |
| 3.583   | 2                                    | .2      | 0 | 2  | 24.829               |
| 3.165   | 36                                   | 0       | 2 | 4  | 28.172               |
| 3.053   | 1                                    | 1       | 0 | 7  | 29.232               |
| 2.933   | 6                                    | 2       | 0 | 5  | 30.451               |
| 2.900   | 100                                  | 1       | 1 | 6  | 30.804               |
| 2.825   | 12                                   | 2       | 1 | 1  | 31.646               |
| 2.766   | 1                                    | 1       | 2 | 2  | 32.341               |
| 2.726   | 5                                    | 0       | 1 | 8  | 32.830               |
| 2.5579  | 10                                   | 2       | 1 | 4  | 35.053               |
| 2.5084  | 34                                   | 3       | 0 | 0  | 35.768               |
| 2.4307  | 4                                    | 1       | 2 | 5  | 36.951               |
| 2.3884  | 3                                    | 3       | 0 | 3  | 37.630               |
| 2.3089  | 5                                    | 2       | 0 | 8  | 38.977               |
| 2.2305  | 5                                    | 1       | 1 | 9  | 40.406               |
| 2.1736  | 8                                    | 2       | 2 | 0  | 41.512               |
| 2.1665  | 8                                    | 2       | 1 | 7  | 41.655               |
| 2.1098  | 13                                   | 3       | 0 | 6  | 42.827               |
| 2.0933  | 4                                    | 2       | 2 | 3  | 43.182               |
| 2.0395  | 16                                   | 1       | 2 | 8  | 44.381               |
| 1.9862  | 7                                    | 0       | 2 | 10 | 45.639               |
| 1.9664  | 7                                    | 1       | 3 | 4  | 46.125               |
| 1.9486  | 2                                    | 0       | 0 | 12 | 46.570               |
| 1.9067  | 4                                    | 3       | 1 | 5  | 47.655               |
| 1.8980  | 29                                   | 2       | 2 | 6  | 47.888               |
| 1.8762  | 1                                    | 4       | 0 | 1  | 48.480               |
| 1.8582  | 2                                    | 0       | 4 | 2  | 48.981               |
| 1.8526  | 1                                    | 2       | 0 | 11 | 49.138               |
| 1.8064M   | 16                                   | 2       | 1 | 10 | 50.482               |
| 1.8064M   |                                      | 3       | 0 | 9  | 50.482               |
| 1.7702  | 3                                    | 1       | 3 | 7  | 51.588               |
| 1.7495  | 1                                    | 1       | 0 | 13 | 52.245               |
| 1.7456  | 1                                    | 0       | 4 | 5  | 52.372               |
| 1.6989  | 8                                    | 3       | 1 | 8  | 53.926               |
| 1.6665  | 1                                    | 2       | 2 | 9  | 55.061               |
| 1.6561  | 6                                    | 3       | 2 | 4  | 55.438               |
| 1.6426  | 20                                   | 4       | 1 | 0  | 55.931               |
| 1.6308  | 5                                    | 0       | 1 | 14 | 56.374               |

Strontium Zirconium Phosphate,  $\text{SrZr}_4(\text{PO}_4)_6$  - (continued)

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

# Tantalum Tungsten Oxide, Ta<sub>2</sub>WO<sub>8</sub>

## Synonym

Tantalum tungstate

## Sample

The single phase composition was prepared by heating 52.4 mole % of Ta<sub>2</sub>O<sub>5</sub> with 47.6 mole % of WO<sub>3</sub> for 30 hours at 1350 °C. (A mixture of 50 mole % each yielded 2 phases.) The composition reported here may be regarded either as oxygen deficient (Ta,W)<sub>3</sub>O<sub>7.986</sub> or as containing excess metal (Ta, W)<sub>3.012</sub>O<sub>8</sub> (Santoro et al., 1979).

## Color

Pale yellow gray

## Structure

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

## Crystallographic constants of this sample

a = 16.6997(15) Å

b = 17.7296(15)

c = 3.8798(4)

a/b = 0.9419

c/b = 0.2188

Z = 8

V = 1148.7 Å<sup>3</sup>

Density (calc) = 7.791 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 73.6(0.0074,55)

## Additional patterns

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

## References

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

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

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

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

Tantalum Tungsten Oxide, Ta<sub>2</sub>W<sub>0</sub><sub>8</sub> - (continued)

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

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

Thorium Molybdenum Oxide,  $\alpha$ -Th(MoO<sub>4</sub>)<sub>2</sub>

Synonym

Thorium molybdate

Sample

ThO<sub>2</sub> and MoO<sub>3</sub> in a molar ratio of 1 to 2 were ground together and heated to 700 °C for 70 hours in a Pt crucible.

Color

Colorless

Structure

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

Crystallographic constants of this sample

$$a = 10.3174(7) \text{ \AA}$$

$$b = 14.4835(10)$$

$$c = 9.7491(7)$$

$$a/b = 0.7124$$

$$c/b = 0.6731$$

$$Z = 8$$

$$V = 1456.8 \text{ \AA}^3$$

$$\text{Density (calc)} = 5.032 \text{ g/cm}^3$$

Figure of merit

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

Polymorphism

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

Additional pattern

PDF card 27-1468 (Thoret, 1974)

Reference

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 25.9 °C<br>Internal standard Ag, a = 4.08651 Å |                  |       |  |                     |
|---|------------------|-------|--|---------------------|
| $d(\text{\AA})$   | $I^{\text{rel}}$ | $hkl$ |  | $2\theta(\text{°})$ |
| $\sigma = \pm 3$  |                  |       |  |                     |
| 7.241   | 15               | 0 2 0 |  | 12.213              |
| 6.371   | 8                | 1 1 1 |  | 13.890              |
| 5.929   | 5                | 1 2 0 |  | 14.929              |
| 5.156   | 29               | 2 0 0 |  | 17.185              |
| 5.065   | 77               | 1 2 1 |  | 17.496              |
| 4.874   | 27               | 0 0 2 |  | 18.185              |
| 4.348   | 16               | 2 1 1 |  | 20.408              |
| 4.202   | 6                | 2 2 0 |  | 21.125              |
| 4.045   | 10               | 0 2 2 |  | 21.955              |
| 3.991   | 15               | 1 3 1 |  | 22.256              |
| 3.859   | 10               | 2 2 1 |  | 23.031              |
| 3.766   | 63               | 1 2 2 |  | 23.604              |
| 3.621   | 47               | 0 4 0 |  | 24.563              |
| 3.544   | 100              | 2 0 2 |  | 25.105              |
| 3.417   | 21               | 1 4 0 |  | 26.059              |
| 3.315   | 7                | 2 3 1 |  | 26.877              |
| 3.257   | 11               | 1 3 2 |  | 27.364              |
| 3.225   | 33               | 1 4 1 |  | 27.635              |
| 3.184   | 23               | 2 2 2 |  | 28.003              |
| 3.163   | 7                | 3 1 1 |  | 28.194              |
| 3.107   | 62               | 3 2 0 |  | 28.713              |
| 3.032   | 25               | 1 1 3 |  | 29.437              |
| 2.961M  | 71               | 2 4 0 |  | 30.154              |
| 2.961M  |                  | 3 2 1 |  | 30.154              |
| 2.908   | 31               | 0 4 2 |  | 30.722              |
| 2.850   | 22               | 1 2 3 |  | 31.361              |
| 2.799   | 11               | 1 4 2 |  | 31.947              |
| 2.750   | 2                | 2 0 3 |  | 32.531              |
| 2.701   | 7                | 2 1 3 |  | 33.135              |
| 2.682   | 2                | 1 5 1 |  | 33.382              |
| 2.620   | 17               | 3 2 2 |  | 34.197              |
| 2.609   | 11               | 1 3 3 |  | 34.347              |
| 2.579   | 4                | 4 0 0 |  | 34.755              |
| 2.574   | 3                | 2 2 3 |  | 34.833              |
| 2.5326  | 25               | 2 4 2 |  | 35.414              |
| 2.4936M   | 10               | 3 4 0 |  | 35.987              |
| 2.4936M   |                  | 4 0 1 |  | 35.987              |
| 2.4582  | 6                | 4 1 1 |  | 36.524              |
| 2.4374  | 15               | 0 0 4 |  | 36.846              |
| 2.4297M   | 9                | 4 2 0 |  | 36.968              |
| 2.4297M   |                  | 3 3 2 |  | 36.968              |
| 2.4151M   | 5                | 3 4 1 |  | 37.199              |
| 2.4151M   |                  | 0 6 0 |  | 37.199              |
| 2.3538  | 8                | 1 4 3 |  | 38.205              |
| 2.2849  | 24               | 1 6 1 |  | 39.404              |

Thorium Molybdenum Oxide,  $\alpha$ -Th(MoO<sub>4</sub>)<sub>2</sub> - (continued)

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

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

Thorium Molybdenum Oxide,  $\beta$ -Th(MoO<sub>4</sub>)<sub>2</sub>

Synonym

Thorium molybdate

Sample

The sample was prepared by heating ThO<sub>2</sub> and MoO<sub>3</sub> in a 1 to 2 molar ratio in a Pt crucible at 700 °C for 20 3/4 hours, then reheated at 1000 °C for 2 1/4 hours.

Color

Colorless

Structure

Hexagonal, P<sub>6</sub> (174). The structure was determined by Thoret et al. (1968).

Crystallographic constants of this sample

$$a = 17.5764(6) \text{ \AA}$$

$$c = 6.2265(2)$$

$$c/a = 0.3543$$

$$Z = 9$$

$$V = 1665.84 \text{ \AA}^3$$

$$\text{Density (calc)} = 4.951 \text{ g/cm}^3$$

Figure of merit

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

Polymorphism

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

Additional pattern

PDF card 27-1469 (Thoret, 1974)

References

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 25.6 °C |                  |       |        |  |
|--|------------------|-------|--------|--|
| Internal standard W, $a = 3.16524 \text{ \AA}$                     |                  |       |        |  |
| d(A)   | I <sup>rel</sup> | hkl   | 2θ(°)  |  |
| $\sigma = \pm 3$   |                  |       |        |  |
| 8.79   | 2                | 1 1 0 | 10.051 |  |
| 5.764M   | 8                | 1 0 1 | 15.360 |  |
| 5.764M   |                  | 2 1 0 | 15.360 |  |
| 5.075M   | 48               | 1 1 1 | 17.461 |  |
| 5.075M   |                  | 3 0 0 | 17.461 |  |
| 4.821  | 7                | 2 0 1 | 18.389 |  |
| 4.227M   | 17               | 2 1 1 | 21.002 |  |
| 4.227M   |                  | 3 1 0 | 21.002 |  |
| 3.935  | 51               | 3 0 1 | 22.580 |  |
| 3.592  | 79               | 2 2 1 | 24.768 |  |

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

Thorium Molybdenum Oxide,  $\beta$ -Th(MoO<sub>4</sub>)<sub>2</sub> - (continued)

| $d(\text{\AA})$  | $I^{\text{rel}}$ | $hkl$  | $2\theta(^{\circ})$ |
|------------------|------------------|--------|---------------------|
| $\sigma = \pm 3$ |                  |        |                     |
| 1.6510M          | 3                | 5 4 2  | 55.623              |
| 1.6510M          |                  | 7 3 1  | 55.623              |
| 1.6328M          | 11               | 6 3 2  | 56.297              |
| 1.6328M          |                  | 9 0 1  | 56.297              |
| 1.6048           | 8                | 8 2 1  | 57.371              |
| 1.5972           | 2                | 4 3 3  | 57.667              |
| 1.5787           | 5                | 7 4 0  | 58.408              |
| 1.5569           | 5                | 0 0 4  | 59.308              |
| 1.5458M          | 3                | 6 5 1  | 59.776              |
| 1.5458M          |                  | 8 3 0  | 59.776              |
| 1.5303M          | 19               | 5 5 2  | 60.444              |
| 1.5303M          |                  | 7 4 1  | 60.444              |
| 1.4995M          | 2                | 8 3 1  | 61.822              |
| 1.4995M          |                  | 9 2 0  | 61.822              |
| 1.4881           | 4                | 3 0 4  | 62.347              |
| 1.4797           | 2                | 6 2 3  | 62.744              |
| 1.4650M          | 3                | 8 2 2  | 63.444              |
| 1.4650M          |                  | 6 6 0  | 63.444              |
| 1.4580M          | 2                | 9 2 1  | 63.786              |
| 1.4580M          |                  | 7 5 0  | 63.786              |
| 1.4461           | 16               | 7 1 3  | 64.371              |
| 1.4259           | 4                | 6 6 1  | 65.398              |
| 1.4196M          | 2                | 6 5 2  | 65.724              |
| 1.4196M          |                  | 7 5 1  | 65.724              |
| 1.4096           | 10               | 4 1 4  | 66.248              |
| 1.4075M          | 21               | 7 4 2  | 66.362              |
| 1.4075M          |                  | 10 1 1 | 66.362              |
| 1.4011           | 2                | 8 4 1  | 66.703              |
| 1.3847M          | 2                | 7 2 3  | 67.597              |
| 1.3847M          |                  | 8 3 2  | 67.597              |
| 1.3750           | 8                | 3 3 4  | 68.139              |
| 1.3723           | 5                | 9 3 1  | 68.295              |
| 1.3533           | 1                | 5 1 4  | 69.389              |
| 1.3513M          | 2                | 9 2 2  | 69.508              |
| 1.3513M          |                  | 11 0 1 | 69.508              |
| 1.3412           | 3                | 5 5 3  | 70.106              |
| 1.3353           | 1                | 10 2 1 | 70.464              |
| 1.3268           | 5                | 6 0 4  | 70.981              |
| 1.3206M          | 2                | 7 3 3  | 71.362              |
| 1.3206M          |                  | 7 5 2  | 71.362              |
| 1.3102M          | 20               | 10 1 2 | 72.018              |
| 1.3102M          |                  | 8 5 1  | 72.018              |
| 1.2967           | 4                | 8 2 3  | 72.891              |
| 1.2824           | 4                | 9 3 2  | 73.838              |
| 1.2685           | 5                | 12 0 0 | 74.785              |
| 1.2652           | 4                | 6 5 3  | 75.010              |
| 1.2563           | 6                | 7 4 3  | 75.635              |
| 1.2412           | 1                | 1 0 5  | 76.718              |
| 1.2396           | 1                | 8 3 3  | 76.838              |
| 1.2308M          | 10               | 8 5 2  | 77.486              |

| $d(\text{\AA})$  | $I^{\text{rel}}$ | $hkl$  | $2\theta(^{\circ})$ |
|------------------|------------------|--------|---------------------|
| $\sigma = \pm 3$ |                  |        |                     |
| 1.2308M          |                  | 7 7 1  | 77.486              |
| 1.2169           | 2                | 2 1 5  | 78.542              |
| 1.2145M          | 1                | 9 5 1  | 78.726              |
| 1.2145M          |                  | 12 1 0 | 78.726              |
| 1.2085           | 12               | 6 3 4  | 79.199              |
| 1.1982           | 5                | 2 2 5  | 80.015              |
| 1.1962           | 6                | 10 4 1 | 80.173              |
| 1.1858           | 4                | 10 1 3 | 81.019              |
| 1.1745           | 3                | 12 0 2 | 81.968              |
| 1.1660           | 7                | 4 1 5  | 82.699              |
| 1.1641M          | 17               | 7 7 2  | 82.860              |
| 1.1641M          |                  | 9 6 0  | 82.860              |
| 1.1508M          | 1                | 8 7 1  | 84.039              |
| 1.1508M          |                  | 10 5 0 | 84.039              |
| 1.1453           | 3                | 9 0 4  | 84.531              |
| 1.1441           | 1                | 9 6 1  | 84.646              |
| 1.1426           | 2                | 4 2 5  | 84.780              |
| 1.1411           | 1                | 12 2 1 | 84.913              |
| 1.1348           | 7                | 10 4 2 | 85.495              |
| 1.1258           | 7                | 8 5 3  | 86.348              |
| 1.1134M          | 1                | 11 3 2 | 87.557              |
| 1.1134M          |                  | 11 4 1 | 87.557              |
| 1.1089           | 2                | 5 2 5  | 88.002              |
| 1.1072M          | 6                | 13 1 1 | 88.167              |
| 1.1072M          |                  | 12 3 0 | 88.167              |
| 1.0902M          | 6                | 9 6 2  | 89.913              |
| 1.0902M          |                  | 12 3 1 | 89.913              |
| 1.0818           | 1                | 8 8 1  | 90.808              |
| 1.0806           | 1L               | 5 3 5  | 90.934              |
| 1.0792M          | 1                | 10 5 2 | 91.085              |
| 1.0792M          |                  | 9 7 1  | 91.085              |
| 1.0742           | 3                | 7 7 3  | 91.624              |
| 1.0715           | 2                | 8 6 3  | 91.932              |
| 1.0668           | 2                | 6 6 4  | 92.447              |
| 1.0631M          | 1                | 11 4 2 | 92.864              |
| 1.0631M          |                  | 13 2 1 | 92.864              |
| 1.0596           | 3                | 7 1 5  | 93.269              |
| 1.0581M          | 4                | 13 1 2 | 93.443              |
| 1.0581M          |                  | 11 5 1 | 93.443              |
| 1.0509           | 2                | 10 4 3 | 94.272              |
| 1.0484           | 2                | 12 1 3 | 94.567              |
| 1.0440           | 4                | 9 3 4  | 95.099              |
| 1.0379           | 3                | 0 0 6  | 95.839              |
| 1.0360           | 1                | 8 8 2  | 96.072              |
| 1.0334M          | 1                | 14 1 1 | 96.385              |
| 1.0334M          |                  | 9 8 0  | 96.385              |
| 1.0307           | 1                | 1 1 6  | 96.724              |
| 1.0281           | 1                | 2 0 6  | 97.056              |
| 1.0196M          | 1                | 13 2 2 | 98.141              |
| 1.0196M          |                  | 9 8 1  | 98.141              |

Thorium Silicate (Huttonite),  $\beta$ -ThSiO<sub>4</sub>

**Sample**

The sample was prepared by heating an equimolar mixture of ThO<sub>2</sub> and SiO<sub>2</sub> for a total of 60 hours at 1550 °C, with periodic grinding. The sample contains a small amount of ThO<sub>2</sub> as a second phase.

**Color**

Colorless

**Structure**

Monoclinic, P2<sub>1</sub>/n (14). Isostructural with monazite (Pabst and Hutton, 1951). The structure of monazite, CePO<sub>4</sub>, was determined by Mooney (1948).

**Crystallographic constants of this sample**

$$a = 6.7759(4) \text{ \AA}$$

$$b = 6.9648(4)$$

$$c = 6.4982(4)$$

$$\beta = 104.99(1)^\circ$$

$$Z = 4$$

$$V = 296.23 \text{ \AA}^3$$

$$\text{Density (calc)} = 7.267 \text{ g/cm}^3$$

**Figure of merit**

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

**Polymorphism**

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

**Additional pattern**

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

**References**

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

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 27.1 °C<br>Internal standards W, a = 3.16524 Å<br>Fluorophlogopite, SRM 675 |                                      |       |   |   |                      |
|--|--------------------------------------|-------|---|---|----------------------|
| $d(\text{\AA})$  | $I^{\text{rel}}$<br>$\sigma = \pm 2$ | $hkl$ |   |   | $2\theta (\text{°})$ |
| 5.260  | 19                                   | -1    | 0 | 1 | 16.842               |
| 4.769  | 8                                    | 1     | 1 | 0 | 18.591               |
| 4.663  | 42                                   | 0     | 1 | 1 | 19.017               |
| 4.198  | 74                                   | -1    | 1 | 1 | 21.145               |
| 4.039  | 31                                   | 1     | 0 | 1 | 21.988               |
| 3.493  | 30                                   | 1     | 1 | 1 | 25.478               |
| 3.2726   | 60                                   | 2     | 0 | 0 | 27.228               |
| 3.1395   | 7                                    | 0     | 0 | 2 | 28.406               |
| 3.0743   | 100                                  | 1     | 2 | 0 | 29.021               |
| 3.0440   | 13                                   | 0     | 2 | 1 | 29.317               |
| 2.9618   | 26                                   | 2     | 1 | 0 | 30.149               |
| 2.8830   | 27                                   | -1    | 1 | 2 | 30.994               |
| 2.8622   | 61                                   | 0     | 1 | 2 | 31.225               |
| 2.6302   | 21                                   | -2    | 0 | 2 | 34.059               |
| 2.4614   | 18                                   | -2    | 1 | 2 | 36.475               |
| 2.4210   | 13                                   | 1     | 1 | 2 | 37.105               |
| 2.3835   | 7                                    | -2    | 2 | 1 | 37.711               |
| 2.3432   | 7                                    | -1    | 2 | 2 | 38.384               |
| 2.2493   | 1                                    | -3    | 0 | 1 | 40.054               |
| 2.1774   | 25                                   | 0     | 3 | 1 | 41.437               |
| 2.1617   | 23                                   | -1    | 0 | 3 | 41.751               |
| 2.1402   | 25                                   | -3    | 1 | 1 | 42.191               |
| 2.1020   | 23                                   | 2     | 2 | 1 | 42.995               |
| 2.0821   | 4                                    | 3     | 1 | 0 | 43.426               |
| 2.0129   | 3                                    | 1     | 3 | 1 | 45.000               |
| 1.9733   | 6                                    | -3    | 1 | 2 | 45.953               |
| 1.9392   | 27                                   | 2     | 1 | 2 | 46.810               |
| 1.9129   | 10                                   | 3     | 0 | 1 | 47.492               |
| 1.8924   | 19                                   | -2    | 3 | 1 | 48.040               |
| 1.8721   | 24                                   | -1    | 3 | 2 | 48.593               |
| 1.8584   | 8                                    | 1     | 0 | 3 | 48.975               |
| 1.8488   | 15                                   | 3     | 2 | 0 | 49.247               |
| 1.7933   | 13                                   | 0     | 2 | 3 | 50.876               |
| 1.7715   | 16                                   | -3    | 2 | 2 | 51.549               |
| 1.7533   | 8                                    | -3    | 0 | 3 | 52.123               |
| 1.7424   | 16                                   | 2     | 3 | 1 | 52.473               |
| 1.7261   | 19                                   | 1     | 3 | 2 | 53.010               |
| 1.7002   | 1                                    | -3    | 1 | 3 | 53.881               |
| 1.6828   | 11                                   | 1     | 4 | 0 | 54.484               |
| 1.6778   | 6                                    | 0     | 4 | 1 | 54.660               |
| 1.6527   | 1                                    | -1    | 4 | 1 | 55.560               |
| 1.6458   | 5                                    | -4    | 1 | 1 | 55.816               |
| 1.6351   | 10                                   | -4    | 0 | 2 | 56.213               |
| 1.6154   | 2                                    | -3    | 3 | 1 | 56.960               |
| 1.5992   | 3                                    | 1     | 4 | 1 | 57.590               |

Thorium Silicate (Huttonite),  $\beta\text{-ThSiO}_4$  - (continued)

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

Thorium Tantalum Oxide,  $\text{Th}_2\text{Ta}_2\text{O}_9$

Synonym

Thorium tantalate

Sample

The sample was prepared from stoichiometric proportions of  $\text{ThO}_2$  and  $\text{Ta}_2\text{O}_5$ . The following heating schedule, alternating with further grinding, yielded a nearly single phase product: 1400 °C for 4½ days, at 1625 °C for 2 hours, at 1625 °C again for 2 hours, and finally at 1625 °C for 2½ hours. Traces of unreacted  $\text{ThO}_2$  remained.

Comment

Due to the minor radiation hazard, only one intensity chart was processed. Because of the  $\text{ThO}_2$  impurity and lack of repetitive measurements, the intensities may be in error by a few percent.

Color

Yellowish white

Structure

Monoclinic. The cell was found by use of the Visser program, followed by calculation of the supercell given below. The data may also be indexed on a C-centered orthorhombic cell with twice the volume of the given monoclinic cell. The phase is apparently not isostructural with  $\text{Th}_2\text{Nb}_2\text{O}_9$ , for which single crystal work has been done by Cava et al. (1981).

Crystallographic constants of this sample

$$a = 9.681(2) \text{ \AA}$$

$$b = 7.4006(11)$$

$$c = 9.6766(15)$$

$$\beta = 106.398(10)^\circ$$

$$a/b = 1.3081$$

$$c/b = 1.3075$$

$$Z = 4 \text{ (assumed)}$$

$$V = 665.08 \text{ \AA}^3$$

$$\text{Density (calc)} = 9.687 \text{ g/cm}^3$$

Figures of merit

$$F_{30} = 30.4(0.0092, 107)$$

$$M_{20} = 24.0$$

Reference

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

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 25.8 °C<br>Internal standards W, a = 3.16524 Å<br>Fluorophlogopite, SRM 675 |                  |         |     |                      |
|--|------------------|---------|-----|----------------------|
| $d(\text{\AA})$  | $I^{\text{rel}}$ | $h k l$ |     | $2\theta (\text{°})$ |
| 4.722M   | 2                | -2      | 0 1 | 18.777               |
| 4.722M   |                  | -1      | 0 2 | 18.777               |
| 3.976M   | 4                | -2      | 1 1 | 22.344               |
| 3.976M   |                  | -1      | 1 2 | 22.344               |
| 3.932M   | 3                | 2       | 1 0 | 22.596               |
| 3.932M   |                  | 0       | 1 2 | 22.596               |
| 3.749M   | 4                | 2       | 0 1 | 23.711               |
| 3.749M   |                  | 1       | 0 2 | 23.711               |
| 3.701  | 6                | 0       | 2 0 | 24.024               |
| 3.437M   | 8                | 1       | 2 0 | 25.900               |
| 3.437M   |                  | 0       | 2 1 | 25.900               |
| 3.336  | 7                | -1      | 2 1 | 26.700               |
| 3.223M   | 100              | -3      | 0 1 | 27.659               |
| 3.223M   |                  | -1      | 0 3 | 27.659               |
| 3.119  | 64               | 1       | 2 1 | 28.594               |
| 3.094M   | 7                | 3       | 0 0 | 28.837               |
| 3.094M   |                  | 0       | 0 3 | 28.837               |
| 2.995M   | 5                | -3      | 0 2 | 29.810               |
| 2.995M   |                  | -2      | 0 3 | 29.810               |
| 2.955M   | 3                | -3      | 1 1 | 30.221               |
| 2.955M   |                  | -1      | 1 3 | 30.221               |
| 2.912M   | 48               | -2      | 2 1 | 30.679               |
| 2.912M   |                  | -1      | 2 2 | 30.679               |
| 2.894M   | 46               | 2       | 2 0 | 30.869               |
| 2.894M   |                  | 0       | 2 2 | 30.869               |
| 2.856M   | 1                | 3       | 1 0 | 31.291               |
| 2.856M   |                  | 0       | 1 3 | 31.291               |
| 2.676  | 39               | -2      | 2 2 | 33.462               |
| 2.634M   | 11               | 2       | 2 1 | 34.004               |
| 2.634M   |                  | 1       | 2 2 | 34.004               |
| 2.430M   | 5                | -3      | 2 1 | 36.959               |
| 2.430M   |                  | -1      | 2 3 | 36.959               |
| 2.375M   | 3                | 3       | 2 0 | 37.859               |
| 2.375M   |                  | 0       | 2 3 | 37.859               |
| 2.350  | 1                | -1      | 3 1 | 38.271               |
| 2.299M   | 1                | -4      | 1 1 | 39.154               |
| 2.299M   |                  | -1      | 1 4 | 39.154               |
| 2.2821   | 1                | 2       | 2 2 | 39.454               |
| 2.1895+  | 7                | 3       | 2 1 | 41.196               |
| 2.1895+  |                  | 1       | 2 3 | 41.196               |
| 2.1742M  | 1                | -4      | 0 3 | 41.500               |
| 2.1742M  |                  | -3      | 0 4 | 41.500               |
| 2.1180   | 1                | -3      | 2 3 | 42.654               |
| 2.0875M  | 2                | -4      | 1 3 | 43.309               |
| 2.0875M  |                  | -3      | 1 4 | 43.309               |
| 2.0811   | 2                | -2      | 3 2 | 43.449               |
| 2.0342M  | 1                | 4       | 1 1 | 44.503               |
| 2.0342M  |                  | 1       | 1 4 | 44.503               |
| 1.9887M  | 2                | -4      | 2 2 | 45.579               |
| 1.9887M  |                  | -2      | 2 4 | 45.579               |

Thorium Tantalum Oxide,  $\text{Th}_2\text{Ta}_2\text{O}_9$  - (continued)

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

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

Thorium Tungsten Oxide,  $\alpha$ -Th(WO<sub>4</sub>)<sub>2</sub>

Synonym

Thorium tungstate

Sample

The sample was prepared by grinding together stoichiometric amounts of ThO<sub>2</sub> and WO<sub>3</sub>, heating with daily intermittent grinding for extended periods at temperatures up to 875 °C. The sample contained a small amount of ThO<sub>2</sub> as impurity. Hence, the intensity of lines 2θ = 27.370, 31.927, 45.765, and 54.293 may be somewhat in error.

Color

Colorless

Structure

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

Crystallographic constants of this sample

$$a = 10.3709(14) \text{ \AA}$$

$$b = 14.518(2)$$

$$c = 9.7133(13)$$

$$a/b = 0.7143$$

$$c/b = 0.6601$$

$$Z = 8$$

$$V = 1462.5 \text{ \AA}^3$$

$$\text{Density (calc)} = 6.610 \text{ g/cm}^3$$

Figure of merit

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

Polymorphism

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

Additional pattern

PDF card 28-1373 (Thoret, 1974)

References

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

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

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

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

Thorium Tungsten Oxide,  $\alpha$ -Th(WO<sub>4</sub>)<sub>2</sub> - (continued)

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

Vanadium Oxide (Karelianite), V<sub>2</sub>O<sub>3</sub>

Synonyms

Vanadium sesquioxide  
Vanadium trioxide  
Vanadic oxide

Sample

The sample was prepared by reducing V<sub>2</sub>O<sub>5</sub> in a controlled atmosphere with the partial pressure of oxygen less than or equal to 10<sup>-20</sup> atm. It was then heated at 600 °C for 8 hours, at 925 °C for 18 hours, and at 900 °C for 30 hours with intermittent grinding.

Color

Black

Structure

Rhombohedral, R̄3c (167). The structure was solved by Zachariasen (1928).

Crystallographic constants of this sample

(Hexagonal axes)

a = 4.9540(2) Å

c = 14.0083(10)

c/a = 2.8277

Z = 6

V = 297.7 Å<sup>3</sup>

Density (calc) = 5.016 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 64.6(0.0097,48)

Additional pattern

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

References

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

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

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 27.4 °C<br>Internal standard W, a = 3.16524 Å |                            |     |   |    |         |
|--|----------------------------|-----|---|----|---------|
| d(Å)   | I <sup>rel</sup><br>σ = ±2 | hkl |   |    | 2θ(°)   |
| 3.658  | 71                         | 0   | 1 | 2  | 24.314  |
| 2.713  | 100                        | 1   | 0 | 4  | 32.987  |
| 2.477  | 80                         | 1   | 1 | 0  | 36.231  |
| 2.336  | 6                          | 0   | 0 | 6  | 38.514  |
| 2.189  | 36                         | 1   | 1 | 3  | 41.216  |
| 2.0519   | 7                          | 2   | 0 | 2  | 44.099  |
| 1.8292   | 34                         | 0   | 2 | 4  | 49.811  |
| 1.6990   | 85                         | 1   | 1 | 6  | 53.923  |
| 1.6210   | 1                          | 0   | 1 | 8  | 56.745  |
| 1.5798   | 7                          | 1   | 2 | 2  | 58.366  |
| 1.4718   | 24                         | 2   | 1 | 4  | 63.115  |
| 1.4298   | 31                         | 3   | 0 | 0  | 65.195  |
| 1.3316   | 14                         | 1   | 0 | 10 | 70.688  |
| 1.3180   | 3                          | 1   | 1 | 9  | 71.527  |
| 1.2385   | 6                          | 2   | 2 | 0  | 76.916  |
| 1.2193   | 4                          | 3   | 0 | 6  | 78.357  |
| 1.1972   | 1                          | 2   | 2 | 3  | 80.092  |
| 1.1728M  | 9                          | 3   | 1 | 2  | 82.114  |
| 1.1728M  |                            | 0   | 2 | 10 | 82.114  |
| 1.1674   | 2                          | 0   | 0 | 12 | 82.575  |
| 1.1267   | 4                          | 1   | 3 | 4  | 86.267  |
| 1.0940   | 12                         | 2   | 2 | 6  | 89.515  |
| 1.0601M  | 9                          | 0   | 4 | 2  | 93.207  |
| 1.0601M  |                            | 2   | 1 | 10 | 93.207  |
| 1.0559   | 3                          | 1   | 1 | 12 | 93.693  |
| 1.0255   | 1                          | 4   | 0 | 4  | 97.381  |
| .9745M   | 1                          | 2   | 3 | 2  | 104.456 |
| .9745M   |                            | 0   | 1 | 14 | 104.456 |
| .9690  | 1L                         | 2   | 2 | 9  | 105.295 |
| .9476  | 8                          | 3   | 2 | 4  | 108.760 |
| .9363  | 4                          | 4   | 1 | 0  | 110.711 |
| .9068M   | 4                          | 1   | 3 | 10 | 116.309 |
| .9068M   |                            | 2   | 0 | 14 | 116.309 |
| .9044  | 5                          | 3   | 0 | 12 | 116.799 |
| .8689  | 5                          | 4   | 1 | 6  | 124.874 |

Ytterbium Fluoride, YbF<sub>3</sub>

CAS registry no.  
13760-80-0

**Sample**

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

**Structure**

Orthorhombic, Pnma (62); isostructural with  
YF<sub>3</sub>. The structure of YF<sub>3</sub> was determined by  
Zalkin and Templeton (1953).

**Crystallographic constants of this sample**

$$a = 6.2164(2) \text{ \AA}$$

$$b = 6.7857(2)$$

$$c = 4.4316(2)$$

$$a/b = 0.9161$$

$$c/b = 0.6531$$

$$Z = 4$$

$$V = 186.94 \text{ \AA}^3$$

$$\text{Density (calc)} = 8.173 \text{ g/cm}^3$$

**Figure of merit**

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

**Polymorphism**

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

**Additional patterns**

PDF card 5-551 (Zalkin, Thesis, U. Calif., Berkeley, 1951)

PDF card 32-1418 (Greis, Thesis, U. Freiburg i. Br., Germany, 1976)

**References**

Thoma, R. E. and Brunton, G. D. (1966).

Inorg. Chem. 11, 1937.

Zalkin, A. and Templeton, D. H. (1953).

J. Am. Chem. Soc. 75, 2453.

| CuKα <sub>1</sub> λ = 1.540598 °<br>Internal standards W, a = 3.16524 °<br>Fluorophlogopite, SRM 675 |                            |     |   |   |        |
|--|----------------------------|-----|---|---|--------|
| d(Å)   | I <sup>rel</sup><br>σ = ±2 | hkl |   |   | 2θ(°)  |
| 3.712  | 19                         | 0   | 1 | 1 | 23.956 |
| 3.610  | 60                         | 1   | 0 | 1 | 24.641 |
| 3.394  | 62                         | 0   | 2 | 0 | 26.239 |
| 3.187  | 100                        | 1   | 1 | 1 | 27.973 |
| 3.107  | 1L                         | 2   | 0 | 0 | 28.711 |
| 2.826  | 66                         | 2   | 1 | 0 | 31.638 |
| 2.5447   | 3                          | 2   | 0 | 1 | 35.240 |
| 2.4720   | 27                         | 1   | 2 | 1 | 36.312 |
| 2.3828   | 3                          | 2   | 1 | 1 | 37.722 |
| 2.2912   | 1L                         | 2   | 2 | 0 | 39.291 |
| 2.2162   | 12                         | 0   | 0 | 2 | 40.679 |
| 2.0869   | 2                          | 1   | 0 | 2 | 43.322 |
| 2.0355   | 15                         | 2   | 2 | 1 | 44.473 |
| 2.0142   | 1L                         | 0   | 3 | 1 | 44.970 |
| 1.9956   | 20                         | 1   | 1 | 2 | 45.411 |
| 1.9164   | 40                         | 1   | 3 | 1 | 47.401 |
| 1.8769   | 26                         | 3   | 0 | 1 | 48.461 |
| 1.8551   | 15                         | 0   | 2 | 2 | 49.068 |
| 1.8286   | 32                         | 2   | 3 | 0 | 49.828 |
| 1.8090   | 18                         | 3   | 1 | 1 | 50.404 |
| 1.7778   | 14                         | 1   | 2 | 2 | 51.354 |
| 1.7437   | 23                         | 2   | 1 | 2 | 52.432 |
| 1.6962   | 12                         | 0   | 4 | 0 | 54.017 |
| 1.6425   | 17                         | 3   | 2 | 1 | 55.938 |
| 1.5539   | 6                          | 4   | 0 | 0 | 59.435 |
| 1.5349   | 12                         | 1   | 4 | 1 | 60.245 |
| 1.5135   | 2                          | 3   | 0 | 2 | 61.190 |
| 1.4771   | 6                          | 3   | 1 | 2 | 62.866 |
| 1.4664   | 1L                         | 4   | 0 | 1 | 63.377 |
| 1.4443   | 12                         | 3   | 3 | 1 | 64.461 |
| 1.4334   | 8                          | 4   | 1 | 1 | 65.014 |
| 1.4130   | 1                          | 4   | 2 | 0 | 66.072 |
| 1.4107   | 16                         | 2   | 3 | 2 | 66.192 |
| 1.4058   | 5                          | 1   | 1 | 3 | 66.452 |
| 1.3821   | 2                          | 3   | 2 | 2 | 67.744 |
| 1.3469   | 5                          | 0   | 4 | 2 | 69.766 |
| 1.3343   | 3                          | 2   | 0 | 3 | 70.525 |
| 1.3234   | 1                          | 1   | 2 | 3 | 71.189 |
| 1.3165   | 1                          | 1   | 4 | 2 | 71.620 |
| 1.3090   | 1L                         | 2   | 1 | 3 | 72.096 |
| 1.2976   | 1L                         | 0   | 5 | 1 | 72.827 |
| 1.2808   | 1L                         | 4   | 3 | 0 | 73.942 |
| 1.2725   | 6                          | 4   | 0 | 2 | 74.508 |
| 1.2703   | 6                          | 1   | 5 | 1 | 74.656 |
| 1.2585   | 7                          | 3   | 4 | 1 | 75.477 |

Ytterbium Fluoride,  $\text{YbF}_3$  - (continued)

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

Zinc Vanadium Oxide,  $\text{Zn}_3(\text{VO}_4)_2$

Synonym

Zinc vanadate

Sample

The sample was made by heating a 3:1 molar mixture of  $\text{ZnO}$  and  $\text{V}_2\text{O}_5$  at  $780^\circ\text{C}$  for 3 days, with several regroundings.

Color

Yellowish white

Structure

Orthorhombic, Abam (64) (Brisi, 1960). Isostructural with  $\text{Co}_3(\text{VO}_4)_2$ .

Crystallographic constants of this sample

$$a = 8.299(1) \text{ \AA}$$

$$b = 11.5284(14)$$

$$c = 6.1116(7)$$

$$a/b = 0.7199$$

$$c/b = 0.5301$$

$$Z = 4$$

$$V = 584.72 \text{ \AA}^3$$

$$\text{Density (calc)} = 4.839 \text{ g/cm}^3$$

Figure of merit

$$F_{30} = 66.6(0.010, 44)$$

Polymorphism

Brown and Hummel (1965) report two polymorphic changes in  $\text{Zn}_3(\text{VO}_4)_2$  at  $795^\circ$  and  $815^\circ\text{C}$ . This is disputed by Makarov et al. (1971).

Additional patterns

PDF card 16-830 (Brisi, 1960)

PDF card 19-1469 (Brown and Hummel, 1965)

Makarov et al. (1971)

References

Brisi, C. (1960). Ric. Sci. 30, 1339.

Brown, J. J. and Hummel, F. A. (1965). Trans. Br. Ceram. Soc. 64, 419.

Makarov, V. A., Fotiev, A. A., and Serebryakova, L. N. (1971). Russ. J. Inorg. Chem. Eng. Transl. 16, 1515.

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $26 \pm 1^\circ\text{C}$<br>Internal standard Si, SRM 640a |                                      |     |   |                         |
|--|--------------------------------------|-----|---|-------------------------|
| d(A)<br>$^\circ$   | I <sup>rel</sup><br>$\sigma = \pm 5$ | hkl |   | 2 $\theta$ ( $^\circ$ ) |
| 5.762  | 13                                   | 0   | 2 | 0                       |
| 4.731  | 18                                   | 1   | 2 | 0                       |
| 4.147  | 7                                    | 2   | 0 | 0                       |
| 3.367  | 20                                   | 2   | 2 | 0                       |
| 3.290  | 27                                   | 2   | 1 | 1                       |
| 3.059  | 1                                    | 0   | 0 | 2                       |
| 3.030  | 57                                   | 1   | 3 | 1                       |
| 2.882  | 30                                   | 0   | 4 | 0                       |
| 2.723  | 4                                    | 1   | 4 | 0                       |
| 2.700  | 9                                    | 0   | 2 | 2                       |
| 2.568  | 100                                  | 1   | 2 | 2                       |
| 2.494  | 47                                   | 3   | 2 | 0                       |
| 2.462M   | 25                                   | 3   | 1 | 1                       |
| 2.462M   |                                      | 2   | 0 | 2                       |
| 2.367  | 3                                    | 2   | 4 | 0                       |
| 2.263  | 3                                    | 2   | 2 | 2                       |
| 2.0964   | 37                                   | 0   | 4 | 2                       |
| 2.0878   | 36                                   | 1   | 5 | 1                       |
| 2.0747   | 1                                    | 4   | 0 | 0                       |
| 2.0323   | 1                                    | 1   | 4 | 2                       |
| 1.9533   | 3                                    | 4   | 2 | 0                       |
| 1.9319   | 4                                    | 3   | 2 | 2                       |
| 1.9203   | 4                                    | 0   | 6 | 0                       |
| 1.9154   | 4                                    | 2   | 5 | 1                       |
| 1.8716M  | 5                                    | 1   | 6 | 0                       |
| 1.8716M  |                                      | 2   | 4 | 2                       |
| 1.8061   | 4                                    | 2   | 1 | 3                       |
| 1.7588   | 6                                    | 1   | 3 | 3                       |
| 1.7167   | 8                                    | 4   | 0 | 2                       |
| 1.6509   | 3                                    | 2   | 3 | 3                       |
| 1.6457   | 4                                    | 4   | 2 | 2                       |
| 1.6237   | 7                                    | 3   | 1 | 3                       |
| 1.5963   | 23                                   | 1   | 6 | 2                       |
| 1.5863   | 8                                    | 5   | 1 | 1                       |
| 1.5778   | 12                                   | 3   | 6 | 0                       |
| 1.5276   | 13                                   | 0   | 0 | 4                       |
| 1.5145   | 6                                    | 2   | 6 | 2                       |
| 1.5014   | 3                                    | 1   | 5 | 3                       |
| 1.4848   | 4                                    | 2   | 7 | 1                       |
| 1.4748   | 38                                   | 4   | 4 | 2                       |
| 1.4542   | 2                                    | 1   | 2 | 4                       |
| 1.4414   | 13                                   | 0   | 8 | 0                       |
| 1.4377   | 2                                    | 5   | 4 | 0                       |
| 1.4331M  | 1                                    | 2   | 0 | 4                       |
| 1.4331M  |                                      | 2   | 5 | 3                       |

Zinc Vanadium Oxide,  $\text{Zn}_3(\text{VO}_4)_2$  - (continued)

| $d(\text{\AA})$  | $I^{\text{rel}}$ | $h k \ell$ | $2\theta(^{\circ})$ |
|------------------|------------------|------------|---------------------|
| $\sigma = \pm 5$ |                  |            |                     |
| 1.4095           | 1                | 4 6 0      | 66.254              |
| 1.3918           | 1                | 2 2 4      | 67.211              |
| 1.3786           | 2                | 3 7 1      | 67.937              |
| 1.3495           | 3                | 0 4 4      | 69.610              |
| 1.3400           | 1L               | 6 1 1      | 70.180              |
| 1.3028           | 9                | 3 2 4      | 72.493              |
| 1.2838           | 2                | 2 4 4      | 73.744              |
| 1.2789           | 4                | 5 1 3      | 74.070              |
| 1.2563           | 1                | 5 6 0      | 75.638              |
| 1.2471           | 3                | 6 4 0      | 76.290              |
| 1.2436           | 2                | 2 8 2      | 76.543              |
| 1.2302           | 3                | 4 0 4      | 77.534              |

Zirconium Boride, ZrB<sub>2</sub>

Synonym

Zirconium diboride

CAS registry no.

12045-64-6

Sample

The sample was prepared at NBS by S. Lang.

Color

Very dark gray

Structure

Hexagonal, P6/mmm (191). Kiessling (1949) and Norton et al. (1949) studied the structure of ZrB<sub>2</sub>. This phase is isomorphous with AlB<sub>2</sub>.

Crystallographic constants of this sample

$$a = 3.16870(8) \text{ \AA}$$

$$c = 3.53002(10)$$

$$c/a = 1.1140$$

$$Z = 1$$

$$V = 30.70 \text{ \AA}^3$$

$$\text{Density (calc)} = 6.104 \text{ g/cm}^3$$

Figure of merit

$$F_{23} = 175.3(0.0057, 23)$$

Additional pattern

PDF card 6-610 (Am. Electro Metal Co.)

References

Kiessling, R. (1949). Acta Chem. Scand. 3, 90.

Norton, J. T., Blumenthal, H., and Sindeband, J. (1949). Metall. Trans. 185, 749.

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 24.9 $^{\circ}\text{C}$ |                  |     |   |   |                  |
|--|------------------|-----|---|---|------------------|
| Internal standard Si, SRM 640a   |                  |     |   |   |                  |
| d(A)   | I <sup>rel</sup> | hkl |   |   | 20( $^{\circ}$ ) |
|  | $\sigma = \pm 1$ |     |   |   |                  |
| 3.530  | 30               | 0   | 0 | 1 | 25.205           |
| 2.7445   | 67               | 1   | 0 | 0 | 32.601           |
| 2.1663   | 100              | 1   | 0 | 1 | 41.658           |
| 1.7652   | 9                | 0   | 0 | 2 | 51.746           |
| 1.5843   | 19               | 1   | 1 | 0 | 58.184           |
| 1.4845   | 21               | 1   | 0 | 2 | 62.515           |
| 1.4455   | 16               | 1   | 1 | 1 | 64.404           |
| 1.3722   | 8                | 2   | 0 | 0 | 68.298           |
| 1.2789   | 16               | 2   | 0 | 1 | 74.071           |
| 1.1790   | 13               | 1   | 1 | 2 | 81.585           |
| 1.1769   | 1                | 0   | 0 | 3 | 81.770           |
| 1.0832   | 8                | 2   | 0 | 2 | 90.654           |
| 1.0813   | 10               | 1   | 0 | 3 | 90.853           |
| 1.0372   | 7                | 2   | 1 | 0 | 95.918           |
| .9951  | 14               | 2   | 1 | 1 | 101.442          |
| .9446  | 4                | 1   | 1 | 3 | 109.266          |
| .9147  | 3                | 3   | 0 | 0 | 114.733          |
| .8942  | 10               | 2   | 1 | 2 | 118.958          |
| .8932  | 6                | 2   | 0 | 3 | 119.185          |
| .8855  | 4                | 3   | 0 | 1 | 120.899          |
| .8825  | 2                | 0   | 0 | 4 | 121.593          |
| .8402  | 4                | 1   | 0 | 4 | 132.938          |
| .8122  | 7                | 3   | 0 | 2 | 143.047          |

Zirconium Hydrogen Phosphate Hydrate,  $\text{Zr}(\text{HPO}_4)_2 \cdot \text{H}_2\text{O}$

Synonym

Zirconium hydrogen orthophosphate hydrate

CAS registry no.

13933-56-7

Sample

The sample was prepared by the method of Alberti and Torracca (1968).  $\text{ZrOCl} \cdot 8\text{H}_2\text{O}$  was dissolved in  $\text{H}_2\text{O}$ . HF and  $\text{H}_3\text{PO}_4$  were added and the solution allowed to evaporate slowly at room temperature. The crystals formed were very fine needles.

Color

Colorless

Structure

Monoclinic,  $P2_1/n$  (14) (Ahrland and Albertsson, 1969). The structure was determined by Clearfield and Smith (1969).

Crystallographic constants of this sample

$$a = 15.463(4) \text{ \AA}$$

$$b = 5.294(2)$$

$$c = 9.0674(15)$$

$$\beta = 101.70(2)^\circ$$

$$a/b = 2.9209$$

$$c/b = 1.7128$$

$$Z = 4$$

$$V = 726.83 \text{ \AA}^3$$

$$\text{Density (calc)} = 2.753 \text{ g/cm}^3$$

Figure of merit

$$F_{30} = 21.0(0.013, 108)$$

Additional patterns

PDF card 19-1489 (Sedlakova and Pekarks, 1966)

PDF card 21-396 (Michel and Weiss, 1967)

PDF card 21-397 (Priv. Comm., Winkler, 1968)

PDF card 22-1022 (Ahrland and Albertsson, 1969)

References

Ahrland, S. and Albertsson, J. (1969). Acta Chem. Scand. 23, 1446.

Alberti, G. and Torracca, E. (1968). J. Inorg. Nucl. Chem. 30, 317.

Clearfield, A. and Smith, G. D. (1969). Inorg. Chem. 8, 431.

Michel, E. and Weiss, A. (1967). Z. Naturforsch. 22B, 1100.

Sedlakova, L. and Pekarks, V. (1966). J. Less-Common Met. 10, 130.

| $d(\text{\AA})$ | $I^{\text{rel}}$<br>$\sigma = \pm 1$ | $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ mean } T = 26 \pm 2 \text{ }^\circ\text{C}$ |     |     |                            |
|-----------------|--------------------------------------|--|-----|-----|----------------------------|
|                 |                                      | Internal standards Si, SRM 640a  |     |     |                            |
|                 |                                      | Fluorophlogopite, SRM 675  |     |     |                            |
| $d(\text{\AA})$ | $I^{\text{rel}}$<br>$\sigma = \pm 1$ | $h$  | $k$ | $l$ | $2\theta (\text{ }^\circ)$ |
| 7.59            | 100                                  | 2  | 0   | 0   | 11.653                     |
| 4.489           | 14                                   | -1   | 1   | 1   | 19.761                     |
| 4.441           | 8                                    | 0  | 0   | 2   | 19.978                     |
| 4.052           | 1L                                   | 3  | 0   | 1   | 21.917                     |
| 3.785           | 1                                    | 4  | 0   | 0   | 23.483                     |
| 3.568           | 51                                   | -3   | 1   | 1   | 24.934                     |
| 3.531           | 31                                   | 2  | 0   | 2   | 25.198                     |
| 3.220           | 3                                    | -4   | 0   | 2   | 27.683                     |
| 3.082           | 1                                    | 4  | 1   | 0   | 28.948                     |
| 3.045           | 2                                    | -3   | 1   | 2   | 29.309                     |
| 3.022           | 1L                                   | -1   | 0   | 3   | 29.539                     |
| 2.649M          | 14                                   | -5   | 1   | 1   | 33.811                     |
| 2.649M          |                                      | 0  | 2   | 0   | 33.811                     |
| 2.626           | 14                                   | -1   | 1   | 3   | 34.112                     |
| 2.524M          | 4                                    | -1   | 2   | 1   | 35.539                     |
| 2.524M          |                                      | 6  | 0   | 0   | 35.539                     |
| 2.475           | 1L                                   | 1  | 1   | 3   | 36.263                     |
| 2.408           | 6                                    | 5  | 1   | 1   | 37.305                     |
| 2.353           | 2                                    | 3  | 0   | 3   | 38.219                     |
| 2.277           | 1L                                   | 6  | 1   | 0   | 39.544                     |
| 2.219           | 1L                                   | 0  | 0   | 4   | 40.631                     |
| 2.197           | 1                                    | -6   | 1   | 2   | 41.059                     |
| 2.169           | 3                                    | 4  | 2   | 0   | 41.600                     |
| 2.164           | 2                                    | -5   | 1   | 3   | 41.705                     |
| 2.118           | 3                                    | 2  | 2   | 2   | 42.663                     |
| 2.111           | 2                                    | -4   | 0   | 4   | 42.806                     |
| 2.045           | 5                                    | -4   | 2   | 2   | 44.258                     |
| 2.038           | 4                                    | -7   | 1   | 1   | 44.425                     |
| 2.023           | 3                                    | 2  | 0   | 4   | 44.769                     |
| 1.996           | 1                                    | 3  | 2   | 2   | 45.407                     |
| 1.968           | 1L                                   | -7   | 1   | 2   | 46.077                     |
| 1.930           | 1L                                   | 5  | 0   | 3   | 47.055                     |
| 1.8922M         | 5                                    | 8  | 0   | 0   | 48.044                     |
| 1.8922M         |                                      | 5  | 2   | 1   | 48.044                     |
| 1.8791          | 5                                    | 7  | 1   | 1   | 48.400                     |
| 1.8647M         | 5                                    | 4  | 2   | 2   | 48.800                     |
| 1.8647M         |                                      | -6   | 0   | 4   | 48.800                     |

# Zirconium Titanium Oxide, ZrTiO<sub>4</sub>

## Synonym

Zirconium titanate

CAS registry no.  
12036-70-3

## Sample

The sample was prepared by heating equimolar amounts of ZrO<sub>2</sub> and TiO<sub>2</sub> at 1500 °C for 66 hours. It was then heat-treated at 1500 °C for 17 hours and quenched in distilled water.

## Color

Pale pink

## Structure

Orthorhombic, Pnab (60). The unit cell was determined by Coughanour et al. (1954) and the space group by Newnham (1967).

## Crystallographic constants of this sample

$$a = 5.0358(5) \text{ Å}$$

$$b = 5.4874(6)$$

$$c = 4.8018(6)$$

$$a/b = 0.9177$$

$$c/b = 0.8751$$

$$Z = 2$$

$$V = 132.69 \text{ Å}^3$$

$$\text{Density (calc)} = 5.084 \text{ g/cm}^3$$

## Figure of merit

$$F_{30} = 68.0(0.011, 41)$$

## Additional pattern

PDF card 7-290 (Coughanour et al., 1954)

## References

Coughanour, L. W., Roth, R. S., and DeProssse, V. A. (1954). J. Res. Natl. Bur. Stand. (U.S.), 52, 37.

Newnham, R. E. (1967). J. Am. Ceram. Soc. 50, 216.

| CuKα <sub>1</sub> λ = 1.540598 Å; mean T = 25.5 °C<br>Internal standard W, a = 3.16524 Å |                  |     |   |   |        |
|--|------------------|-----|---|---|--------|
| d(Å)   | I <sup>rel</sup> | hkl |   |   | 2θ(°)  |
| σ = ±1   |                  |     |   |   |        |
| 3.614  | 16               | 0   | 1 | 1 | 24.614 |
| 2.934  | 100              | 1   | 1 | 1 | 30.443 |
| 2.744  | 13               | 0   | 2 | 0 | 32.612 |
| 2.517  | 10               | 2   | 0 | 0 | 35.642 |
| 2.408  | 9                | 1   | 2 | 0 | 37.312 |
| 2.229  | 3                | 2   | 0 | 1 | 40.431 |
| 2.154  | 10               | 1   | 2 | 1 | 41.911 |
| 2.0661   | 4                | 2   | 1 | 1 | 43.781 |
| 2.0158   | 1L               | 1   | 1 | 2 | 44.931 |
| 1.8542   | 13               | 2   | 2 | 0 | 49.092 |
| 1.8067   | 11               | 0   | 2 | 2 | 50.472 |
| 1.7376   | 13               | 2   | 0 | 2 | 52.632 |
| 1.7096   | 9                | 0   | 3 | 1 | 53.562 |
| 1.7013   | 12               | 1   | 2 | 2 | 53.843 |
| 1.6192   | 6                | 1   | 3 | 1 | 56.813 |
| 1.5366   | 1L               | 0   | 1 | 3 | 60.174 |
| 1.5224   | 10               | 3   | 1 | 1 | 60.794 |
| 1.4679   | 11               | 2   | 2 | 2 | 63.305 |
| 1.4318   | 4                | 3   | 2 | 0 | 65.096 |
| 1.4144   | 6                | 2   | 3 | 1 | 65.996 |
| 1.3506   | 1L               | 2   | 0 | 3 | 69.548 |
| 1.3345   | 1L               | 3   | 1 | 2 | 70.508 |
| 1.3233   | 4                | 1   | 4 | 0 | 71.199 |
| 1.3121   | 1L               | 2   | 1 | 3 | 71.899 |
| 1.2763   | 1                | 1   | 4 | 1 | 74.250 |
| 1.2590   | 1                | 4   | 0 | 0 | 75.441 |
| 1.2298   | 1L               | 3   | 2 | 2 | 77.562 |
| 1.2174   | 1L               | 4   | 0 | 1 | 78.503 |
| 1.2046M  | 2                | 2   | 4 | 0 | 79.504 |
| 1.2046M  |                  | 0   | 3 | 3 | 79.504 |
| 1.2003   | 1                | 0   | 0 | 4 | 79.844 |
| 1.1978   | 1                | 3   | 3 | 1 | 80.044 |
| 1.1910   | 1                | 0   | 4 | 2 | 80.594 |
| 1.1890   | 1                | 4   | 1 | 1 | 80.764 |
| 1.1716   | 1L               | 1   | 3 | 3 | 82.215 |
| 1.1591   | 3                | 1   | 4 | 2 | 83.296 |
| 1.1443   | 1                | 4   | 2 | 0 | 84.627 |
| 1.1336   | 1                | 3   | 1 | 3 | 85.608 |
| 1.1152   | 1                | 4   | 0 | 2 | 87.379 |
| 1.0997M  | 1L               | 0   | 2 | 4 | 88.930 |
| 1.0997M  |                  | 3   | 3 | 2 | 88.930 |
| 1.0864   | 2                | 2   | 3 | 3 | 90.312 |

# Zirconium Titanium Oxide, $Zr_5Ti_7O_{24}$

## Synonym

Zirconium titanate

## Sample

The sample was prepared by blending  $ZrO_2$  and  $TiO_2$  in the molar ratio of 5:7, doped with 1/2 mole % of  $Y_2O_3$  to promote crystallinity, and calcined at 1000 °C for 24 hours, twice reground and fired at 1500 °C for 20 hours, heat-treated at 1300 °C for several hours and cooled at 1 °C/hour to 650 °C (McHale et al., 1983).

## Color

Pale yellowish pink

## Structure

Orthorhombic, Pcan (60). The material has the columbite structure (McHale et al., 1983). The structure was confirmed by neutron powder diffraction (Bourdotted, 1983).

## Crystallographic constants of this sample

$$a = 5.3255(5) \text{ \AA}$$

$$b = 14.374(2)$$

$$c = 5.0236(5)$$

$$a/b = 0.3705$$

$$c/b = 0.3495$$

$$Z = 1$$

$$V = 384.55 \text{ \AA}^3$$

$$\text{Density (calc)} = 5.075 \text{ g/cm}^3$$

## Figure of merit

$$F_{30} = 66.8(0.011, 43)$$

## References

Bourdotted, P. (1983). Private communication.

McHale, A. E., Roth, R. S., Santoro, A., and Simmons, J. (1983). Am. Ceram. Soc. Bull. 62, 387.

| CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; mean T = 26.0 °C<br>Internal standard Si, SRM 640a |                                      |     |   |   |        |
|--|--------------------------------------|-----|---|---|--------|
| d(A)<br>°  | I <sup>rel</sup><br>$\sigma = \pm 1$ | hkl |   |   | 2θ(°)  |
| 7.19   | 4                                    | 0   | 2 | 0 | 12.305 |
| 3.592  | 6                                    | 0   | 4 | 0 | 24.765 |
| 3.561  | 14                                   | 1   | 3 | 0 | 24.986 |
| 3.543  | 11                                   | 1   | 1 | 1 | 25.116 |
| 3.257  | 8                                    | 1   | 2 | 1 | 27.358 |
| 2.904  | 100                                  | 1   | 3 | 1 | 30.760 |
| 2.663  | 15                                   | 2   | 0 | 0 | 33.628 |
| 2.561  | 3                                    | 1   | 4 | 1 | 35.013 |
| 2.513  | 9                                    | 0   | 0 | 2 | 35.704 |
| 2.498  | 4                                    | 2   | 2 | 0 | 35.921 |
| 2.475  | 2                                    | 0   | 1 | 2 | 36.264 |
| 2.396  | 4                                    | 0   | 6 | 0 | 37.506 |
| 2.353  | 4                                    | 2   | 0 | 1 | 38.217 |
| 2.321  | 1L                                   | 2   | 1 | 1 | 38.758 |
| 2.260  | 4                                    | 1   | 5 | 1 | 39.863 |
| 2.225  | 1                                    | 0   | 3 | 2 | 40.513 |
| 2.1389   | 4                                    | 2   | 4 | 0 | 42.218 |
| 2.1123   | 10                                   | 2   | 3 | 1 | 42.776 |
| 2.0594   | 5                                    | 0   | 4 | 2 | 43.931 |
| 2.0531   | 4                                    | 1   | 3 | 2 | 44.071 |
| 1.9680   | 1                                    | 2   | 4 | 1 | 46.084 |
| 1.9190   | 2                                    | 1   | 4 | 2 | 47.332 |
| 1.8904   | 2                                    | 0   | 5 | 2 | 48.092 |
| 1.8267   | 14                                   | 2   | 0 | 2 | 49.883 |
| 1.8127   | 2                                    | 2   | 1 | 2 | 50.293 |
| 1.7905   | 3                                    | 1   | 7 | 1 | 50.964 |
| 1.7814   | 15                                   | 2   | 6 | 0 | 51.241 |
| 1.7705   | 6                                    | 2   | 2 | 2 | 51.580 |
| 1.7333   | 10                                   | 0   | 6 | 2 | 52.772 |
| 1.6788   | 7                                    | 2   | 6 | 1 | 54.626 |
| 1.6651   | 11                                   | 3   | 3 | 0 | 55.112 |
| 1.6620   | 8                                    | 3   | 1 | 1 | 55.222 |
| 1.6285   | 2                                    | 2   | 4 | 2 | 56.461 |
| 1.5880   | 5                                    | 1   | 1 | 3 | 58.035 |
| 1.5804   | 11                                   | 3   | 3 | 1 | 58.342 |
| 1.5592   | 3                                    | 1   | 2 | 3 | 59.211 |
| 1.5425   | 1                                    | 2   | 5 | 2 | 59.920 |
| 1.5293   | 1L                                   | 1   | 9 | 0 | 60.489 |
| 1.5153   | 5                                    | 1   | 3 | 3 | 61.108 |
| 1.4895   | 1                                    | 2   | 8 | 0 | 62.283 |
| 1.4634   | 6                                    | 1   | 9 | 1 | 63.520 |
| 1.4612   | 5                                    | 0   | 8 | 2 | 63.627 |
| 1.4592   | 4                                    | 1   | 4 | 3 | 63.724 |
| 1.4534   | 4                                    | 2   | 6 | 2 | 64.012 |
| 1.4459   | 2                                    | 3   | 5 | 1 | 64.381 |

Zirconium Titanium Oxide,  $\text{Zr}_5\text{Ti}_7\text{O}_{24}$  - (continued)

| d(Å)    | $I^{\text{rel}}$ | hkl              |    |   | $2\theta (\circ)$ |
|---------|------------------|------------------|----|---|-------------------|
|         |                  | $\sigma = \pm 1$ |    |   |                   |
| 1.4209  | 1L               | 3                | 2  | 2 | 65.655            |
| 1.4176  | 1                | 2                | 0  | 3 | 65.827            |
| 1.4109  | 3                | 2                | 1  | 3 | 66.179            |
| 1.3877  | 2                | 3                | 3  | 2 | 67.434            |
| 1.3649  | 1                | 2                | 7  | 2 | 68.714            |
| 1.3448  | 1L               | 3                | 4  | 2 | 69.889            |
| 1.3093  | 2                | 4                | 2  | 0 | 72.076            |
| 1.2971  | 1L               | 3                | 7  | 1 | 72.862            |
| 1.2872  | 2                | 4                | 0  | 1 | 73.517            |
| 1.2817  | 1                | 4                | 1  | 1 | 73.886            |
| 1.2612  | 1L               | 1                | 7  | 3 | 75.292            |
| 1.2556  | 1L               | 0                | 0  | 4 | 75.681            |
| 1.2511  | 1                | 0                | 1  | 4 | 76.007            |
| 1.2371  | 1                | 0                | 2  | 4 | 77.022            |
| 1.2135  | 1                | 3                | 1  | 3 | 78.804            |
| 1.2050  | 1L               | 1                | 2  | 4 | 79.470            |
| 1.1979  | 1L               | 0                | 12 | 0 | 80.041            |
| 1.1874  | 1                | 3                | 9  | 0 | 80.892            |
| 1.1846M | 1L               | 1                | 3  | 4 | 81.121            |
| 1.1846M |                  | 3                | 7  | 2 | 81.121            |
| 1.1807  | 1                | 3                | 3  | 3 | 81.443            |
| 1.1762  | 1                | 4                | 0  | 2 | 81.827            |
| 1.1636  | 2                | 4                | 6  | 0 | 82.901            |
| 1.1607  | 2                | 4                | 2  | 2 | 83.156            |
| 1.1553  | 2                | 3                | 9  | 1 | 83.632            |
| 1.1336  | 2                | 4                | 6  | 1 | 85.613            |
| 1.1297M | 1L               | 2                | 10 | 2 | 85.981            |
| 1.1297M |                  | 1                | 9  | 3 | 85.981            |

# Molybdenum Oxide (Molybdite), MoO<sub>3</sub>

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

Synonym  
Molybdenum trioxide

CAS registry no.  
1313-27-5

## Structure

Orthorhombic, PbNm (62). The structure was refined from single crystal data (Kihlborg, 1963).

Atom positions  
All atoms were in special positions 4(c).

## Intensities

The peak intensities here differ from those on PDF card 5-508 (Swanson et al., 1954), especially at  $h\bar{k}\ell$ 's 040 and 060. From a spray-dried sample, recent experimental intensity measurements at NBS support the intensity values given in this calculated pattern.

## Crystallographic constants of this sample

$$\begin{aligned}a &= 3.9630 \text{ \AA} \\b &= 13.856 \\c &= 3.6966\end{aligned}$$

$$\begin{aligned}a/b &= 0.2860 \\c/b &= 0.2668\end{aligned}$$

(published values: 3.9628, 13.855, 3.6964  $\text{\AA}$ ; Kihlborg, 1963)

$$\begin{aligned}Z &= 4 \\V &= 202.99 \text{ \AA}^3 \\ \text{Density (calc)} &= 4.710 \text{ g/cm}^3\end{aligned}$$

## Thermal parameters

Isotropic (Kihlborg, 1963)

## Scattering factors

$O^{+2}$  (Suzuki, 1960)  
 $Mo^0$  (Thomas and Umeda, 1957), corrected for the real part of the anomalous dispersion (Cromer and Liberman, 1970).

## Scale factors

$\gamma = 0.686 \times 10^{-3}$   
 $I/I_{\text{corundum}}$  (calculated) = 4.80, for the scale reflection  $h\bar{k}\ell = 021$ .

## Polymorphism

A hexagonal form has been reported (PDF card 21-569, Spangenberg, Westinghouse Electric Corp., Horseheads, NY).

## Additional pattern

PDF card 5-508 (Swanson et al., 1954)

## References

Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.

Kihlborg, L. (1963). Ark. Kemi 21, 357.

Suzuki, T. (1960). Acta Crystallogr. 13, 279.

Swanson, H. E., Fuyat, R. K., and Ugrinic, G. M. (1954). Natl. Bur. Stand. (U.S.) Circ. 539, 3, 30.

Thomas, L. H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.

| Calculated Pattern (Peak heights) |                  |                |                          |  |
|-----------------------------------|------------------|----------------|--------------------------|--|
| $d(\text{\AA})^\circ$             | $I^{\text{rel}}$ | $h\bar{k}\ell$ | $2\theta(\text{^\circ})$ |  |
| 6.921                             | 36               | 0 2 0          | 12.78                    |  |
| 3.808                             | 77               | 1 1 0          | 23.34                    |  |
| 3.464                             | 38               | 0 4 0          | 25.70                    |  |
| 3.440                             | 31               | 1 2 0          | 25.88                    |  |
| 3.259                             | 100              | 0 2 1          | 27.34                    |  |
| 3.008                             | 7                | 1 3 0          | 29.68                    |  |
| 2.703                             | 15               | 1 0 1          | 33.12                    |  |
| 2.653                             | 26               | 1 1 1          | 33.76                    |  |
| 2.608                             | 3                | 1 4 0          | 34.36                    |  |
| 2.5267                            | 7                | 0 4 1          | 35.50                    |  |
| 2.3329                            | 8                | 1 3 1          | 38.56                    |  |
| 2.3088                            | 21               | 0 6 0          | 38.98                    |  |
| 2.2707                            | 13               | 1 5 0          | 39.66                    |  |
| 2.1311                            | 7                | 1 4 1          | 42.38                    |  |
| 1.9953                            | 2                | 1 6 0          | 45.42                    |  |
| 1.9812                            | 8                | 2 0 0          | 45.76                    |  |
| 1.9586+                           | 12               | 0 6 1          | 46.32                    |  |
| 1.9349                            | 1                | 1 5 1          | 46.92                    |  |
| 1.9051                            | 1                | 2 2 0          | 47.70                    |  |
| 1.8483                            | 15               | 0 0 2          | 49.26                    |  |
| 1.8206                            | 9                | 2 3 0          | 50.06                    |  |
| 1.7860                            | 2                | 0 2 2          | 51.10                    |  |
| 1.7705                            | 2                | 1 7 0          | 51.58                    |  |
| 1.7559                            | 4                | 1 6 1          | 52.04                    |  |
| 1.7324                            | 13               | 2 1 1          | 52.80                    |  |
| 1.7203                            | 2                | 2 4 0          | 53.20                    |  |
| 1.6933                            | 5                | 2 2 1          | 54.12                    |  |
| 1.6627                            | 10               | 1 1 2          | 55.20                    |  |
| 1.6301                            | 9                | 0 4 2          | 56.40                    |  |
| 1.6285                            | 9                | 1 2 2          | 56.46                    |  |
| 1.5969                            | 12               | 1 7 1          | 57.68                    |  |
| 1.5869                            | 3                | 1 8 0          | 58.08                    |  |
| 1.5745                            | 2                | 1 3 2          | 58.58                    |  |
| 1.5682                            | 11               | 0 8 1          | 58.84                    |  |
| 1.5079                            | 1                | 1 4 2          | 61.44                    |  |
| 1.5039                            | 3                | 2 6 0          | 61.62                    |  |
| 1.4776                            | 10               | 2 5 1          | 62.84                    |  |
| 1.4585                            | 1                | 1 8 1          | 63.76                    |  |
| 1.4431                            | 7                | 0 6 2          | 64.52                    |  |
| 1.4337+                           | 8                | 1 5 2          | 65.00                    |  |

Molybdenum Oxide (Molybdite), MoO<sub>3</sub> - (continued)

| d(A) <sup>o</sup>            | I <sup>rel</sup> | hkl    | 2θ(°) |
|------------------------------|------------------|--------|-------|
| 1.4004                       | 4                | 2 7 0  | 66.74 |
| 1.3931                       | 1                | 2 6 1  | 67.14 |
| 1.3854                       | 3                | 0 10 0 | 67.56 |
| 1.3558                       | 1                | 1 6 2  | 69.24 |
| 1.3518                       | 3                | 2 0 2  | 69.48 |
| 1.3453                       | 3                | 2 1 2  | 69.86 |
| 1.3380                       | 1                | 1 9 1  | 70.30 |
| 1.3096                       | 1                | 2 7 1  | 72.06 |
| 1.2975+                      | 8                | 2 3 2  | 72.84 |
| 1.2788                       | 1                | 1 7 2  | 74.08 |
| 1.2591                       | 1                | 2 4 2  | 75.44 |
| 1.2440                       | 4                | 3 0 1  | 76.52 |
| 1.2331+                      | 2                | 1 10 1 | 77.32 |
| 1.2299                       | 3                | 2 8 1  | 77.56 |
| 1.2157                       | 1                | 2 9 0  | 78.64 |
| 1.2131                       | 4                | 0 2 3  | 78.84 |
| 1.2041                       | 2                | 1 8 2  | 79.54 |
| 1.2011+                      | 2                | 3 3 1  | 79.78 |
| + More than one hkl possible |                  |        |       |

| d(A) <sup>o</sup> | I <sup>rel</sup> | hkl    | 2θ(°) |
|-------------------|------------------|--------|-------|
| 1.7559            | 4                | 1 6 1  | 52.04 |
| 1.7327            | 15               | 2 1 1  | 52.79 |
| 1.7200            | 2                | 2 4 0  | 53.21 |
| 1.6935            | 6                | 2 2 1  | 54.11 |
| 1.6629            | 12               | 1 1 2  | 55.19 |
| 1.6335            | 2                | 2 3 1  | 56.27 |
| 1.6306            | 7                | 0 4 2  | 56.38 |
| 1.6282            | 5                | 1 2 2  | 56.47 |
| 1.5969            | 14               | 1 7 1  | 57.68 |
| 1.5871            | 2                | 1 8 0  | 58.07 |
| 1.5748            | 2                | 1 3 2  | 58.57 |
| 1.5684            | 13               | 0 8 1  | 58.83 |
| 1.5081            | 1                | 1 4 2  | 61.43 |
| 1.5037            | 3                | 2 6 0  | 61.63 |
| 1.4774            | 12               | 2 5 1  | 62.85 |
| 1.4583            | 1                | 1 8 1  | 63.77 |
| 1.4429            | 8                | 0 6 2  | 64.53 |
| 1.4350            | 4                | 1 9 0  | 64.93 |
| 1.4334            | 7                | 1 5 2  | 65.01 |
| 1.4004            | 5                | 2 7 0  | 66.74 |
| 1.3929            | 1                | 2 6 1  | 67.15 |
| 1.3856            | 3                | 0 10 0 | 67.55 |
| 1.3558            | 1                | 1 6 2  | 69.24 |
| 1.3516            | 4                | 2 0 2  | 69.49 |
| 1.3452            | 4                | 2 1 2  | 69.87 |
| 1.3378            | 1                | 1 9 1  | 70.31 |
| 1.3096            | 1                | 2 7 1  | 72.06 |
| 1.2976            | 4                | 3 2 0  | 72.83 |
| 1.2972            | 7                | 2 3 2  | 72.86 |
| 1.2786            | 1                | 1 7 2  | 74.09 |
| 1.2591            | 1                | 2 4 2  | 75.44 |
| 1.2440            | 4                | 3 0 1  | 76.52 |
| 1.2343            | 1                | 3 4 0  | 77.23 |
| 1.2331            | 2                | 1 10 1 | 77.32 |
| 1.2297            | 3                | 2 8 1  | 77.57 |
| 1.2158            | 1                | 2 9 0  | 78.63 |
| 1.2132            | 4                | 0 2 3  | 78.83 |
| 1.2040            | 2                | 1 8 2  | 79.55 |
| 1.2011            | 1                | 3 3 1  | 79.78 |
| 1.2005            | 1                | 1 11 0 | 79.83 |

| Calculated Pattern (Integrated) |                  |       |       |
|---------------------------------|------------------|-------|-------|
| d(A) <sup>o</sup>               | I <sup>rel</sup> | hkl   | 2θ(°) |
| 6.927                           | 31               | 0 2 0 | 12.77 |
| 3.8098                          | 73               | 1 1 0 | 23.33 |
| 3.4636                          | 34               | 0 4 0 | 25.70 |
| 3.4399                          | 25               | 1 2 0 | 25.88 |
| 3.2618                          | 100              | 0 2 1 | 27.32 |
| 3.0076                          | 7                | 1 3 0 | 29.68 |
| 2.7034                          | 15               | 1 0 1 | 33.11 |
| 2.6528                          | 27               | 1 1 1 | 33.76 |
| 2.6079                          | 3                | 1 4 0 | 34.36 |
| 2.5274                          | 7                | 0 4 1 | 35.49 |
| 2.5185                          | 1                | 1 2 1 | 35.62 |
| 2.3329                          | 8                | 1 3 1 | 38.56 |
| 2.3093                          | 22               | 0 6 0 | 38.97 |
| 2.2713                          | 14               | 1 5 0 | 39.65 |
| 2.1311                          | 8                | 1 4 1 | 42.38 |
| 1.9953                          | 2                | 1 6 0 | 45.42 |
| 1.9816                          | 8                | 2 0 0 | 45.75 |
| 1.9613                          | 8                | 2 1 0 | 46.25 |
| 1.9586                          | 8                | 0 6 1 | 46.32 |
| 1.9349                          | 1                | 1 5 1 | 46.92 |
| 1.9051                          | 1                | 2 2 0 | 47.70 |
| 1.8483                          | 17               | 0 0 2 | 49.26 |
| 1.8210                          | 11               | 2 3 0 | 50.05 |
| 1.7860                          | 2                | 0 2 2 | 51.10 |
| 1.7708                          | 2                | 1 7 0 | 51.57 |

## INORGANIC NAMES

|   | Vol. or<br>Sec. | Page |   | Vol. or<br>Sec. | Page |
|---|-----------------|------|---|-----------------|------|
| Aluminum, Al .....  | 1               | 11   | Ammonium aluminum fluoride,<br>$(\text{NH}_4)_3\text{AlF}_6$ .....  | 9m              | 5    |
| Aluminum antimony, AlSb .....   | 4               | 72   | Ammonium aluminum selenate hydrate,<br>$\text{NH}_4\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....              | 9m              | 6    |
| Aluminum bismuth oxide, $\text{Al}_4\text{Bi}_2\text{O}_9$ .....  | 11m             | 5    | Ammonium aluminum sulfate,<br>$\text{NH}_4\text{Al}(\text{SO}_4)_2$ .....   | 10m             | 5    |
| Aluminum borate, $\text{Al}_{18}\text{B}_4\text{O}_{33}$ .....  | 17m             | 5    | Ammonium aluminum sulfate hydrate<br>(tschermigite), $\text{NH}_4\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ ..... | 6               | 3    |
| Aluminum chloride, $\text{AlCl}_3$ .....  | 9m              | 61   | Ammonium azide, $\text{NH}_4\text{N}_3$ .....   | 9               | 4    |
| Aluminum chloride hydrate<br>(chloraluminate), $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ .....                    | 7               | 3    | Ammonium beryllium fluoride,<br>$(\text{NH}_4)_2\text{BeF}_4$ .....   | 3m              | 5    |
| Aluminum copper, $\text{Al}_4\text{Cu}_9$ .....   | 11m             | 79   | Ammonium borate hydrate,<br>$\text{NH}_4\text{B}_5\text{O}_8 \cdot 4\text{H}_2\text{O}$ .....                               | 17m             | 7    |
| Aluminum fluoride hydroxide silicate,<br>topaz, $\text{Al}_2(\text{F},\text{OH})_2\text{SiO}_4$ .....             | 1m              | 4    | Ammonium boron fluoride, $\text{NH}_4\text{BF}_4$ ...   | 3m              | 6    |
| Aluminum iron, $\text{AlFe}$ .....  | 18m             | 5    | Ammonium bromide, $\text{NH}_4\text{Br}$ .....  | 2               | 49   |
| Aluminum iron antimony oxide, bahianite,<br>$\text{Al}_{5.66}\text{Fe}_{0.09}\text{Sb}_{2.95}\text{O}_{16}$ ..... | 16m             | 87   | Ammonium cadmium bromide, $(\text{NH}_4)_4\text{CdBr}_6$  | 15m             | 9    |
| Aluminum iron oxide, $\text{AlFeO}_3$ .....   | 15m             | 7    | Ammonium cadmium chloride, $\text{NH}_4\text{CdCl}_3$   | 5m              | 6    |
| Aluminum lithium, $\text{Al}_4\text{Li}_9$ .....  | 10m             | 98   | Ammonium cadmium phosphate hydrate,<br>$\text{NH}_4\text{CdPO}_4 \cdot \text{H}_2\text{O}$ .....                            | 19m             | 13   |
| Aluminum nickel, $\text{AlNi}$ .....  | 6m              | 82   | Ammonium cadmium sulfate,<br>$(\text{NH}_4)_2\text{Cd}_2(\text{SO}_4)_3$ .....  | 7m              | 5    |
| Aluminum nitride, $\text{AlN}$ .....  | 12m             | 5    | Ammonium cadmium sulfate hydrate,<br>$(\text{NH}_4)_2\text{Cd}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....              | 8m              | 5    |
| Aluminum nitrate hydrate,<br>$\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ .....                           | 11m             | 6    | Ammonium calcium sulfate,<br>$(\text{NH}_4)_2\text{Ca}_2(\text{SO}_4)_3$ .....  | 8m              | 7    |
| Aluminum oxide (corundum), $\alpha\text{-Al}_2\text{O}_3$ ..  | 9               | 3    | Ammonium cerium nitrate,<br>$(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$ .....   | 18m             | 6    |
| Aluminum oxide hydrate (boehmite),<br>$\alpha\text{-Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$ .....               | 3               | 38   | Ammonium chlorate, $\text{NH}_4\text{ClO}_4$<br>(orthorhombic) .....  | 7               | 6    |
| Aluminum oxide hydrate, diaspore,<br>$\beta\text{-Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$ .....                 | 3               | 41   | Ammonium chloride (salammoniac),<br>$\text{NH}_4\text{Cl}$ .....  | 1               | 59   |
| Aluminum phosphate, $\text{Al}(\text{PO}_3)_3$ .....  | 2m              | 3    | Ammonium chromium sulfate hydrate,<br>$\text{NH}_4\text{Cr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....                | 6               | 7    |
| Aluminum phosphate (berlinite),<br>$\text{AlPO}_4$ (trigonal) .....   | 10              | 3    | Ammonium cobalt (II) chloride,<br>$\text{NH}_4\text{CoCl}_3$ .....  | 6m              | 5    |
| Aluminum phosphate, $\text{AlPO}_4$<br>(orthorhombic) .....   | 10              | 4    | Ammonium cobalt fluoride, $\text{NH}_4\text{CoF}_3$   | 8m              | 9    |
| Aluminum plutonium, $\text{Al}_3\text{Pu}$ .....  | 15m             | 77   | Ammonium copper bromide hydrate,<br>$(\text{NH}_4)_2\text{CuBr}_4 \cdot 2\text{H}_2\text{O}$ .....                          | 10m             | 6    |
| Aluminum rhenium, $\text{AlRe}$ .....   | 15m             | 79   | Ammonium copper chloride, $\text{NH}_4\text{CuCl}_3$  | 7m              | 7    |
| Aluminum rhenium, $\text{Al}_{12}\text{Re}$ .....   | 15m             | 80   | Ammonium copper chloride hydrate,<br>$(\text{NH}_4)_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$ .....                         | 12m             | 6    |
| Aluminum rhodium, $\text{AlRh}$ .....   | 15m             | 82   | Ammonium copper fluoride, $\text{NH}_4\text{CuF}_3$   | 11m             | 8    |
| Aluminum ruthenium, $\text{AlRu}$ .....   | 15m             | 83   | Ammonium gallium sulfate hydrate,<br>$\text{NH}_4\text{Ga}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....                 | 6               | 9    |
| Aluminum ruthenium, $\text{Al}_6\text{Ru}$ .....  | 15m             | 84   | Ammonium germanium fluoride,<br>$(\text{NH}_4)_2\text{GeF}_6$ .....   | 6               | 8    |
| Aluminum samarium, $\text{AlSm}_2$ .....  | 15m             | 86   | Ammonium hydrogen arsenate,<br>$\text{NH}_4\text{H}_2\text{AsO}_4$ .....  | 16m             | 9    |
| Aluminum samarium, $\text{AlSm}_3$ .....  | 15m             | 88   | Ammonium hydrogen carbonate<br>(teschemacherite), $(\text{NH}_4)\text{HCO}_3$ .....   | 9               | 5    |
| Aluminum samarium, $\text{Al}_2\text{Sm}$ .....   | 15m             | 90   | Ammonium hydrogen phosphate,<br>$\text{NH}_4\text{H}_2\text{PO}_4$ .....  | 4               | 64   |
| Aluminum samarium, $\text{Al}_3\text{Sm}$ .....   | 15m             | 91   | Ammonium iodate, $\text{NH}_4\text{IO}_3$ .....   | 10m             | 7    |
| Aluminum silicate (mullite),<br>$\text{Al}_6\text{Si}_2\text{O}_{13}$ .....                                       | 3m              | 3    | Ammonium iodide, $\text{NH}_4\text{I}$ .....  | 4               | 56   |
| Aluminum sulfate, $\text{Al}_2(\text{SO}_4)_3$ .....  | 15m             | 8    | Ammonium iridium chloride,<br>$(\text{NH}_4)_2\text{IrCl}_6$ .....  | 8               | 6    |
| Aluminum technetium, $\text{Al}_6\text{Tc}$ .....   | 15m             | 93   | Ammonium iron chloride hydrate,<br>$(\text{NH}_4)_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ .....                            | 14m             | 7    |
| Aluminum terbium, $\text{Al}_2\text{Tb}$ .....  | 15m             | 95   | Ammonium iron fluoride, $(\text{NH}_4)_3\text{FeF}_6$   | 9m              | 9    |
| Aluminum terbium, $\text{Al}_2\text{Tb}_3$ .....  | 15m             | 96   | Ammonium iron sulfate, $\text{NH}_4\text{Fe}(\text{SO}_4)_2$  | 10m             | 8    |
| Aluminum thorium uranium, $\text{Al}_6\text{ThU}$ .....   | 15m             | 98   | Ammonium iron sulfate hydrate,<br>$\text{NH}_4\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....                    | 6               | 10   |
| Aluminum tungsten, $\text{Al}_5\text{W}$ , $\delta$ -phase .....  | 15m             | 100  | Ammonium lead chloride, $(\text{NH}_4)_2\text{PbCl}_6$  | 11m             | 10   |
| Aluminum tungsten oxide, $\text{Al}_2(\text{WO}_4)_3$ ..  | 11m             | 7    | Ammonium magnesium aluminum fluoride,<br>$\text{NH}_4\text{MgAlF}_6$ .....  | 10m             | 9    |
| Aluminum vanadium, $\text{Al}_{10}\text{V}$ .....   | 15m             | 102  |   |                 |      |
| Aluminum vanadium, $\text{Al}_{10.25}\text{V}$ .....  | 15m             | 104  |   |                 |      |
| Aluminum vanadium, $\text{Al}_{23}\text{V}_4$ .....   | 15m             | 106  |   |                 |      |
| Aluminum vanadium, $\text{Al}_{45}\text{V}_7$ , $\alpha'$ -phase ..   | 15m             | 108  |   |                 |      |
| Aluminum ytterbium, $\text{Al}_2\text{Yb}$ .....  | 15m             | 111  |   |                 |      |
| Aluminum yttrium, $\text{Al}_3\text{Y}$ .....   | 15m             | 112  |   |                 |      |
| Aluminium yttrium oxide, $\text{AlY}_3$ .....   | 19m             | 7    |   |                 |      |
| Aluminium yttrium oxide, $\text{Al}_2\text{Y}_4\text{O}_9$ .....  | 19m             | 9    |   |                 |      |
| Aluminium yttrium oxide, $\text{Al}_5\text{Y}_3\text{O}_{12}$ .....   | 19m             | 11   |   |                 |      |

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   | Antimony cerium, $\text{CeSb}$ .....  | 4m              | 40   |
| Ammonium magnesium phosphate hydrate (struvite), $\text{NH}_4\text{MgPO}_4 \cdot 6\text{H}_2\text{O}$ ....                    | 3m              | 41   | Antimony cobalt, $\text{CoSb}$ .....  | 15m             | 121  |
| Ammonium manganese chloride hydrate, $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$ ....                            | 11m             | 11   | Antimony cobalt, $\text{CoSb}_2$ .....  | 15m             | 122  |
| Ammonium manganese(II) fluoride, $\text{NH}_4\text{MnF}_3$ .....  | 5m              | 8    | Antimony cobalt titanium, $\text{CoSbTi}$ ..  | 15m             | 124  |
| Ammonium manganese sulfate, $(\text{NH}_4)_2\text{Mn}_2(\text{SO}_4)_3$ .....   | 7m              | 8    | Antimony cobalt vanadium, $\text{CoSbV}$ ..   | 15m             | 125  |
| Ammonium manganese sulfate hydrate, $(\text{NH}_4)_2\text{Mn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ ....                  | 8m              | 12   | Antimony dysprosium, $\text{DySb}$ .....  | 4m              | 41   |
| Ammonium mercury chloride, $\text{NH}_4\text{HgCl}_3$ .....   | 8m              | 14   | Antimony erbium, $\text{ErSb}$ .....  | 4m              | 41   |
| 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   | Antimony(III) fluoride, $\text{SbF}_3$ .....  | 2m              | 4    |
| Ammonium nickel(II) chloride, $\text{NH}_4\text{NiCl}_3$ .....  | 6m              | 6    | Antimony gadolinium, $\text{GdSb}$ .....  | 4m              | 42   |
| Ammonium nickel chromium oxide hydrate, $(\text{NH}_4)_2\text{Ni}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ ....             | 8m              | 16   | Antimony gallium, $\text{GaSb}$ .....   | 6               | 30   |
| Ammonium nickel sulfate hydrate, $(\text{NH}_4)_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....                    | 17m             | 9    | Antimony gold (aurostibite), $\text{AuSb}_2$ ..   | 7               | 18   |
| Ammonium nitrate (nitrammite), $\text{NH}_4\text{NO}_3$ .....   | 7               | 4    | Antimony indium, $\text{InSb}$ .....  | 4               | 73   |
| Ammonium osmium bromide, $(\text{NH}_4)_2\text{OsBr}_6$ .....   | 3               | 71   | Antimony(III) iodide, $\text{SbI}_3$ .....  | 6               | 16   |
| Ammonium osmium chloride, $(\text{NH}_4)_2\text{OsCl}_6$ .....  | 1m              | 6    | Antimony iron titanium oxide hydroxide, derbylite, $\text{SbFe}_4\text{Ti}_3\text{O}_{13}(\text{OH})$ ..... | 16m             | 89   |
| Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_4$ .....   | 6               | 6    | Antimony lanthanum, $\text{LaSb}$ .....   | 4m              | 42   |
| Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_6$ .....   | 8               | 7    | Antimony neodymium, $\text{NdSb}$ .....   | 4m              | 43   |
| Ammonium platinum bromide, $(\text{NH}_4)_2\text{PtBr}_6$ .....   | 9               | 6    | Antimony(III) oxide (senarmontite), $\text{Sb}_2\text{O}_3$ (cubic) .....                                   | 3               | 31   |
| Ammonium platinum chloride, $(\text{NH}_4)_2\text{PtCl}_6$ .....  | 5               | 3    | Antimony(III) oxide, valentinite, $\text{Sb}_2\text{O}_3$ (orthorhombic) .....                              | 10              | 6    |
| Ammonium potassium iron chloride hydrate (kremersite), $(\text{NH}_4,\text{K})_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ ..... | 14m             | 8    | Antimony(IV) oxide (cervantite), $\text{Sb}_2\text{O}_4$ .....  | 10              | 8    |
| Ammonium rhenium oxide, $\text{NH}_4\text{ReO}_4$ .....   | 9               | 7    | Antimony oxide, $\text{Sb}_6\text{O}_{13}$ .....  | 16m             | 14   |
| Ammonium selenium bromide, $(\text{NH}_4)_2\text{SeBr}_6$ .....   | 8               | 4    | Antimony praseodymium, $\text{PrSb}$ .....  | 4m              | 43   |
| Ammonium silicon fluoride (cryptothalite), $(\text{NH}_4)_2\text{SiF}_6$ .....  | 5               | 5    | Antimony scandium, $\text{SbSc}$ .....  | 4m              | 44   |
| Ammonium strontium chromium oxide, $(\text{NH}_4)_2\text{Sr}(\text{CrO}_4)_2$ .....   | 14m             | 9    | Antimony selenide, $\text{Sb}_2\text{Se}_3$ .....   | 3m              | 7    |
| Ammonium strontium sulfate, $(\text{NH}_4)_2\text{Sr}(\text{SO}_4)_2$ .....   | 15m             | 11   | Antimony silver sulfide, $\text{AgSbS}_2$ (cubic) .....   | 5m              | 48   |
| Ammonium sulfate (mascagnite), $(\text{NH}_4)_2\text{SO}_4$ .....   | 9               | 8    | Antimony silver sulfide (miargyrite), $\text{AgSbS}_2$ (monoclinic) .....                                   | 5m              | 49   |
| Ammonium sulfate, $(\text{NH}_4)_2\text{S}_2\text{O}_3$ .....   | 17m             | 11   | Antimony silver sulfide (pyrargyrite), $\text{Ag}_3\text{SbS}_3$ (trigonal) .....                           | 5m              | 51   |
| Ammonium sulfate, $(\text{NH}_4)_2\text{S}_2\text{O}_8$ .....   | 17m             | 13   | Antimony silver telluride, $\text{AgSbTe}_2$ .....  | 3m              | 47   |
| Ammonium tellurium bromide, $(\text{NH}_4)_2\text{TeBr}_6$ .....  | 8               | 5    | Antimony(III) sulfide (stibnite), $\text{Sb}_2\text{S}_3$ .....   | 5               | 6    |
| Ammonium tellurium chloride, $(\text{NH}_4)_2\text{TeCl}_6$ .....   | 8               | 8    | Antimony telluride, $\text{Sb}_2\text{Te}_3$ .....  | 3m              | 8    |
| Ammonium tin chloride, $(\text{NH}_4)_2\text{SnCl}_6$ .....   | 5               | 4    | Antimony terbium, $\text{SbTb}$ .....   | 5m              | 61   |
| Ammonium tin fluoride, $\text{NH}_4\text{SnF}_3$ .....  | 18m             | 8    | Antimony thorium, $\text{SbTh}$ .....   | 4m              | 44   |
| Ammonium titanium fluoride, $(\text{NH}_4)_2\text{TiF}_6$ .....   | 16m             | 10   | Antimony thulium, $\text{SbTm}$ .....   | 4m              | 45   |
| Ammonium vanadium oxide, $\text{NH}_4\text{VO}_3$ .....   | 8               | 9    | Antimony tin, $\text{SbSn}$ .....   | 16m             | 15   |
| Ammonium zinc chloride, $(\text{NH}_4)_3\text{ZnCl}_5$ .....  | 15m             | 12   | Antimony ytterbium, $\text{SbYb}$ .....   | 4m              | 45   |
| Ammonium zinc fluoride, $\text{NH}_4\text{ZnF}_3$ .....   | 8m              | 18   | Antimony yttrium, $\text{SbY}$ .....  | 4m              | 46   |
| Ammonium zirconium fluoride, $(\text{NH}_4)_3\text{ZrF}_7$ .....  | 6               | 14   | Arsenic, As .....   | 3               | 6    |
| Antimonic acid, $\text{H}_{14}\text{Sb}_{14}\text{O}_{21}(\text{OH})_{42}$ ..   | 16m             | 13   | Arsenic bromide, $\text{AsBr}_3$ .....  | 18m             | 9    |
| Antimony, Sb .....  | 3               | 14   | Arsenic cerium, $\text{AsCe}$ .....   | 4m              | 51   |
| Antimony bromide, $\alpha\text{-SbBr}_3$ .....  | 15m             | 13   | Arsenic(III) iodide, $\text{AsI}_3$ .....   | 13m             | 7    |
|   |                 |      | Arsenic oxide (arsenolite), $\text{As}_2\text{O}_3$ (cubic) .....   | 1               | 51   |
|   |                 |      | Arsenic oxide, claudetite, $\text{As}_2\text{O}_3$ (monoclinic) .....                                       | 3m              | 9    |
|   |                 |      | Barium, Ba .....  | 4               | 7    |
|   |                 |      | Barium aluminum oxide, $\text{BaAl}_2\text{O}_4$ .....  | 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, $\text{BaB}_4\text{O}_7$ .....   | 4m              | 6    |
|   |                 |      | Barium borate, high form, $\text{BaB}_2\text{O}_4$ ..   | 4m              | 4    |
|   |                 |      | Barium borate, $\text{BaB}_8\text{O}_{13}$ .....  | 7m              | 10   |
|   |                 |      | Barium boride, $\text{BaB}_6$ .....   | 19m             | 18   |

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| Barium bromate hydrate,<br>$\text{Ba}(\text{BrO}_3)_2 \cdot \text{H}_2\text{O}$ .....  | 8m              | 19   | Barium silicate, $\text{Ba}_2\text{Si}_3\text{O}_8$ .....   | 13m             | 13   |
| Barium bromide, $\text{BaBr}_2$ .....  | 10m             | 63   | Barium silicate, $\text{Ba}_3\text{SiO}_5$ .....  | 13m             | 15   |
| Barium bromide fluoride, $\text{BaBrF}$ .....  | 10m             | 10   | Barium silicate, $\text{Ba}_3\text{Si}_5\text{O}_{13}$ .....  | 13m             | 17   |
| Barium bromide hydrate, $\text{BaBr}_2 \cdot \text{H}_2\text{O}$ .....                 | 3m              | 10   | Barium silicon fluoride, $\text{BaSiF}_6$ ...   | 4m              | 7    |
| Barium bromide hydrate, $\text{BaBr}_2 \cdot 2\text{H}_2\text{O}$ .....                | 16m             | 16   | Barium strontium nitrate,<br>$\text{Ba}_{.25}\text{Sr}_{.75}(\text{NO}_3)_2$ .....  | 12m             | 42   |
| Barium cadmium chloride hydrate,<br>$\text{BaCdCl}_4 \cdot 4\text{H}_2\text{O}$ .....  | 15m             | 14   | Barium strontium nitrate,<br>$\text{Ba}_{.50}\text{Sr}_{.50}(\text{NO}_3)_2$ .....  | 12m             | 42   |
| Barium cadmium phosphate,<br>$\text{BaCd}(\text{PO}_3)_4$ .....                        | 20m             | 7    | Barium strontium nitrate,<br>$\text{Ba}_{.75}\text{Sr}_{.25}(\text{NO}_3)_2$ .....  | 12m             | 42   |
| Barium calcium nitrate,<br>$\text{Ba}_{.25}\text{Ca}_{.75}(\text{NO}_3)_2$ .....       | 12m             | 38   | Barium sulfate (baryte), $\text{BaSO}_4$ ....   | 10m             | 12   |
| Barium calcium nitrate,<br>$\text{Ba}_{.50}\text{Ca}_{.50}(\text{NO}_3)_2$ .....       | 12m             | 38   | Barium sulfide, $\text{BaS}$ .....  | 7               | 8    |
| Barium calcium nitrate,<br>$\text{Ba}_{.75}\text{Ca}_{.25}(\text{NO}_3)_2$ .....       | 12m             | 38   | Barium thiosulfate hydrate,<br>$\text{BaS}_2\text{O}_3 \cdot \text{H}_2\text{O}$ .....  | 16m             | 20   |
| Barium calcium tungsten oxide,<br>$\text{Ba}_2\text{CaW}_6$ .....                      | 9m              | 10   | Barium titanium oxide, $\text{BaSnO}_3$ .....   | 3m              | 11   |
| Barium carbonate (witherite), $\text{BaCO}_3$<br>(orthorhombic) .....                  | 2               | 54   | Barium titanium oxide, $\text{BaTiO}_3$<br>(hexagonal) .....  | 20m             | 9    |
| Barium carbonate, $\text{BaCO}_3$ (cubic)<br>at 1075 °C .....                          | 10              | 11   | Barium titanium oxide, $\text{BaTiO}_3$<br>(tetragonal) .....   | 3               | 45   |
| Barium chlorate, $\text{Ba}(\text{ClO}_3)_2$ .....                                     | 16m             | 17   | Barium titanium oxide, $\text{BaTi}_{205}$ ....   | 20m             | 11   |
| Barium chlorate hydrate,<br>$\text{Ba}(\text{ClO}_3)_2 \cdot \text{H}_2\text{O}$ ..... | 8m              | 21   | Barium titanium oxide, $\text{BaTi}_{409}$ ....   | 20m             | 13   |
| Barium chlorate, $\text{Ba}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$ .....           | 2m              | 7    | Barium titanium phosphate,<br>$\text{BaTi}_4(\text{PO}_4)_6$ .....  | 20m             | 15   |
| Barium chloride, $\text{BaCl}_2$ , (cubic) ...   | 9m              | 13   | Barium titanium silicate (fresnoite),<br>$\text{Ba}_2\text{TiSi}_2\text{O}_8$ .....   | 9m              | 14   |
| Barium chloride, $\text{BaCl}_2$ ,<br>(orthorhombic) .....                             | 9m              | 11   | Barium tungsten oxide, $\text{BaW}_4$ .....   | 7               | 9    |
| Barium chloride fluoride, $\text{BaClF}$ ...   | 10m             | 11   | Barium tungsten oxide, $\text{Ba}_2\text{W}_5$ ....   | 12m             | 14   |
| Barium chloride hydrate, $\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$ .....               | 12m             | 9    | Barium tungsten oxide, $\text{Ba}_3\text{W}_6$ ....   | 19m             | 21   |
| Barium chromium oxide,<br>$\text{Ba}_3(\text{CrO}_4)_2$ .....                          | 15m             | 16   | Barium vanadium oxide, $\text{Ba}_3(\text{VO}_4)_2$ ..  | 14m             | 10   |
| Barium fluoride, $\text{BaF}_2$ .....  | 1               | 70   | Barium zirconium oxide, $\text{BaZrO}_3$ ....   | 5               | 8    |
| Barium hydroxide phosphate,<br>$\text{Ba}_5(\text{OH})(\text{PO}_4)_3$ .....           | 11m             | 12   | Barium zirconium phosphate,<br>$\text{BaZr}_4(\text{PO}_4)_6$ .....   | 20m             | 17   |
| Barium iodide, $\text{BaI}_2$ .....  | 10m             | 66   | Beryllium, alpha, $\text{Be}$ .....   | 9m              | 64   |
| Barium iodide hydrate, $\text{BaI}_2 \cdot 2\text{H}_2\text{O}$ ..                     | 16m             | 18   | Beryllium aluminum oxide<br>(chrysoberyl), $\text{BeAl}_2\text{O}_4$ .....  | 9               | 10   |
| Barium lead chloride, $\text{BaPbCl}_4$ .....  | 11m             | 13   | Beryllium aluminum silicate, beryl,<br>$\text{Be}_3\text{Al}_2(\text{SiO}_3)_6$ .....   | 9               | 13   |
| Barium lead nitrate,<br>$\text{Ba}_{.33}\text{Pb}_{.67}(\text{NO}_3)_2$ .....          | 12m             | 40   | Beryllium calcium iron magnesium<br>aluminum phosphate hydroxide<br>hydrate, roscherite (monoclinic),<br>$\text{Be}_2\text{Ca}(\text{Fe}_{.3}\text{Mg}_{.7})_2\text{Al}_{.67}(\text{PO}_4)_3(\text{OH})_3 \cdot 2\text{H}_2\text{O}$  | 16m             | 96   |
| Barium lead nitrate,<br>$\text{Ba}_{.67}\text{Pb}_{.33}(\text{NO}_3)_2$ .....          | 12m             | 40   | Beryllium calcium manganese<br>aluminum iron phosphate hydroxide<br>hydrate, roscherite (triclinic),<br>$\text{Be}_4\text{Ca}_2(\text{Mn}_{3.91}\text{Mg}_{.04}\text{Ca}_{.05})(\text{Al}_{.13}\text{Fe}_{.42}\text{Mn}_{.12})(\text{PO}_4)_6(\text{OH})_4 \cdot 6\text{H}_2\text{O}$ ..... | 16m             | 100  |
| Barium manganese oxide, $\text{BaMnO}_4$ .....   | 18m             | 11   | Beryllium calcium oxide,<br>$\text{Be}_{17}\text{Ca}_{12}\text{O}_{29}$ .....   | 7m              | 89   |
| Barium manganese oxide,<br>$\text{Ba}(\text{MnO}_4)_2$ .....                           | 15m             | 17   | Beryllium carbide, $\text{Be}_2\text{C}$ .....  | 19m             | 23   |
| Barium molybdenum oxide, $\text{BaMoO}_4$ .....  | 7               | 7    | Beryllium chromium oxide, $\text{BeCr}_2\text{O}_4$ .....   | 10              | 12   |
| Barium molybdenum oxide, $\text{Ba}_2\text{MoO}_5$ ..                                  | 12m             | 10   | Beryllium cobalt, $\text{BeCo}$ .....   | 5m              | 62   |
| Barium neodymium titanium oxide,<br>$\text{BaNd}_2\text{Ti}_3\text{O}_{10}$ .....      | 18m             | 12   | Beryllium germanium oxide, $\text{Be}_2\text{GeO}_4$ .....  | 10              | 13   |
| Barium neodymium titanium oxide,<br>$\text{BaNd}_2\text{Ti}_5\text{O}_{14}$ .....      | 19m             | 19   | Beryllium lanthanum oxide, $\text{Be}_2\text{La}_2\text{O}_5$ .....   | 9m              | 65   |
| Barium nitrate (nitrobarite),<br>$\text{Ba}(\text{NO}_3)_2$ .....                      | 11m             | 14   | Beryllium niobium, $\text{Be}_2\text{Nb}$ .....   | 7m              | 92   |
| Barium nitrite hydrate,<br>$\text{Ba}(\text{NO}_2)_2 \cdot \text{H}_2\text{O}$ .....   | 15m             | 18   | Beryllium nitride, $\text{Be}_3\text{N}_2$ .....  | 18m             | 15   |
| Barium oxide, $\text{BaO}$ .....   | 9m              | 63   | Beryllium oxide (bromellite), $\text{BeO}$ .....  | 1               | 36   |
| Barium oxide, $\text{BaO}_2$ .....   | 6               | 18   | Beryllium palladium, $\text{BePd}$ .....  | 5m              | 62   |
| Barium phosphate, $\text{Ba}_2\text{P}_2\text{O}_7$ ,<br>(high form) .....             | 16m             | 19   | Beryllium silicate, phenakite,<br>$\text{Be}_2\text{SiO}_4$ .....   | 8               | 11   |
| Barium phosphate, $\text{Ba}_3(\text{PO}_4)_2$ .....                                   | 12m             | 12   | Beryllium sulfate, $\text{BeSO}_4$ .....  | 15m             | 20   |
| Barium selenide, $\text{BaSe}$ .....   | 5m              | 61   | Bismuth, Bi .....   | 3               | 20   |
| Barium silicate, $\beta\text{-BaSiO}_3$ .....  | 13m             | 8    | Bismuth bromide oxide, $\text{BiOBr}$ .....   | 8               | 14   |
| Barium silicate (sanbornite),<br>$\beta\text{-BaSi}_2\text{O}_5$ .....                 | 13m             | 10   | Bismuth cerium, $\text{BiCe}$ .....   | 4m              | 46   |
| Barium silicate, $\text{Ba}_2\text{SiO}_4$ .....                                       | 13m             | 12   | Bismuth chloride oxide (bismoclite),<br>$\text{BiOCl}$ .....  | 4               | 54   |
|  |                 |      | Bismuth dysprosium, $\text{BiDy}$ .....   | 4m              | 47   |
|  |                 |      | Bismuth erbium, $\text{BiEr}$ .....   | 4m              | 47   |

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| Bismuth fluoride, $\text{BiF}_3$ .....   | 1m              | 7    | Cadmium sulfide (greenockite), $\text{CdS}$  | 4               | 15   |
| Bismuth germanium oxide,<br>$\text{Bi}_4(\text{GeO}_4)_3$ .....                          | 20m             | 18   | Cadmium telluride, $\text{CdTe}$ .....   | 3m              | 21   |
| Bismuth germanium oxide,<br>$\text{Bi}_{12}\text{GeO}_{20}$ .....                        | 20m             | 19   | Cadmium titanium oxide, $\text{CdTiO}_3$ .....   | 15m             | 21   |
| Bismuth holmium, $\text{BiHo}$ .....   | 4m              | 48   | Cadmium tungsten oxide, $\text{CdWO}_4$ .....  | 2m              | 8    |
| Bismuth(III) iodide, $\text{BiI}_3$ .....  | 6               | 20   | Cadmium zinc phosphate,<br>$\text{Cd}_{0.9}\text{Zn}_{2.1}(\text{PO}_4)_2$ .....   | 20m             | 26   |
| Bismuth iodide oxide, $\text{BiOI}$ .....  | 9               | 16   | Calcium, Ca .....  | 9m              | 68   |
| Bismuth lanthanum, $\text{BiLa}$ .....   | 4m              | 48   | Calcium aluminum germanium oxide,<br>$\text{Ca}_3\text{Al}_2(\text{GeO}_4)_3$ .....  | 10              | 15   |
| Bismuth neodymium, $\text{BiNd}$ .....   | 4m              | 49   | Calcium aluminum hydroxide,<br>$\text{Ca}_3\text{Al}_2(\text{OH})_{12}$ .....  | 11m             | 16   |
| Bismuth oxide (bismite), $\alpha\text{-Bi}_2\text{O}_3$ ..                               | 3m              | 17   | Calcium aluminum iron oxide<br>(brownmillerite), $\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$ ..   | 16m             | 28   |
| Bismuth phosphate, $\text{BiPO}_4$<br>(monoclinic) .....                                 | 3m              | 11   | Calcium aluminum oxide, $\text{Ca}_3\text{Al}_2\text{O}_6$ ..  | 5               | 10   |
| Bismuth phosphate, $\text{BiPO}_4$ (trigonal)  | 3m              | 13   | Calcium aluminum oxide (mayenite),<br>$\text{Ca}_{12}\text{Al}_{14}\text{O}_{33}$ .....  | 9               | 20   |
| Bismuth praseodymium, $\text{BiPr}$ .....  | 4m              | 49   | Calcium aluminum oxide hydrate,<br>$\text{Ca}_4\text{Al}_6\text{O}_{13} \cdot 3\text{H}_2\text{O}$ .....   | 19m             | 25   |
| Bismuth selenide (paraguanajuatite),<br>$\text{Bi}_2\text{Se}_3$ .....                   | 18m             | 16   | Calcium aluminum silicate hydrate,<br>chabazite, $\text{Ca}_2\text{Al}_4\text{Si}_8\text{O}_{24} \cdot 12\text{H}_2\text{O}$ ..  | 19m             | 27   |
| Bismuth sulfide (bismuthinite),<br>$\text{Bi}_2\text{S}_3$ .....                         | 5m              | 13   | Calcium aluminum sulfate hydrate<br>(ettringite), $\text{Ca}_6\text{Al}_2\text{S}_3\text{O}_{18} \cdot 31\text{H}_2\text{O}$ ..  | 8               | 3    |
| Bismuth telluride, $\text{BiTe}$ .....   | 4m              | 50   | Calcium borate, $\text{CaB}_2\text{O}_4$ .....   | 18m             | 17   |
| Bismuth telluride (tellurobis-muthite), $\text{Bi}_2\text{Te}_3$ .....                   | 3m              | 16   | Calcium borate, $\text{CaB}_2\text{O}_4$<br>(calculated pattern) .....   | 15m             | 136  |
| Bismuth titanium oxide, $\text{Bi}_{12}\text{TiO}_{20}$ ..                               | 20m             | 21   | Calcium borate hydrate,<br>hexahydroborite, $\text{Ca}[\text{B}(\text{OH})_4]_2 \cdot 2\text{H}_2\text{O}$   | 16m             | 104  |
| Bismuth vanadium oxide, high form,<br>$\text{BiVO}_4$ (monoclinic) .....                 | 3m              | 14   | Calcium boride, $\text{CaB}_6$ .....   | 16m             | 29   |
| Bismuth vanadium oxide, low form,<br>$\text{BiVO}_4$ (tetragonal) .....                  | 3m              | 14   | Calcium bromide, $\text{CaBr}_2$ .....   | 11m             | 70   |
| Boron nitride, $\text{BN}$ .....   | 20m             | 22   | Calcium bromide hydrate, $\text{CaBr}_2 \cdot 6\text{H}_2\text{O}$   | 8               | 15   |
| Boron oxide, $\text{B}_2\text{O}_3$ , phase 1 .....                                      | 10m             | 70   | Calcium carbonate (aragonite),<br>$\text{CaCO}_3$ (orthorhombic) .....   | 3               | 53   |
| Boron phosphate, $\text{BPO}_4$ .....  | 20m             | 23   | Calcium carbonate (aragonite),<br>$\text{CaCO}_3$ (orthorhombic, calculated<br>pattern) .....  | 14m             | 44   |
| Cadmium, Cd .....  | 3               | 10   | Calcium carbonate (calcite),<br>$\text{CaCO}_3$ (hexagonal) .....  | 2               | 51   |
| Cadmium aluminum oxide, $\text{CdAl}_2\text{O}_4$ ..                                     | 20m             | 24   | Calcium chloride (hydrophilite),<br>$\text{CaCl}_2$ .....  | 11m             | 18   |
| Cadmium ammine chloride,<br>$\text{Cd}(\text{NH}_3)_2\text{Cl}_2$ .....                  | 10m             | 14   | Calcium chloride fluoride, $\text{CaClF}$ ..   | 10m             | 17   |
| Cadmium borate, $\text{CdB}_4\text{O}_7$ .....   | 16m             | 24   | Calcium chloride hydrate,<br>$\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ .....   | 11m             | 73   |
| Cadmium bromate hydrate,<br>$\text{Cd}(\text{BrO}_3) \cdot 2\text{H}_2\text{O}$ .....    | 17m             | 14   | Calcium chloride hydrate<br>(antarcticite), $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$ .....  | 12m             | 16   |
| Cadmium bromide, $\text{CdBr}_2$ .....   | 9               | 17   | Calcium chromium germanium oxide,<br>$\text{Ca}_3\text{Cr}_2(\text{GeO}_4)_3$ .....  | 10              | 16   |
| Cadmium bromide chloride, $\text{CdBrCl}$ ..   | 11m             | 15   | Calcium chromium iron titanium<br>oxide, loveringite, $\text{Ca}_{.72}\text{RE}_{.33}(\text{Y},$<br>$\text{Th},\text{U},\text{Pb})_{.05}\text{Ti}_{12.48}\text{Fe}_{3.38}\text{Cr}_{2.24}$ | 16m             | 106  |
| Cadmium carbonate (otavite), $\text{CdCO}_3$ ..  | 7               | 11   | $\text{Mg}_{.92}\text{Zr}_{.58}\text{Al}_{.39}\text{V}_{.21}\text{Mn}_{.04}\text{O}_{38}$ ..   |                 |      |
| Cadmium cerium, $\text{CdCe}$ .....  | 5m              | 63   | Calcium chromium oxide (chromatite),<br>$\text{CaCrO}_4$ .....   | 7               | 13   |
| Cadmium chlorate hydrate,<br>$\text{Cd}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ ..... | 3m              | 19   | Calcium chromium oxide, $\text{Ca}_3(\text{CrO}_4)_2$  | 15m             | 22   |
| Cadmium chloride, $\text{CdCl}_2$ .....  | 9               | 18   | Calcium chromium silicate<br>(uvarovite), $\text{Ca}_3\text{Cr}_2(\text{SiO}_4)_3$ .....   | 10              | 17   |
| Cadmium chromium oxide, $\text{CdCr}_2\text{O}_4$ ..                                     | 5m              | 16   | Calcium cyanamide, $\text{CaCN}_2$ .....   | 18m             | 19   |
| Cadmium copper, $\text{Cd}_8\text{Cu}_5$ .....   | 11m             | 81   | Calcium fluoride (fluorite), $\text{CaF}_2$ ..   | 1               | 69   |
| Cadmium cyanide, $\text{Cd}(\text{CN})_2$ .....  | 2m              | 8    | Calcium fluoride phosphate<br>(fluorapatite), $\text{Ca}_5\text{F}(\text{PO}_4)_3$ .....   | 3m              | 22   |
| Cadmium fluoride, $\text{CdF}_2$ .....   | 10m             | 15   | Calcium fluoride phosphate hydrate,<br>$\text{CaFPO}_3 \cdot 2\text{H}_2\text{O}$ .....  | 15m             | 24   |
| Cadmium iodide, $\alpha\text{-CdI}_2$ .....  | 19m             | 24   | Calcium gallium germanium oxide,<br>$\text{Ca}_3\text{Ga}_2(\text{GeO}_4)_3$ .....   | 10              | 18   |
| Cadmium iron oxide, $\text{CdFe}_2\text{O}_4$ .....                                      | 9m              | 16   | Calcium hydrogen phosphate hydrate,<br>$\text{Ca}_8\text{H}_2(\text{PO}_4)_6 \cdot 5\text{H}_2\text{O}$ .....  | 13m             | 21   |
| Cadmium lanthanum, $\text{CdLa}$ .....   | 5m              | 63   | Calcium hydrogen phosphate sulfate<br>hydrate, $\text{Ca}_2\text{HPO}_4\text{SO}_4 \cdot 4\text{H}_2\text{O}$ .....  | 16m             | 109  |
| Cadmium manganese oxide, $\text{CdMn}_2\text{O}_4$ ..                                    | 10m             | 16   |  |                 |      |
| Cadmium molybdenum oxide, $\text{CdMo}_4$ ..   | 6               | 21   |  |                 |      |
| Cadmium nitrate hydrate,<br>$\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ .....   | 7m              | 93   |  |                 |      |
| Cadmium oxide, $\text{CdO}$ .....  | 2               | 27   |  |                 |      |
| Cadmium oxide, $\text{CdO}$ (ref. standard)  | 8m              | 2    |  |                 |      |
| Cadmium phosphate, $\text{Cd}_2\text{P}_2\text{O}_7$ .....                               | 16m             | 26   |  |                 |      |
| Cadmium phosphate, $\text{Cd}_3(\text{PO}_4)_2$ .....                                    | 16m             | 27   |  |                 |      |
| Cadmium praseodymium, $\text{CdPr}$ .....  | 5m              | 64   |  |                 |      |
| Cadmium selenide (cadmoselite),<br>$\text{CdSe}$ (hexagonal) .....                       | 7               | 12   |  |                 |      |
| Cadmium silicate, $\text{Cd}_2\text{SiO}_4$ .....  | 13m             | 19   |  |                 |      |
| Cadmium silicate, $\text{Cd}_3\text{SiO}_5$ .....  | 13m             | 20   |  |                 |      |
| Cadmium sulfate, $\text{CdSO}_4$ .....   | 3m              | 20   |  |                 |      |
| Cadmium sulfate hydrate, $\text{CdSO}_4 \cdot \text{H}_2\text{O}$                        | 6m              | 10   |  |                 |      |
| Cadmium sulfate hydrate,<br>$3\text{CdSO}_4 \cdot 8\text{H}_2\text{O}$ .....             | 6m              | 8    |  |                 |      |

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| Calcium hydroxide (portlandite),<br>$\text{Ca}(\text{OH})_2$ .....   | 1               | 58   | Cerium copper, $\text{CeCu}_6$ .....  | 7m              | 99   |
| Calcium iodate (lautarite),<br>$\text{Ca}(\text{IO}_3)_2$ .....  | 14m             | 12   | Cerium(III) fluoride, $\text{CeF}_3$ .....  | 8               | 17   |
| Calcium iodate hydrate,<br>$\text{Ca}(\text{IO}_3)_2 \cdot 6\text{H}_2\text{O}$ .....  | 14m             | 13   | Cerium gallium, $\text{CeGa}_2$ .....   | 13m             | 54   |
| Calcium iron germanium oxide,<br>$\text{Ca}_3\text{Fe}_2(\text{GeO}_4)_3$ .....  | 10              | 19   | Cerium magnesium, $\text{CeMg}$ .....   | 5m              | 65   |
| Calcium iron oxide, $\text{CaFe}_2\text{O}_4$ .....  | 18m             | 20   | Cerium magnesium, $\text{CeMg}_3$ .....   | 13m             | 56   |
| Calcium iron silicate (kirschsteinite),<br>$\text{CaFeSiO}_4$ .....  | 20m             | 28   | Cerium nickel, $\text{CeNi}_2$ .....  | 13m             | 58   |
| Calcium iron silicate (andradite),<br>$\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_{12}$ .....   | 9               | 22   | Cerium niobium oxide, $\text{CeNbO}_4$ .....  | 18m             | 25   |
| Calcium iron silicate<br>hydroxide, julgoldite,<br>$\text{Ca}_2\text{Fe}_3\text{Si}_3\text{O}_{10}(\text{OH},\text{O})_2(\text{OH})_2$ ..... | 10m             | 72   | Cerium niobium titanium oxide<br>(aeschyrite), $\text{CeNbTiO}_6$ .....                                 | 3m              | 24   |
| Calcium lead nitrate,<br>$\text{Ca}_{.33}\text{Pb}_{.67}(\text{NO}_3)_2$ .....   | 12m             | 44   | Cerium nitrate hydrate,<br>$\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ .....                   | 17m             | 20   |
| Calcium lead nitrate,<br>$\text{Ca}_{.67}\text{Pb}_{.33}(\text{NO}_3)_2$ .....   | 12m             | 44   | Cerium nitride, $\text{CeN}$ .....  | 4m              | 51   |
| Calcium magnesium silicate (monticellite), $\text{CaMgSiO}_4$ .....  | 20m             | 30   | Cerium oxide, $\text{CeO}_2$ .....  | 20m             | 38   |
| Calcium magnesium silicate<br>(diopside), $\text{CaMg}(\text{SiO}_3)_2$ .....  | 5m              | 17   | Cerium(IV) oxide (cerianite), $\text{CeO}_2$ .....  | 1               | 56   |
| Calcium magnesium silicate (akermanite),<br>$\text{Ca}_2\text{MgSi}_2\text{O}_7$ .....   | 20m             | 32   | Cerium phosphide, $\text{CeP}$ .....  | 4m              | 52   |
| Calcium magnesium silicate (merwinite),<br>$\text{Ca}_3\text{Mg}(\text{SiO}_4)_2$ .....  | 20m             | 34   | Cerium tantalum oxide, $\text{CeTaO}_4$ .....   | 18m             | 27   |
| Calcium manganese phosphate fluoride,<br>$\text{Ca}_8\text{Mn}_2(\text{PO}_4)_6\text{F}_2$ .....   | 20m             | 35   | Cerium thallium, $\text{CeTl}$ .....  | 13m             | 59   |
| Calcium molybdenum oxide<br>(powellite), $\text{CaMoO}_4$ .....  | 6               | 22   | Cerium thallium, $\text{CeTl}_3$ .....  | 13m             | 60   |
| Calcium nitrate, $\text{Ca}(\text{NO}_3)_2$ .....  | 7               | 14   | Cerium thallium, $\text{Ce}_3\text{Tl}$ .....   | 13m             | 61   |
| Calcium oxide (lime), $\text{CaO}$ .....   | 1               | 43   | Cerium(III) vanadium oxide, $\text{CeVO}_4$ .....   | 1m              | 9    |
| Calcium oxide (lime), $\text{CaO}$<br>(calculated pattern) .....   | 14m             | 49   | Cerium zinc, $\text{CeZn}$ .....  | 5m              | 65   |
| Calcium oxide phosphate, $\text{Ca}_4\text{O}(\text{PO}_4)_2$ .....  | 12m             | 17   | Cerium zinc, $\text{CeZn}_3$ .....  | 14m             | 50   |
| Calcium phosphate, $\beta\text{-Ca}_2\text{P}_2\text{O}_7$ .....   | 7m              | 95   | Cerium zinc, $\text{CeZn}_5$ .....  | 14m             | 53   |
| Calcium platinum oxide, $\text{Ca}_4\text{PtO}_6$ .....  | 10m             | 18   | Cerium zinc, $\text{Ce}_2\text{Zn}_{17}$ .....  | 14m             | 55   |
| Calcium selenide, $\text{CaSe}$ .....  | 5m              | 64   | Cesium aluminum sulfate hydrate,<br>$\text{CsAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....       | 6               | 25   |
| Calcium silicate (larnite),<br>$\beta\text{-Ca}_2\text{SiO}_4$ .....   | 19m             | 29   | Cesium antimony fluoride, $\text{CsSbF}_6$ .....  | 4m              | 9    |
| Calcium silicon fluoride hydrate,<br>$\text{CaSiF}_6 \cdot 2\text{H}_2\text{O}$ .....  | 19m             | 31   | Cesium beryllium fluoride, $\text{CsBeF}_3$ .....   | 9m              | 69   |
| Calcium strontium nitrate,<br>$\text{Ca}_{.33}\text{Sr}_{.67}(\text{NO}_3)_2$ .....  | 12m             | 46   | Cesium boron fluoride, $\text{CsBF}_4$ .....  | 8               | 22   |
| Calcium strontium nitrate,<br>$\text{Ca}_{.67}\text{Sr}_{.33}(\text{NO}_3)_2$ .....  | 12m             | 46   | Cesium bromate, $\text{CsBrO}_3$ .....  | 8               | 18   |
| Calcium sulfate (anhydrite), $\text{CaSO}_4$ .....   | 4               | 65   | Cesium bromide, $\text{CsBr}$ .....   | 3               | 49   |
| Calcium sulfate hydrate (bassanite),<br>$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$ .....  | 18m             | 22   | Cesium cadmium bromide, $\text{CsCdBr}_3$<br>(hexagonal) .....  | 10m             | 20   |
| Calcium sulfate hydrate (gypsum),<br>$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ .....   | 17m             | 16   | Cesium cadmium chloride, $\text{CsCdCl}_3$<br>(hexagonal) .....   | 5m              | 19   |
| Calcium sulfide (oldhamite), $\text{CaS}$ .....  | 7               | 15   | Cesium calcium chloride, $\text{CsCaCl}_3$ .....  | 5m              | 21   |
| Calcium telluride, $\text{CaTe}$ .....   | 4m              | 50   | Cesium calcium fluoride, $\text{CsCaF}_3$ .....   | 8m              | 25   |
| Calcium tin oxide, $\text{CaSnO}_3$ .....  | 17m             | 18   | Cesium calcium sulfate,<br>$\text{Cs}_2\text{Ca}_2(\text{SO}_4)_3$ .....                                | 7m              | 12   |
| Calcium titanium oxide<br>(perovskite), $\text{CaTiO}_3$ .....   | 9m              | 17   | Cesium cerium chloride, $\text{Cs}_2\text{CeCl}_6$ .....  | 14m             | 58   |
| Calcium tungsten oxide, $\text{Ca}_3\text{W}_2\text{O}_6$ .....  | 9m              | 19   | Cesium chlorate, $\text{CsClO}_3$ .....   | 8               | 20   |
| Calcium tungsten oxide, scheelite,<br>$\text{CaWO}_4$ .....  | 6               | 23   | Cesium chlorate, $\text{CsClO}_4$ ,<br>(orthorhombic) .....   | 1m              | 10   |
| Calcium zirconium phosphate,<br>$\text{CaZr}_4(\text{PO}_4)_6$ .....   | 20m             | 36   | Cesium chloride, $\text{CsCl}$ .....  | 2               | 44   |
| Carbon, diamond, C .....   | 2               | 5    | Cesium chromium oxide, $\text{Cs}_2\text{CrO}_4$ .....  | 3m              | 25   |
| Cerium arsenate, $\text{CeAsO}_4$ .....  | 4m              | 8    | Cesium chromium sulfate hydrate,<br>$\text{CsCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....       | 8               | 21   |
| Cerium(III) chloride, $\text{CeCl}_3$ .....  | 1m              | 8    | Cesium cobalt(II) chloride, $\text{CsCoCl}_3$ .....   | 6m              | 11   |
| Cerium cobalt, $\text{CeCo}_2$ .....   | 13m             | 50   | Cesium cobalt chloride, $\text{Cs}_2\text{CoCl}_4$ .....  | 11m             | 19   |
| Cerium cobalt, $\text{Ce}_2\text{Co}_{11}$ .....   | 13m             | 51   | Cesium copper(II) chloride, $\text{CsCuCl}_3$ .....   | 5m              | 22   |
|  |                 |      | Cesium copper chloride, $\text{Cs}_2\text{CuCl}_4$ .....  | 11m             | 20   |
|  |                 |      | Cesium copper sulfate hydrate,<br>$\text{Cs}_2\text{Cu}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ ..... | 7m              | 14   |
|  |                 |      | Cesium fluoride, $\text{CsF}$ .....   | 3m              | 26   |
|  |                 |      | Cesium gallium sulfate hydrate,<br>$\text{CsGa}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....        | 8               | 23   |
|  |                 |      | Cesium germanium fluoride, $\text{Cs}_2\text{GeF}_6$ .....  | 5               | 17   |
|  |                 |      | Cesium hydrogen phosphate,<br>$\text{CsH}_5(\text{PO}_4)_2$ .....                                       | 20m             | 39   |
|  |                 |      | Cesium iodate, $\text{CsIO}_3$ .....  | 15m             | 26   |
|  |                 |      | Cesium iodide, $\text{CsI}$ .....   | 4               | 47   |
|  |                 |      | Cesium iodide, $\text{CsI}_3$ .....   | 19m             | 33   |
|  |                 |      | Cesium iodine bromide, $\text{CsI}_2\text{Br}$ .....  | 7m              | 103  |
|  |                 |      | Cesium iodine chloride, $\text{CsICl}_2$ .....  | 3               | 50   |
|  |                 |      | Cesium iron chloride hydrate,<br>$\text{Cs}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ .....              | 14m             | 14   |
|  |                 |      | Cesium iron sulfate hydrate,<br>$\text{Cs}_2\text{Fe}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....   | 7m              | 16   |

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| Cesium iron sulfate hydrate,<br>$\text{CsFe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....                      | 6               | 28   | Chromium rhodium, $\text{Cr}_3\text{Rh}$ .....  | 6m              | 15   |
| Cesium lead(II) chloride, $\text{CsPbCl}_3$<br>(tetragonal) .....  | 5m              | 24   | Chromium silicide, $\text{Cr}_3\text{Si}$ .....   | 6               | 29   |
| Cesium lead fluoride, $\text{CsPbF}_3$ .....   | 8m              | 26   | Chromium sulfate, $\text{Cr}_2(\text{SO}_4)_3$ .....  | 16m             | 33   |
| Cesium lithium cobalt cyanide,<br>$\text{CsLiCo}(\text{CN})_6$ .....   | 10m             | 79   | Chromium tungsten oxide, $\text{CrWO}_4$ .....  | 20m             | 43   |
| Cesium lithium fluoride, $\text{CsLiF}_2$ .....  | 7m              | 105  | Cobalt, Co (cubic) .....  | 4m              | 10   |
| Cesium magnesium chromium oxide,<br>$\text{Cs}_2\text{Mg}_2(\text{CrO}_4)_3$ .....                                 | 8m              | 27   | Cobalt aluminum oxide, $\text{CoAl}_2\text{O}_4$ .....  | 9               | 27   |
| Cesium magnesium chromium oxide<br>hydrate, $\text{Cs}_2\text{Mg}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ ..... | 8m              | 29   | Cobalt ammine iodide, $\text{Co}(\text{NH}_3)_6\text{I}_3$ .....                                      | 10m             | 83   |
| Cesium magnesium sulfate hydrate,<br>$\text{Cs}_2\text{Mg}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....         | 7m              | 18   | Cobalt antimony oxide, $\text{CoSb}_2\text{O}_6$ .....  | 5m              | 26   |
| Cesium magnesium titanium oxide,<br>$\text{Cs}_{1.45}\text{Mg}_{0.72}\text{Ti}_{7.27}\text{O}_{16}$ .....          | 18m             | 29   | Cobalt arsenate hydrate (erythrite),<br>$\text{Co}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$ ..... | 19m             | 39   |
| Cesium manganese fluoride, $\text{CsMnF}_3$ .....  | 10m             | 21   | Cobalt arsenide, $\text{CoAs}_2$ .....  | 4m              | 10   |
| Cesium manganese sulfate hydrate,<br>$\text{Cs}_2\text{Mn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....         | 7m              | 20   | Cobalt arsenide (skutterudite),<br>$\text{CoAs}_3$ .....  | 10              | 21   |
| Cesium mercury chloride, $\text{CsHgCl}_3$ .....   | 7m              | 22   | Cobalt borate, $\text{Co}_3(\text{BO}_3)_2$ .....   | 12m             | 20   |
| Cesium molybdenum oxide,<br>$\text{Cs}_2\text{Mo}_3\text{O}_{10}$ .....  | 19m             | 35   | Cobalt bromide hydrate, $\text{CoBr}_2 \cdot 6\text{H}_2\text{O}$ .....                               | 12m             | 21   |
| Cesium nickel(II) chloride, $\text{CsNiCl}_3$ .....  | 6m              | 12   | Cobalt(II) carbonate (sphaero-<br>cobaltite), $\text{CoCO}_3$ .....                                   | 10              | 24   |
| Cesium nickel sulfate hydrate,<br>$\text{Cs}_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....            | 7m              | 23   | Cobalt chlorate hydrate,<br>$\text{Co}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....               | 3m              | 28   |
| Cesium nitrate, $\text{CsNO}_3$ .....  | 9               | 25   | Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$ .....                              | 11m             | 22   |
| Cesium osmium(IV) bromide, $\text{Cs}_2\text{OsBr}_6$ .....  | 2m              | 10   | Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ .....                              | 11m             | 23   |
| Cesium osmium chloride, $\text{Cs}_2\text{OsCl}_6$ .....   | 2m              | 11   | Cobalt chromium oxide, $\text{CoCr}_2\text{O}_4$ .....  | 9m              | 21   |
| Cesium platinum bromide, $\text{Cs}_2\text{PtBr}_6$ .....  | 8               | 19   | Cobalt copper tin, $\text{CoCu}_2\text{Sn}$ .....   | 14m             | 64   |
| Cesium platinum chloride, $\text{Cs}_2\text{PtCl}_6$ .....   | 5               | 14   | Cobalt dysprosium, $\text{Co}_2\text{Dy}$ .....   | 13m             | 63   |
| Cesium platinum fluoride, $\text{Cs}_2\text{PtF}_6$ .....  | 6               | 27   | Cobalt erbium, $\text{Co}_2\text{Er}$ .....   | 13m             | 64   |
| Cesium selenium bromide, $\text{Cs}_2\text{SeBr}_6$ .....  | 8               | 20   | Cobalt erbium, $\text{Co}_7\text{Er}_2$ .....   | 13m             | 65   |
| Cesium silicon fluoride, $\text{Cs}_2\text{SiF}_6$ .....   | 5               | 19   | Cobalt fluoride, $\text{CoF}_2$ .....   | 18m             | 31   |
| Cesium strontium chloride, $\text{CsSrCl}_3$ .....   | 6m              | 13   | Cobalt fluoride, $\text{CoF}_2$ (calculated<br>pattern) .....   | 10m             | 85   |
| Cesium sulfate, $\text{Cs}_2\text{SO}_4$ .....   | 7               | 17   | Cobalt fluoride hydrate, $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$ .....                               | 11m             | 24   |
| Cesium tellurium bromide, $\text{Cs}_2\text{TeBr}_6$ .....   | 9               | 24   | Cobalt gadolinium, $\text{CoGd}_3$ .....  | 13m             | 68   |
| Cesium tin chloride, $\text{Cs}_2\text{SnCl}_6$ .....  | 5               | 16   | Cobalt gadolinium, $\text{Co}_2\text{Gd}$ .....   | 13m             | 71   |
| Cesium vanadium sulfate hydrate,<br>$\text{CsV}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....                   | 1m              | 11   | Cobalt gadolinium, $\text{Co}_7\text{Gd}_2$ .....   | 13m             | 72   |
| Cesium zinc sulfate hydrate,<br>$\text{Cs}_2\text{Zn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....              | 7m              | 25   | Cobalt gallium hafnium, $\text{Co}_2\text{GaHf}$ .....  | 14m             | 65   |
| Cesium zirconium phosphate<br>$\text{CsZr}_2(\text{PO}_4)_3$ .....   | 20m             | 41   | Cobalt gallium manganese, $\text{Co}_2\text{GaMn}$ .....  | 13m             | 75   |
| Chromium, Cr .....   | 5               | 20   | Cobalt gallium niobium,<br>$\text{Co}_{1.5}\text{Ga}_{0.5}\text{Nb}$ .....                            | 15m             | 144  |
| Chromium boride, $\zeta\text{-CrB}$ .....  | 17m             | 22   | Cobalt gallium niobium, $\text{Co}_2\text{GaNb}$ .....  | 14m             | 66   |
| Chromium boride, $\text{CrB}_2$ .....  | 19m             | 37   | Cobalt gallium oxide, $\text{CoGa}_2\text{O}_4$ .....   | 10              | 27   |
| Chromium boride, $\text{Cr}_5\text{B}_3$ .....   | 18m             | 30   | Cobalt gallium tantalum,<br>$\text{Co}_{1.5}\text{Ga}_{0.5}\text{Ta}$ .....                           | 15m             | 146  |
| Chromium chloride, $\text{CrCl}_2$ .....   | 11m             | 77   | Cobalt gallium tantalum, $\text{Co}_2\text{GaTa}$ .....   | 13m             | 76   |
| Chromium chloride, $\text{CrCl}_3$ .....   | 17m             | 23   | Cobalt gallium titanium, $\text{Co}_2\text{GaTi}$ .....   | 13m             | 77   |
| Chromium chloride hydrate, $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$ .....   | 16m             | 31   | Cobalt gallium vanadium, $\text{Co}_2\text{GaV}$ .....  | 13m             | 78   |
| Chromium cobalt niobium, $\text{CoCrNb}$ .....   | 15m             | 140  | Cobalt germanium, $\text{Co}_3\text{Ge}_2$ .....  | 14m             | 67   |
| Chromium cobalt silicide,<br>$\text{Co}_9\text{Cr}_{15}\text{Si}_6$ .....  | 14m             | 62   | Cobalt germanium, $\text{Co}_5\text{Ge}_7$ .....  | 15m             | 148  |
| Chromium cobalt tantalum, $\text{CoCrTa}$ .....  | 15m             | 142  | Cobalt germanium hafnium,<br>$\text{Co}_{16}\text{Ge}_7\text{Hf}_6$ .....                             | 14m             | 69   |
| Chromium fluoride, $\text{CrF}_2$ .....  | 10m             | 81   | Cobalt germanium manganese,<br>$\text{Co}_2\text{GeMn}$ .....   | 13m             | 79   |
| Chromium fluoride, $\text{CrF}_5$ .....  | 7m              | 108  | Cobalt germanium niobium,<br>$\text{Co}_{1.5}\text{Ge}_{0.5}\text{Nb}$ .....                          | 15m             | 150  |
| Chromium(III) fluoride hydrate,<br>$\text{CrF}_3 \cdot 3\text{H}_2\text{O}$ .....                                  | 5m              | 25   | Cobalt germanium niobium,<br>$\text{Co}_{16}\text{Ge}_7\text{Nb}_6$ .....                             | 14m             | 71   |
| Chromium iridium, $\text{Cr}_3\text{Ir}$ .....   | 6m              | 14   | Cobalt germanium oxide, $\text{Co}_2\text{GeO}_4$ .....   | 10              | 27   |
| Chromium iron oxide,<br>$\text{Cr}_{1.3}\text{Fe}_{0.7}\text{O}_3$ .....   | 17m             | 24   | Cobalt germanium tantalum,<br>$\text{Co}_{1.5}\text{Ge}_{0.5}\text{Ta}$ .....                         | 15m             | 152  |
| Chromium niobium oxide, $\text{CrNbO}_4$ .....   | 19m             | 38   | Cobalt germanium tantalum,<br>$\text{Co}_{16}\text{Ge}_7\text{Ta}_6$ .....                            | 14m             | 73   |
| Chromium oxide, $\text{CrO}_3$ .....   | 17m             | 25   | Cobalt germanium titanium, $\text{Co}_2\text{GeTi}$ .....   | 13m             | 80   |
| Chromium(III) oxide, $\text{Cr}_2\text{O}_3$ .....   | 5               | 22   | Cobalt hafnium tin, $\text{Co}_2\text{HfSn}$ .....  | 14m             | 75   |
| Chromium phosphate, $\alpha\text{-CrPO}_4$ .....   | 2m              | 12   | Cobalt holmium, $\text{Co}_2\text{Ho}$ .....  | 14m             | 76   |
| Chromium phosphate, $\beta\text{-CrPO}_4$ .....  | 9               | 26   | Cobalt holmium, $\text{Co}_{9.2}\text{Ho}_{12}$ .....   | 15m             | 154  |
| Chromium phosphate hydrate,<br>$\text{CrPO}_4 \cdot 6\text{H}_2\text{O}$ .....                                     | 15m             | 27   | Cobalt hydroxide, $\beta\text{-Co(OH)}_2$ .....   | 15m             | 29   |
|  |                 |      | Cobalt indium, $\text{CoIn}_3$ .....  | 13m             | 81   |
|  |                 |      | Cobalt iodide, $\text{CoI}_2$ .....   | 4m              | 52   |
|  |                 |      | Cobalt iron arsenide<br>(safflorite), $\text{CoFeAs}_4$ .....   | 10              | 28   |

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| Cobalt iron oxide, $\text{CoFe}_2\text{O}_4$ .....   | 9m              | 22   | Copper ammine sulfate hydrate,<br>$\text{Cu}(\text{NH}_3)_4\text{SO}_4 \cdot \text{H}_2\text{O}$ .....   | 10m             | 90   |
| Cobalt iron sulfide, $\text{Co}_8\text{FeS}_8$ .....   | 14m             | 77   | Copper antimony oxide, $\text{CuSb}_2\text{O}_6$ ....  | 5m              | 27   |
| Cobalt iron vanadium,<br>$\text{Co}_{4.35}\text{Fe}_{13.47}\text{V}_{12.18}$ .....           | 14m             | 79   | Copper arsenate (trippkeite),<br>$\text{CuAs}_2\text{O}_4$ .....   | 16m             | 120  |
| Cobalt lanthanum, $\text{CoLa}_3$ .....  | 13m             | 83   | Copper(I) bromide, $\text{CuBr}$ .....   | 4               | 36   |
| Cobalt lutetium, $\text{Co}_2\text{Lu}$ .....  | 13m             | 86   | Copper(I) chloride (nantokite),<br>$\text{CuCl}$ .....   | 4               | 35   |
| Cobalt magnesium, $\text{Co}_2\text{Mg}$ .....   | 15m             | 156  | Copper chloride hydrate<br>(eriochalcite), $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ .....   | 18m             | 33   |
| Cobalt manganese silicide, $\text{Co}_2\text{MnSi}$  | 14m             | 81   | Copper chromium oxide, $\text{CuCr}_2\text{O}_4$ ....  | 20m             | 46   |
| Cobalt mercury thiocyanate,<br>$\text{Co}[\text{Hg}(\text{CNS})_4]$ .....                    | 2m              | 13   | Copper fluoride hydrate, $\text{CuF}_2 \cdot 2\text{H}_2\text{O}$ .....  | 11m             | 25   |
| Cobalt molybdenum, $\text{Co}_2\text{Mo}$ .....  | 14m             | 82   | Copper hydrogen phosphite hydrate,<br>$\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ .....   | 11m             | 83   |
| Cobalt molybdenum, $\text{Co}_2\text{Mo}_3$ .....  | 15m             | 158  | Copper hydroxide carbonate,<br>azurite, $\text{Cu}_3(\text{OH})_2(\text{CO}_3)_2$ .....  | 10              | 30   |
| Cobalt molybdenum, $\text{Co}_7\text{Mo}_6$ .....  | 15m             | 160  | Copper hydroxide carbonate<br>(malachite), $\text{Cu}_2(\text{OH})_2\text{CO}_3$ .....   | 10              | 31   |
| Cobalt molybdenum silicide,<br>$\text{Co}_3\text{Mo}_2\text{Si}$ .....                       | 15m             | 162  | Copper hydroxide phosphate<br>(libethenite), $\text{Cu}_2(\text{OH})\text{PO}_4$ .....   | 17m             | 30   |
| Cobalt neodymium, $\text{Co}_2\text{Nd}$ .....   | 13m             | 87   | Copper(I) iodide (marshite), $\text{CuI}$ ..   | 4               | 38   |
| Cobalt nickel tin,<br>$\text{Co}_{.75}\text{Ni}_{.75}\text{Sn}_{.75}$ .....                  | 13m             | 88   | Copper iron oxide, $\text{CuFe}_2\text{O}_4$ .....   | 20m             | 47   |
| Cobalt niobium silicide, $\text{Co}_3\text{Nb}_4\text{Si}_7$                                 | 15m             | 164  | Copper lead hydroxide sulfate,<br>linarite, $\text{CuPb}(\text{OH})_2(\text{SO}_4)$ .....  | 16m             | 34   |
| Cobalt niobium tin, $\text{Co}_2\text{NbSn}$ .....   | 15m             | 166  | Copper mercury iodide, $\beta\text{-Cu}_2\text{HgI}_4$ ..  | 20m             | 48   |
| Cobalt nitrate hydrate,<br>$\alpha\text{-Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ ..... | 12m             | 22   | Copper(I) oxide (cuprite), $\text{Cu}_2\text{O}$ ..  | 2               | 23   |
| Cobalt(II) oxide, $\text{CoO}$ .....   | 9               | 28   | Copper(II) oxide (tenorite), $\text{CuO}$ ..   | 1               | 49   |
| Cobalt(II,III) oxide, $\text{Co}_3\text{O}_4$ .....  | 9               | 29   | Copper phosphate, $\text{Cu}(\text{PO}_3)_2$ .....   | 14m             | 15   |
| Cobalt phosphate, $\text{Co}(\text{PO}_3)_2$ .....   | 13m             | 23   | Copper phosphate, $\alpha\text{-Cu}_2\text{P}_2\text{O}_7$ .....   | 7m              | 113  |
| Cobalt phosphate hydrate,<br>$\text{Co}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$ .....    | 19m             | 40   | Copper sulfate (chalcocyanite),<br>$\text{CuSO}_4$ .....   | 3m              | 29   |
| Cobalt phosphide, $\text{CoP}$ .....   | 14m             | 83   | Copper(II) sulfide (covellite), $\text{CuS}$ ..  | 4               | 13   |
| Cobalt phosphide, $\text{CoP}_3$ .....   | 14m             | 85   | Copper uranium oxide, $\text{CuUO}_4$ .....  | 10m             | 93   |
| Cobalt phosphide, $\text{Co}_2\text{P}$ .....  | 18m             | 32   | Dichlorotetraaquochromium (III)<br>chloride dihydrate,<br>$[\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2] \text{Cl} \cdot 2\text{H}_2\text{O}$ ..... | 16m             | 31   |
| Cobalt platinum, $\text{CoPt}$ (disordered)  | 15m             | 167  | Dysprosium arsenate, $\text{DyAsO}_4$ .....  | 3m              | 30   |
| Cobalt platinum, $\text{CoPt}$ (ordered) ...   | 15m             | 168  | Dysprosium arsenide, $\text{DyAs}$ .....   | 4m              | 53   |
| Cobalt platinum, $\text{CoPt}_3$<br>(disordered) .....                                       | 15m             | 169  | Dysprosium gallium oxide,<br>$\text{Dy}_3\text{Ga}_5\text{O}_{12}$ .....   | 2m              | 15   |
| Cobalt platinum, $\text{CoPt}_3$ (ordered) ..  | 15m             | 170  | Dysprosium gold, $\text{DyAu}$ .....   | 5m              | 66   |
| Cobalt plutonium, $\text{CoPu}_2$ .....  | 14m             | 87   | Dysprosium nitride, $\text{DyN}$ .....   | 4m              | 53   |
| Cobalt plutonium, $\text{CoPu}_3$ .....  | 15m             | 171  | Dysprosium oxide, $\text{Dy}_2\text{O}_3$ .....  | 9               | 30   |
| Cobalt plutonium, $\text{CoPu}_6$ .....  | 14m             | 89   | Dysprosium silver, $\text{DyAg}$ .....   | 5m              | 66   |
| Cobalt plutonium, $\text{Co}_2\text{Pu}$ .....   | 14m             | 91   | Dysprosium telluride, $\text{DyTe}$ .....  | 4m              | 54   |
| Cobalt plutonium, $\text{Co}_3\text{Pu}$ .....   | 14m             | 92   | Dysprosium vanadium oxide, $\text{DyVO}_4$ ..  | 4m              | 15   |
| Cobalt plutonium, $\text{Co}_{17}\text{Pu}_2$ .....  | 14m             | 94   | Erbium arsenate, $\text{ErAsO}_4$ .....  | 3m              | 31   |
| Cobalt praseodymium, $\text{Co}_2\text{Pr}$ .....  | 14m             | 97   | Erbium arsenide, $\text{ErAs}$ .....   | 4m              | 54   |
| Cobalt rhodium sulfide, $\text{Co}_8\text{RhS}_8$ ..   | 14m             | 98   | Erbium gallium oxide, $\text{Er}_3\text{Ga}_5\text{O}_{12}$ ..   | 1m              | 12   |
| Cobalt ruthenium sulfide, $\text{Co}_8\text{RuS}_8$ ..                                       | 14m             | 100  | Erbium iron, $\text{ErFe}_2$ .....   | 19m             | 42   |
| Cobalt samarium, $\text{Co}_2\text{Sm}$ .....  | 15m             | 173  | Erbium manganese oxide, $\text{ErMnO}_3$ .....   | 2m              | 16   |
| Cobalt samarium, $\text{Co}_5\text{Sm}$ .....  | 13m             | 90   | Erbium nitride, $\text{ErN}$ .....   | 4m              | 55   |
| Cobalt silicate, $\text{Co}_2\text{SiO}_4$<br>(orthorhombic) .....                           | 4m              | 11   | Erbium oxide, $\text{Er}_2\text{O}_3$ .....  | 8               | 25   |
| Cobalt silicon fluoride hydrate,<br>$\text{CoSiF}_6 \cdot 6\text{H}_2\text{O}$ .....         | 3m              | 27   | Erbium phosphate, $\text{ErPO}_4$ .....  | 9               | 31   |
| Cobalt sulfate, $\beta\text{-CoSO}_4$ .....  | 2m              | 14   | Erbium silver, $\text{ErAg}$ .....   | 5m              | 67   |
| Cobalt tantalum silicide,<br>$\text{Co}_{16}\text{Ta}_6\text{Si}_7$ .....                    | 14m             | 102  | Erbium telluride, $\text{ErTe}$ .....  | 4m              | 55   |
| Cobalt telluride, $\text{CoTe}$ .....  | 20m             | 45   | Erbium vanadium oxide, $\text{ErVO}_4$ .....   | 5m              | 29   |
| Cobalt thorium, $\text{Co}_{17}\text{Th}_2$ .....  | 12m             | 64   | Europium arsenate, $\text{EuAsO}_4$ .....  | 3m              | 32   |
| Cobalt tin, $\text{Co}_3\text{Sn}_2$ .....   | 13m             | 92   | Europium(III) chloride, $\text{EuCl}_3$ .....  | 1m              | 13   |
| Cobalt tin oxide, $\text{Co}_2\text{SnO}_4$ .....  | 15m             | 30   | Europium chloride oxide, $\text{EuClO}$ .....  | 1m              | 13   |
| Cobalt tin vanadium, $\text{Co}_2\text{SnV}$ .....   | 15m             | 174  | Europium gallium oxide,<br>$\text{Eu}_3\text{Ga}_5\text{O}_{12}$ .....   | 2m              | 17   |
| Cobalt tin zirconium, $\text{Co}_2\text{SnZr}$ .....   | 15m             | 175  | Europium nitride, $\text{EuN}$ .....   | 4m              | 56   |
| Cobalt titanium oxide, $\text{CoTiO}_3$ .....  | 4m              | 13   | Europium oxide, $\text{EuO}$ .....   | 4m              | 56   |
| Cobalt titanium silicide,<br>$\text{Co}_{16}\text{Ti}_6\text{Si}_7$ .....                    | 14m             | 104  | Europium oxide, $\text{Eu}_2\text{O}_3$ (cubic) .....  | 20m             | 50   |
| Cobalt tungsten oxide, $\text{CoWO}_4$ .....   | 4m              | 13   | Europium oxide, $\text{Eu}_2\text{O}_3$ (monoclinic).<br>$\text{Eu}_2\text{O}_3$ .....   | 20m             | 52   |
| Cobalt vanadium silicide, $\text{Co}_2\text{VSi}$ ..   | 15m             | 176  | Europium phosphate, $\text{EuPO}_4$ .....  | 11m             | 26   |
| Copper, Cu .....   | 1               | 15   |  |                 |      |
| Copper ammine selenate,<br>$\text{Cu}(\text{NH}_3)_4\text{SeO}_4$ .....                      | 10m             | 87   |  |                 |      |

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| Europium(III) vanadium oxide, EuVO <sub>4</sub>  | 4m              | 16   | Indium, In .....  | 3               | 12   |
| Gadolinium arsenate, GdAsO <sub>4</sub> .....  | 4m              | 17   | Indium arsenide, InAs .....   | 3m              | 35   |
| Gadolinium arsenide, GdAs .....  | 4m              | 57   | Indium oxide, In <sub>2</sub> O <sub>3</sub> .....  | 5               | 26   |
| Gadolinium chloride hydrate,<br>GdCl <sub>3</sub> ·6H <sub>2</sub> O .....               | 7m              | 118  | Indium phosphate, InPO <sub>4</sub> .....   | 8               | 29   |
| Gadolinium chloride oxide, GdClO ..  | 1m              | 17   | Indium sulfide, In <sub>2</sub> S <sub>3</sub> .....  | 11m             | 30   |
| Gadolinium fluoride, GdF <sub>3</sub> .....  | 1m              | 14   | Iodine, I <sub>2</sub> .....  | 3               | 16   |
| Gadolinium gallium oxide,<br>Gd <sub>3</sub> Ga <sub>5</sub> O <sub>12</sub> .....       | 2m              | 18   | Iridium, Ir .....   | 4               | 9    |
| Gadolinium indium, GdIn .....  | 5m              | 67   | Iridium niobium, IrNb <sub>3</sub> .....  | 6m              | 19   |
| Gadolinium nitride, GdN .....  | 4m              | 57   | Iridium oxide, IrO <sub>2</sub> .....   | 4m              | 19   |
| Gadolinium oxide, Gd <sub>2</sub> O <sub>3</sub> .....                                   | 1m              | 16   | Iridium titanium, IrTi <sub>3</sub> .....   | 6m              | 20   |
| Gadolinium silver, GdAg .....  | 6m              | 87   | Iridium vanadium, IrV <sub>3</sub> .....  | 6m              | 21   |
| Gadolinium titanium oxide, Gd <sub>2</sub> TiO <sub>5</sub>                              | 8m              | 32   | Iron, $\alpha$ -Fe .....  | 4               | 3    |
| Gadolinium vanadium oxide, GdVO <sub>4</sub> ..  | 5m              | 30   | Iron aluminum oxide (hercynite),<br>FeAl <sub>2</sub> O <sub>4</sub> .....                                      | 19m             | 48   |
| Gallium, Ga .....  | 2               | 9    | Iron antimony oxide, FeSbO <sub>4</sub> .....   | 19m             | 49   |
| Gallium arsenide, GaAs .....   | 3m              | 33   | Iron arsenide, FeAs .....   | 1m              | 19   |
| Gallium lutetium oxide, Ga <sub>5</sub> Lu <sub>3</sub> O <sub>12</sub>                  | 2m              | 22   | Iron arsenide (loellingite), FeAs <sub>2</sub> .....  | 10              | 34   |
| Gallium magnesium, Ga <sub>2</sub> Mg .....  | 12m             | 48   | Iron boride, FeB .....  | 18m             | 35   |
| Gallium magnesium, Ga <sub>5</sub> Mg <sub>2</sub> .....                                 | 12m             | 51   | Iron bromide, FeBr <sub>2</sub> .....   | 4m              | 59   |
| Gallium neodymium oxide, Ga <sub>5</sub> Nd <sub>3</sub> O <sub>12</sub>                 | 1m              | 34   | Iron carbonate, siderite, FeCO <sub>3</sub> ...   | 15m             | 32   |
| Gallium oxide, $\alpha$ -Ga <sub>2</sub> O <sub>3</sub> .....                            | 4               | 25   | Iron chloride hydrate (rokuhnite),<br>FeCl <sub>2</sub> ·2H <sub>2</sub> O .....                                | 11m             | 32   |
| Gallium phosphate ( $\alpha$ -quartz type),<br>GaPO <sub>4</sub> .....                   | 8               | 27   | Iron chloride hydrate (hydromolysite),<br>FeCl <sub>3</sub> ·6H <sub>2</sub> O .....                            | 17m             | 40   |
| Gallium phosphate hydrate,<br>GaPO <sub>4</sub> ·2H <sub>2</sub> O .....                 | 8m              | 34   | Iron chromium oxide (chromite),<br>FeCr <sub>2</sub> O <sub>4</sub> .....                                       | 19m             | 50   |
| Gallium samarium oxide, Ga <sub>5</sub> Sm <sub>3</sub> O <sub>12</sub>                  | 1m              | 42   | Iron fluoride hydrate, FeF <sub>2</sub> ·4H <sub>2</sub> O .....  | 11m             | 90   |
| Gallium ytterbium oxide, Ga <sub>5</sub> Yb <sub>3</sub> O <sub>12</sub>                 | 1m              | 49   | Iron fluoride, FeF <sub>3</sub> .....   | 18m             | 36   |
| Gallium yttrium oxide, Ga <sub>5</sub> Y <sub>3</sub> O <sub>12</sub> ..                 | 1m              | 50   | Iron fluoride hydrate, $\beta$ -FeF <sub>3</sub> ·3H <sub>2</sub> O .....                                       | 17m             | 41   |
| Germanium, Ge .....  | 1               | 18   | Iron hydroxide sulfate hydrate,<br>butlerite, Fe(OH)SO <sub>4</sub> ·2H <sub>2</sub> O .....                    | 10m             | 95   |
| Germanium iodide, GeI <sub>2</sub> .....   | 4m              | 58   | Iron iodide, FeI <sub>2</sub> .....   | 4m              | 60   |
| Germanium(IV) iodide, GeI <sub>4</sub> .....   | 5               | 25   | Iron niobium oxide, Fe(NbO <sub>3</sub> ) <sub>2</sub> .....  | 20m             | 56   |
| Germanium oxide, GeO <sub>2</sub> (hexagonal)<br>(low form) .....                        | 1               | 51   | Iron niobium oxide, Fe <sub>4</sub> Nb <sub>2</sub> O <sub>9</sub> .....  | 20m             | 58   |
| Germanium oxide, GeO <sub>2</sub><br>(tetragonal) (high form) .....                      | 8               | 28   | Iron oxide (hematite), $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> .....   | 18m             | 37   |
| Gold, Au .....   | 1               | 33   | Iron(II,III) oxide (magnetite),<br>Fe <sub>3</sub> O <sub>4</sub> .....   | 5m              | 31   |
| Gold chloride, AuCl .....  | 16m             | 37   | Iron phosphate, FePO <sub>4</sub> .....   | 15m             | 33   |
| Gold(I) cyanide, AuCN .....  | 10              | 33   | Iron phosphate hydrate (vivianite),<br>Fe <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O ..... | 16m             | 38   |
| Gold holmium, AuHo .....   | 5m              | 68   | Iron silicate (fayalite), Fe <sub>2</sub> SiO <sub>4</sub> .....  | 20m             | 59   |
| Gold magnesium, AuMg .....   | 6m              | 83   | Iron sulfate, Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....   | 16m             | 39   |
| Gold niobium, AuNb <sub>3</sub> .....  | 6m              | 16   | Iron sulfate hydrate (melanterite),<br>FeSO <sub>4</sub> ·7H <sub>2</sub> O .....                               | 8m              | 38   |
| Gold potassium cyanide, AuK(CN) <sub>2</sub> ..  | 8m              | 36   | Iron sulfide (pyrite), FeS <sub>2</sub> .....   | 5               | 29   |
| Gold tin, AuSn .....   | 7               | 19   | Iron thorium, Fe <sub>17</sub> Th <sub>2</sub> .....  | 12m             | 67   |
| Gold titanium, AuTi <sub>3</sub> .....   | 6m              | 17   | Iron titanium oxide (ilmenite),<br>FeTiO <sub>3</sub> .....   | 15m             | 34   |
| Gold vanadium, AuV <sub>3</sub> .....  | 6m              | 18   | Iron titanium oxide (ulvöspinel),<br>Fe <sub>2</sub> TiO <sub>4</sub> .....                                     | 20m             | 61   |
| Hafnium, Hf .....  | 3               | 18   | Iron yttrium oxide, Fe <sub>5</sub> Y <sub>3</sub> O <sub>12</sub> .....  | 18m             | 38   |
| Hafnium nitride, HfN .....   | 19m             | 46   | Lanthanum arsenate, LaAsO <sub>4</sub> .....  | 3m              | 36   |
| Hafnium oxide, HfO <sub>2</sub> .....  | 20m             | 54   | Lanthanum arsenide, LaAs .....  | 4m              | 60   |
| Holmium arsenate, HoAsO <sub>4</sub> .....   | 3m              | 34   | Lanthanum borate, LaBO <sub>3</sub> .....   | 1m              | 20   |
| Holmium fluoride, HoF <sub>3</sub> .....   | 10m             | 23   | Lanthanum boride, LaB <sub>6</sub> .....  | 20m             | 62   |
| Holmium nitride, HoN .....   | 4m              | 58   | Lanthanum chloride, LaCl <sub>3</sub> .....   | 1m              | 20   |
| Holmium oxide, Ho <sub>2</sub> O <sub>3</sub> .....                                      | 9               | 32   | Lanthanum chloride oxide, LaClO .....   | 7               | 22   |
| Holmium selenide, HoSe .....   | 4m              | 59   | Lanthanum fluoride, LaF <sub>3</sub> .....  | 7               | 21   |
| Holmium silver, HoAg .....   | 5m              | 68   | Lanthanum magnesium, LaMg .....   | 5m              | 69   |
| Holmium vanadium oxide, HoVO <sub>4</sub> .....  | 4m              | 18   | Lanthanum nickel platinum,<br>LaNi <sub>0.25</sub> Pt <sub>4.75</sub> .....                                     | 17m             | 42   |
| Hydrazinium sulfate, (NH <sub>3</sub> ) <sub>2</sub> SO <sub>4</sub> .....               | 17m             | 38   | Lanthanum niobium titanium oxide,<br>LaNbTiO <sub>6</sub> .....   | 3m              | 37   |
| Hydrogen amidosulfate, H <sub>2</sub> NSO <sub>3</sub> H ..                              | 7               | 54   | Lanthanum nitrate hydrate,<br>La(NO <sub>3</sub> ) <sub>3</sub> ·6H <sub>2</sub> O .....                        | 8m              | 40   |
| Hydrogen arsenate, H <sub>5</sub> As <sub>3</sub> O <sub>10</sub> .....                  | 7m              | 84   | Lanthanum nitride, LaN .....  | 4m              | 61   |
| Hydrogen borate, $\beta$ -HBO <sub>2</sub> (monoclinic)                                  | 9m              | 71   | Lanthanum oxide, La <sub>2</sub> O <sub>3</sub> .....   | 3               | 33   |
| Hydrogen borate (metaborite),<br>HBO <sub>2</sub> (cubic) .....                          | 4m              | 27   |   |                 |      |
| Hydrogen iodate, HIO <sub>3</sub> .....  | 5               | 28   |   |                 |      |
| Hydrogen iodate, HI <sub>3</sub> O <sub>8</sub> .....                                    | 8m              | 104  |   |                 |      |
| Hydrogen phosphate hydrate,<br>H <sub>3</sub> PO <sub>4</sub> ·0.5H <sub>2</sub> O ..... | 12m             | 56   |   |                 |      |
| Hydrogen tellurate, H <sub>6</sub> TeO <sub>6</sub> .....                                | 12m             | 34   |   |                 |      |

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| Lanthanum phosphide, LaP .....   | 5m              | 69   | Lithium hydroxide, LiOH .....   | 17m             | 46   |
| Lanthanum selenide, LaSe .....   | 4m              | 61   | Lithium hydroxide hydrate, LiOH·H <sub>2</sub> O                                      | 11m             | 92   |
| Lanthanum titanium oxide, La <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub>   | 15m             | 35   | Lithium iodate, LiIO <sub>3</sub> (hexagonal)   | 7               | 26   |
| Lanthanum zinc, LaZn .....   | 5m              | 70   | Lithium iodate, LiIO <sub>3</sub> (tetragonal)  | 10m             | 33   |
| Lead, Pb .....   | 1               | 34   | Lithium iodide hydrate, LiI·3H <sub>2</sub> O ..                                      | 18m             | 40   |
| Lead borate, PbB <sub>4</sub> O <sub>7</sub> .....   | 4m              | 19   | Lithium molybdenum oxide, Li <sub>2</sub> MoO <sub>4</sub>                            |                 |      |
| Lead bromide, PbBr <sub>2</sub> .....  | 17m             | 43   | (trigonal) .....  | 1m              | 23   |
| Lead bromide chloride, PbBrCl .....  | 11m             | 33   | Lithium niobium oxide, LiNbO <sub>3</sub> .....                                       | 6m              | 22   |
| Lead bromide fluoride, PbBrF .....   | 10m             | 25   | Lithium nitrate, LiNO <sub>3</sub> .....  | 7               | 27   |
| Lead bromide hydroxide, PbBr(OH) ..  | 16m             | 40   | Lithium oxide, Li <sub>2</sub> O .....  | 1m              | 25   |
| Lead bromide oxide, Pb <sub>3</sub> O <sub>2</sub> Br <sub>2</sub> .....   | 5m              | 32   | Lithium phosphate, high form, Li <sub>3</sub> PO <sub>4</sub>                         | 3m              | 39   |
| Lead carbonate (cerussite), PbCO <sub>3</sub>  | 2               | 56   | Lithium phosphate, low form   |                 |      |
| Lead chloride (cotunnite), PbCl <sub>2</sub> ..  | 12m             | 23   | (lithiophosphate), Li <sub>3</sub> PO <sub>4</sub> .....                              | 4m              | 21   |
| Lead chloride fluoride (matlockite),   |                 |      | Lithium phosphate hydrate,  |                 |      |
| PbClF .....  | 13m             | 25   | Li <sub>3</sub> P <sub>3</sub> O <sub>9</sub> ·3H <sub>2</sub> O .....                | 2m              | 20   |
| Lead chromium oxide, Pb <sub>2</sub> CrO <sub>5</sub> .....  | 14m             | 16   | Lithium potassium sulfate, KLiSO <sub>4</sub>   | 3m              | 43   |
| Lead fluoride, α-PbF <sub>2</sub>  |                 |      | Lithium rubidium fluoride, LiRbF <sub>2</sub>   | 7m              | 128  |
| (orthorhombic) .....   | 5               | 31   | Lithium selenide, Li <sub>2</sub> Se .....  | 10m             | 100  |
| Lead fluoride, β-PbF <sub>2</sub> (cubic) .....  | 5               | 33   | Lithium silicate, Li <sub>2</sub> SiO <sub>3</sub> .....                              | 14m             | 19   |
| Lead fluoride iodide, PbFI .....   | 10m             | 26   | Lithium silver bromide,   |                 |      |
| Lead hydrogen arsenate (schultenite),  |                 |      | Li <sub>2</sub> Ag <sub>8</sub> Br .....  | 12m             | 55   |
| PbHAsO <sub>4</sub> .....  | 14m             | 18   | Lithium silver bromide, Li <sub>4</sub> Ag <sub>6</sub> Br                            | 12m             | 55   |
| Lead hydrogen phosphate, PbHPO <sub>4</sub> ..   | 15m             | 37   | Lithium silver bromide,   |                 |      |
| Lead hydroxide phosphate,  |                 |      | Li <sub>6</sub> Ag <sub>4</sub> Br .....  | 12m             | 55   |
| Pb <sub>5</sub> OH(PO <sub>4</sub> ) <sub>3</sub> .....  | 8               | 33   | Lithium silver bromide,   |                 |      |
| Lead iodate, Pb(IO <sub>3</sub> ) <sub>2</sub> .....   | 17m             | 45   | Li <sub>8</sub> Ag <sub>2</sub> Br .....  | 12m             | 55   |
| Lead(II) iodide, PbI <sub>2</sub> .....  | 5               | 34   | Lithium sodium aluminum fluoride,   |                 |      |
| Lead molybdenum oxide (wulfenite),   |                 |      | cryolithionite, Li <sub>3</sub> Na <sub>3</sub> Al <sub>2</sub> F <sub>12</sub> ..... | 9m              | 23   |
| PbMoO <sub>4</sub> .....   | 7               | 23   | Lithium sodium sulfate, LiNaSO <sub>4</sub> .....                                     | 6m              | 24   |
| Lead nitrate, Pb(NO <sub>3</sub> ) <sub>2</sub> .....  | 5               | 36   | Lithium sulfate, Li <sub>2</sub> SO <sub>4</sub> .....                                | 6m              | 26   |
| Lead oxide (litharge), PbO (red,   |                 |      | Lithium sulfate hydrate,  |                 |      |
| tetragonal) .....  | 2               | 30   | Li <sub>2</sub> SO <sub>4</sub> ·H <sub>2</sub> O .....                               | 4m              | 22   |
| Lead oxide (massicot), PbO (yellow,  |                 |      | Lithium sulfide, Li <sub>2</sub> S .....  | 10m             | 101  |
| orthorhombic) .....  | 2               | 32   | Lithium tantalum oxide, LiTaO <sub>3</sub> .....                                      | 14m             | 20   |
| Lead(II,III) oxide (minium), Pb <sub>3</sub> O <sub>4</sub>  | 8               | 32   | Lithium telluride, Li <sub>2</sub> Te .....   | 10m             | 102  |
| Lead oxide sulfate, Pb <sub>5</sub> O <sub>5</sub> SO <sub>4</sub> .....   | 10m             | 27   | Lithium thorium molybdenum oxide,   |                 |      |
| Lead selenide (clausthalite), PbSe   |                 |      | Li <sub>4</sub> Th <sub>7</sub> (MoO <sub>4</sub> ) <sub>16</sub> .....               | 20m             | 63   |
| Lead strontium nitrate,  |                 |      | Lithium thorium tungsten oxide,   |                 |      |
| Pb <sub>.33</sub> Sr <sub>.67</sub> (NO <sub>3</sub> ) <sub>2</sub> .....  | 12m             | 53   | Li <sub>4</sub> Th <sub>7</sub> (WO <sub>4</sub> ) <sub>16</sub> .....                | 20m             | 64   |
| Lead strontium nitrate,  |                 |      | Lithium tin oxide, Li <sub>2</sub> SnO <sub>3</sub> .....                             | 16m             | 45   |
| Pb <sub>.67</sub> Sr <sub>.33</sub> (NO <sub>3</sub> ) <sub>2</sub> .....  | 12m             | 53   | Lithium titanium oxide, Li <sub>2</sub> Ti <sub>3</sub> O <sub>7</sub> ..             | 20m             | 66   |
| Lead sulfate (anglesite), PbSO <sub>4</sub> ..   | 3               | 67   | Lithium tungsten oxide, Li <sub>2</sub> WO <sub>4</sub>                               |                 |      |
| Lead sulfide (galena), PbS .....   | 2               | 18   | (trigonal) .....  | 1m              | 25   |
| Lead tin oxide, Pb <sub>2</sub> SnO <sub>4</sub> .....   | 10m             | 29   | Lithium tungsten oxide hydrate,   |                 |      |
| Lead titanium oxide (macedonite),  |                 |      | Li <sub>2</sub> WO <sub>4</sub> ·0.5H <sub>2</sub> O .....                            | 2m              | 20   |
| PbTiO <sub>3</sub> .....   | 5               | 39   | Lithium uranium fluoride, LiUF <sub>5</sub> .....                                     | 7m              | 131  |
| Lead tungsten oxide (stolzite),  |                 |      | Lithium zirconium oxide, Li <sub>2</sub> ZrO <sub>3</sub> ..                          | 19m             | 51   |
| PbWO <sub>4</sub> (tetragonal) .....   | 5m              | 34   | Lutetium arsenate, LuAsO <sub>4</sub> .....   | 5m              | 36   |
| Lead uranium oxide, Pb <sub>3</sub> UO <sub>6</sub> .....  | 8m              | 109  | Lutetium manganese oxide, LuMnO <sub>3</sub> ..                                       | 2m              | 23   |
| Lithium aluminum fluoride,   |                 |      | Lutetium nitride, LuN .....   | 4m              | 62   |
| α-Li <sub>3</sub> AlF <sub>6</sub> .....   | 8m              | 111  | Lutetium oxide, Lu <sub>2</sub> O <sub>3</sub> .....                                  | 1m              | 27   |
| Lithium arsenate, Li <sub>3</sub> AsO <sub>4</sub> .....   | 2m              | 19   | Lutetium vanadium oxide, LuVO <sub>4</sub> .....                                      | 5m              | 37   |
| Lithium azide, LiN <sub>3</sub> .....  | 8m              | 113  | Magnesium, Mg .....   | 1               | 10   |
| Lithium barium fluoride, LiBaF <sub>3</sub> ..   | 5m              | 35   | Magnesium aluminum oxide (spinel),  |                 |      |
| Lithium beryllium fluoride, Li <sub>2</sub> BeF <sub>4</sub>   | 7m              | 126  | MgAl <sub>2</sub> O <sub>4</sub> .....  | 9m              | 25   |
| Lithium borate, Li <sub>2</sub> B <sub>4</sub> O <sub>7</sub> .....  | 8m              | 114  | Magnesium aluminum silicate (low  |                 |      |
| Lithium bromide, LiBr .....  | 4               | 30   | cordierite), Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub>          |                 |      |
| Lithium calcium aluminum boron   |                 |      | (orthorhombic) .....  | 1m              | 28   |
| hydroxy silicate, liddicoatite,  |                 |      | Magnesium aluminum silicate   |                 |      |
| Ca(Li,Al) <sub>3</sub> Al <sub>6</sub> B <sub>3</sub> Si <sub>6</sub> O <sub>27</sub> (O,OH) <sub>3</sub> (OH,F) | 16m             | 42   | (indialite) Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub>           |                 |      |
| Lithium carbonate, Li <sub>2</sub> CO <sub>3</sub> .....   | 8m              | 42   | (hexagonal) .....   | 1m              | 29   |
| Lithium chlorate hydrate,  |                 |      | Magnesium aluminum silicate   |                 |      |
| LiClO <sub>4</sub> ·3H <sub>2</sub> O .....  | 8               | 34   | (pyrope), Mg <sub>3</sub> Al <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub> .....      | 4m              | 24   |
| Lithium chloride, LiCl .....   | 1               | 62   | Magnesium arsenate hydrate  |                 |      |
| Lithium chromium oxide hydrate,  |                 |      | (hoernesite), Mg <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O ..  | 19m             | 53   |
| Li <sub>2</sub> CrO <sub>4</sub> ·2H <sub>2</sub> O .....  | 16m             | 44   | Magnesium borate, MgB <sub>4</sub> O <sub>7</sub> .....                               | 17m             | 47   |
| Lithium fluoride, LiF .....  | 1               | 61   | Magnesium borate, Mg <sub>2</sub> B <sub>2</sub> O <sub>5</sub>                       |                 |      |
| Lithium gallium oxide, LiGaO <sub>2</sub> .....  | 10m             | 31   | (triclinic) .....   | 4m              | 25   |

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| Magnesium bromide, $MgBr_2$ .....  | 4m              | 62   | Magnesium sulfide, $MgS$ .....                                     | 7               | 31   |
| Magnesium bromide hydrate,<br>$MgBr_2 \cdot 6H_2O$ .....   | 11m             | 35   | Magnesium sulfite hydrate,<br>$MgSO_3 \cdot 6H_2O$ .....           | 9m              | 26   |
| Magnesium carbonate (magnesite),<br>$MgCO_3$ .....   | 7               | 28   | Magnesium tin, $Mg_2Sn$ .....                                      | 5               | 41   |
| Magnesium cerium nitrate hydrate,<br>$Mg_3Ce_2(NO_3)_{12} \cdot 24H_2O$ .....  | 10              | 20   | Magnesium tin oxide, $Mg_2SnO_4$ .....                             | 10m             | 37   |
| Magnesium chlorate hydrate,<br>$Mg(ClO_4)_2 \cdot 6H_2O$ .....   | 7m              | 30   | Magnesium titanium oxide<br>(geikielite), $MgTiO_3$ .....          | 5               | 43   |
| Magnesium chloride, $MgCl_2$ .....   | 11m             | 94   | Magnesium titanium oxide, $Mg_2TiO_4$ .....                        | 12m             | 25   |
| Magnesium chloride hydrate,<br>$MgCl_2 \cdot 12H_2O$ .....   | 7m              | 135  | Magnesium tungsten oxide, $MgWO_4$ ...                             | 13m             | 27   |
| Magnesium chloride hydrate<br>(bischofite), $MgCl_2 \cdot 6H_2O$ .....   | 11m             | 37   | Manganese, $\alpha$ -Mn (calculated pattern)                       | 7m              | 142  |
| Magnesium chromium oxide<br>(magnesiochromite), $MgCr_2O_4$ .....  | 9               | 34   | Manganese, $\alpha$ -Mn .....                                      | 17m             | 50   |
| Magnesium chromium oxide hydrate,<br>$MgCrO_4 \cdot 5H_2O$ .....   | 15m             | 39   | Manganese, $\beta$ -Mn .....                                       | 18m             | 43   |
| Magnesium fluoride (sellaita), $MgF_2$   | 4               | 33   | Manganese aluminum oxide (galaxite),<br>$MnAl_2O_4$ .....          | 9               | 35   |
| Magnesium fluoride silicate<br>(humite), $Mg_7F_2Si_3O_{12}$ .....   | 1m              | 30   | Manganese bromide, $MnBr_2$ .....                                  | 4m              | 63   |
| Magnesium fluoride silicate<br>(norbergite), $Mg_3F_2SiO_4$ .....  | 10              | 39   | Manganese(II) carbonate<br>(rhodochrosite), $MnCO_3$ .....         | 7               | 32   |
| Magnesium gallium oxide, $MgGa_2O_4$ ..  | 10              | 36   | Manganese chloride (scacchite),<br>$MnCl_2$ .....                  | 8m              | 43   |
| Magnesium germanium oxide,<br>$Mg_2GeO_4$ (cubic) .....  | 10              | 37   | Manganese chloride hydrate,<br>$MnCl_2 \cdot 2H_2O$ .....          | 11m             | 38   |
| Magnesium germanium oxide,<br>$Mg_2GeO_4$ (orthorhombic) .....   | 10              | 38   | Manganese chloride, $MnCl_2 \cdot 4H_2O$ .....                     | 9m              | 28   |
| Magnesium hydrogen phosphate<br>hydrate, newberyite, $MgHPO_4 \cdot 3H_2O$   | 7m              | 139  | Manganese cobalt oxide, $MnCo_2O_4$ ...                            | 9m              | 30   |
| Magnesium hydroxide (brucite),<br>$Mg(OH)_2$ .....   | 6               | 30   | Manganese fluoride, $MnF_2$ .....                                  | 10m             | 105  |
| Magnesium iodate hydrate,<br>$Mg(IO_3)_2 \cdot 4H_2O$ .....  | 17m             | 48   | Manganese iodide, $MnI_2$ .....                                    | 4m              | 63   |
| Magnesium iron hydroxide carbonate<br>hydrate, pyroaurite,<br>$Mg_6Fe_2(OH)_{16}CO_3 \cdot 4H_2O$ (rhomb.) ..                      | 10m             | 104  | Manganese iron oxide (jacobsite),<br>$MnFe_2O_4$ .....             | 9               | 36   |
| Magnesium iron hydroxide carbonate<br>hydrate, sjögrenite,<br>$Mg_6Fe_2(OH)_{16}CO_3 \cdot 4H_2O$ , (hexag.) ...                   | 10m             | 103  | Manganese(II) oxide (manganosite),<br>$MnO$ .....                  | 5               | 45   |
| Magnesium lanthanum nitrate<br>hydrate, $Mg_3La_2(NO_3)_{12} \cdot 24H_2O$ .....   | 1m              | 22   | Manganese oxide (pyrolusite), $\beta$ - $MnO_2$ .....              | 10m             | 39   |
| Magnesium manganese oxide, $MgMn_2O_4$   | 10m             | 35   | Manganese oxide (bixbyite), $\alpha$ - $Mn_2O_3$ .....             | 11m             | 95   |
| Magnesium manganese zinc iron sulfate<br>hydroxide hydrate, zincobotryogen,<br>( $Zn, Mg, Mn$ ) $Fe(SO_4)_2(OH) \cdot 7H_2O$ ..... | 20m             | 67   | Manganese oxide (hausmannite),<br>$Mn_3O_4$ .....                  | 10m             | 38   |
| Magnesium mercury, $MgHg$ .....  | 6m              | 84   | Manganese oxide hydroxide, groutite,<br>$\alpha$ - $MnOOH$ .....   | 11m             | 97   |
| Magnesium molybdenum oxide, $MgMoO_4$  | 7m              | 28   | Manganese phosphate, $Mn(Po_3)_2$ .....                            | 14m             | 21   |
| Magnesium nickel oxide, $MgNiO_2$ .....  | 10m             | 36   | Manganese phosphate, $Mn_2P_2O_7$ .....                            | 15m             | 41   |
| Magnesium oxide (periclase), $MgO$ ..  | 1               | 37   | Manganese phosphate, $Mn_3(Po_4)_2$ .....                          | 16m             | 47   |
| Magnesium phosphate, $Mg(Po_3)_2$ .....  | 13m             | 26   | Manganese selenide, $MnSe$ .....                                   | 10              | 41   |
| Magnesium phosphate, $\alpha$ - $Mg_2P_2O_7$ ....  | 18m             | 41   | Manganese sulfate hydrate<br>(szemkite), $MnSO_4 \cdot H_2O$ ..... | 16m             | 49   |
| Magnesium phosphate (farringtonite),<br>$Mg_3(Po_4)_2$ .....   | 19m             | 55   | Manganese sulfide (alabandite),<br>$\alpha$ - $MnS$ .....          | 4               | 11   |
| Magnesium selenide, $MgSe$ .....   | 5m              | 70   | Manganese titanium oxide<br>(pyrophanite), $MnTiO_3$ .....         | 15m             | 42   |
| Magnesium selenite hydrate,<br>$MgSeO_3 \cdot 6H_2O$ .....   | 8m              | 116  | Manganese(II) tungsten oxide<br>(huebnerite), $MnWO_4$ .....       | 2m              | 24   |
| Magnesium silicate (clinoenstatite),<br>$MgSiO_3$ .....  | 20m             | 69   | Manganese vanadium oxide, $Mn_2V_2O_7$ .....                       | 9m              | 75   |
| Magnesium silicate, enstatite,<br>$MgSiO_3$ .....  | 6               | 32   | Mercury amide chloride, $HgNH_2Cl$ .....                           | 10m             | 40   |
| Magnesium silicate (forsterite),<br>$Mg_2SiO_4$ .....  | 20m             | 71   | Mercury ammine chloride,<br>$Hg(NH_3)_2Cl_2$ .....                 | 11m             | 39   |
| Magnesium sulfate hydrate<br>(kieserite), $MgSO_4 \cdot H_2O$ .....  | 16m             | 46   | Mercury bromate, $Hg(BrO_3)_2$ .....                               | 10m             | 107  |
| Magnesium sulfate hydrate<br>(epsomite), $MgSO_4 \cdot 7H_2O$ .....  | 7               | 30   | Mercury bromide, $HgBr_2$ .....                                    | 10m             | 110  |
|  |                 |      | Mercury bromide, $Hg_2Br_2$ .....                                  | 7               | 33   |
|  |                 |      | Mercury chloride, $HgCl_2$ .....                                   | 13m             | 29   |
|  |                 |      | Mercury chloride (calomel),<br>$Hg_2Cl_2$ .....                    | 13m             | 30   |
|  |                 |      | Mercury chloride sulfide,<br>$\alpha$ - $Hg_3Cl_2S_2$ .....        | 8m              | 118  |
|  |                 |      | Mercury(II) cyanide, $Hg(CN)_2$ .....                              | 6               | 35   |
|  |                 |      | Mercury(II) fluoride, $HgF_2$ .....                                | 2m              | 25   |
|  |                 |      | Mercury hydroxide nitrate,<br>$Hg(OH)NO_3$ .....                   | 17m             | 52   |
|  |                 |      | Mercury(I) iodide, $HgI$ .....                                     | 4               | 49   |
|  |                 |      | Mercury(II) iodide, $HgI_2$ (tetragonal)                           | 7m              | 32   |
|  |                 |      | Mercury(II) oxide (montroydite),<br>$HgO$ .....                    | 9               | 39   |

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| Mercury(II) selenide (tiemannite), HgSe .....  | 7               | 35   | Nickel sulfide, millerite, NiS ....   | 1m              | 37   |
| Mercury sulfate, HgSO <sub>4</sub> .....   | 16m             | 50   | Nickel titanium oxide, NiTiO <sub>3</sub> ....  | 18m             | 54   |
| Mercury sulfate, Hg <sub>2</sub> SO <sub>4</sub> .....   | 16m             | 52   | Nickel tungsten oxide, NiWO <sub>4</sub> ....   | 2m              | 27   |
| Mercury(II) sulfide (cinnabar), HgS (hexagonal) .....  | 4               | 17   | Nickel yttrium, Ni <sub>3</sub> Y ....  | 10m             | 123  |
| Mercury(II) sulfide (metacinnabar), HgS (cubic) .....  | 4               | 21   | Niobium, Nb (monoclinic) ....   | 19m             | 67   |
| Molybdenum, Mo .....   | 1               | 20   | Niobium boride, $\zeta$ -NbB ....   | 17m             | 54   |
| Molybdenum arsenide, Mo <sub>2</sub> As <sub>3</sub> .....   | 10m             | 115  | Niobium chloride oxide, NbCl <sub>3</sub> O ....  | 7m              | 148  |
| Molybdenum osmium, Mo <sub>3</sub> Os .....  | 6m              | 28   | Niobium osmium, Nb <sub>3</sub> Os ....   | 6m              | 30   |
| Molybdenum oxide, MoO <sub>2</sub> .....   | 18m             | 44   | Niobium platinum, Nb <sub>3</sub> Pt ....   | 6m              | 31   |
| Molybdenum oxide (molybdite), MoO <sub>3</sub> .....   | 20m             | 118  | Niobium silicide, NbSi <sub>2</sub> ....  | 8               | 39   |
| Molybdenum oxide (molybdite), MoO <sub>3</sub> .....   | 3               | 30   | Niobium silicide, $\alpha$ -Nb <sub>5</sub> Si <sub>3</sub> ....  | 15m             | 43   |
| Molybdenum silicide, Mo <sub>5</sub> Si <sub>3</sub> .....   | 19m             | 59   | Niobium silicide, $\beta$ -Nb <sub>5</sub> Si <sub>3</sub> ....   | 15m             | 44   |
| Molybdenum sulfide (molybdenite), MoS <sub>2</sub> .....   | 5               | 47   | Osmium, Os ....   | 4               | 8    |
| Neodymium arsenate, NdAsO <sub>4</sub> .....   | 4m              | 28   | Osmium titanium, OsTi ....  | 6m              | 85   |
| Neodymium arsenide, NdAs .....   | 4m              | 64   | Palladium, Pd ....  | 1               | 21   |
| Neodymium borate, NdBO <sub>3</sub> .....  | 1m              | 32   | Palladium hydride, PdH <sub>0.706</sub> ....  | 5m              | 72   |
| Neodymium chloride, NdCl <sub>3</sub> .....  | 1m              | 33   | Palladium oxide, PdO ....   | 4               | 27   |
| Neodymium chloride oxide, NdOCl ...  | 8               | 37   | Palladium selenium (palladseite), Pd <sub>17</sub> Se <sub>15</sub> ....  | 16m             | 139  |
| Neodymium fluoride, NdF <sub>3</sub> .....   | 8               | 36   | Palladium vanadium, PdV <sub>3</sub> ....   | 6m              | 32   |
| Neodymium oxide, Nd <sub>2</sub> O <sub>3</sub> .....  | 4               | 26   | Phosphorus bromide, PBr <sub>7</sub> ....   | 7m              | 150  |
| Neodymium phosphate, NdPO <sub>4</sub> .....   | 11m             | 40   | Phosphorus oxide (stable form I), P <sub>2</sub> O <sub>5</sub> (orthorhombic) ....   | 9m              | 86   |
| Neodymium selenide, NdSe .....   | 5m              | 71   | Phosphorus oxide (stable form II), P <sub>2</sub> O <sub>5</sub> (orthorhombic) ....  | 9m              | 88   |
| Neodymium silver, NdAg .....   | 5m              | 71   | Phosphorus oxide (metastable form), P <sub>4</sub> O <sub>10</sub> (rhombohedral) ....  | 9m              | 91   |
| Neodymium tantalum oxide, Nd <sub>2</sub> TaO <sub>4</sub> ..  | 18m             | 46   | Platinum, Pt ....   | 1               | 31   |
| Neodymium titanium oxide, Nd <sub>2</sub> TiO <sub>5</sub> ..  | 18m             | 48   | Platinum titanium, PtTi <sub>3</sub> ....   | 6m              | 33   |
| Neodymium titanium oxide, Nd <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub> ..                                      | 18m             | 50   | Platinum vanadium, PtV <sub>3</sub> ....  | 6m              | 34   |
| Neodymium titanium oxide, Nd <sub>4</sub> Ti <sub>9</sub> O <sub>24</sub> ..                                     | 18m             | 52   | Plutonium arsenide, PuAs ....   | 4m              | 65   |
| Neodymium vanadium oxide, NdVO <sub>4</sub> ...  | 4m              | 30   | Plutonium phosphide, PuP ....   | 4m              | 65   |
| Neptunium nitride, NpN .....   | 4m              | 64   | Plutonium telluride, PuTe ....  | 4m              | 66   |
| Nickel, Ni .....   | 1               | 13   | Potassium aluminum sulfate, KAl(SO <sub>4</sub> ) <sub>2</sub> ....   | 9m              | 31   |
| Nickel aluminum oxide, NiAl <sub>2</sub> O <sub>4</sub> ....   | 9               | 42   | Potassium aluminum sulfate hydrate (potash alum), KAl(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O ...                        | 6               | 36   |
| Nickel arsenate hydrate (annabergite), Ni <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O ..... | 19m             | 60   | Potassium arsenic fluoride, KAsF <sub>6</sub> ....  | 17m             | 57   |
| Nickel arsenide (rammelsbergite), NiAs <sub>2</sub> .....  | 10              | 42   | Potassium barium chromium oxide, K <sub>2</sub> Ba(CrO <sub>4</sub> ) <sub>2</sub> ....   | 14m             | 23   |
| Nickel arsenic sulfide (gersdorffite), NiAs <sub>2</sub> S .....   | 1m              | 35   | Potassium barium iron titanium oxide, K <sub>1.16</sub> Ba <sub>0.72</sub> Fe <sub>0.36</sub> Ti <sub>5.58</sub> O <sub>13</sub> .. | 16m             | 147  |
| Nickel bromide, NiBr <sub>2</sub> .....  | 10m             | 119  | Potassium barium molybdenum oxide, K <sub>2</sub> Ba(MoO <sub>4</sub> ) <sub>2</sub> ....   | 14m             | 24   |
| Nickel(II) carbonate, NiCO <sub>3</sub> (trigonal) .....   | 1m              | 36   | Potassium barium nickel nitrite, K <sub>2</sub> BaNi(NO <sub>2</sub> ) <sub>6</sub> ....  | 9m              | 32   |
| Nickel chloride, NiCl <sub>2</sub> .....   | 9m              | 81   | Potassium barium niobium oxide, KBa <sub>2</sub> (NbO <sub>3</sub> ) <sub>5</sub> ....  | 20m             | 73   |
| Nickel chloride hydrate, NiCl <sub>2</sub> ·6H <sub>2</sub> O .....  | 11m             | 42   | Potassium barium phosphate, KBaPO <sub>4</sub> ....   | 19m             | 68   |
| Nickel fluoride, NiF <sub>2</sub> .....  | 10m             | 121  | Potassium borate hydroxide hydrate, K <sub>2</sub> B <sub>4</sub> O <sub>5</sub> (OH) <sub>4</sub> ·2H <sub>2</sub> O ....          | 15m             | 46   |
| Nickel fluoride hydrate, NiF <sub>2</sub> ·4H <sub>2</sub> O .....   | 11m             | 43   | Potassium calcium phosphate, KCaPO <sub>4</sub> ....  | 19m             | 70   |
| Nickel gallium oxide, NiGa <sub>2</sub> O <sub>4</sub> .....   | 10              | 45   | Potassium boron hydride, KBH <sub>4</sub> ....  | 9               | 44   |
| Nickel germanium oxide, Ni <sub>2</sub> GeO <sub>4</sub> ...   | 9               | 43   | Potassium bromate, KBrO <sub>3</sub> ....   | 7               | 38   |
| Nickel iron oxide (trevorite), NiFe <sub>2</sub> O <sub>4</sub> .....  | 10              | 44   | Potassium bromide, KBr ....   | 1               | 66   |
| Nickel molybdenum oxide, NiMoO <sub>4</sub> .....  | 19m             | 62   | Potassium bromide chloride, KBr <sub>0.5</sub> Cl <sub>0.5</sub> ....   | 8m              | 46   |
| Nickel nitrate hydrate, Ni(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....                               | 12m             | 26   | Potassium bromide iodide, KBr <sub>.33</sub> I <sub>.67</sub> ....  | 11m             | 44   |
| Nickel(II) oxide (bunsenite), NiO .....  | 1               | 47   | Potassium bromide iodide, KBr <sub>.67</sub> I <sub>.33</sub> ....  | 11m             | 45   |
| Nickel phosphate, Ni(PO <sub>3</sub> ) <sub>2</sub> .....  | 14m             | 22   | Potassium cadmium chloride, KCdCl <sub>3</sub> ....   | 5m              | 38   |
| Nickel phosphate hydrate, Ni <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O .....               | 19m             | 64   | Potassium cadmium fluoride, KCdF <sub>3</sub> ....  | 8m              | 47   |
| Nickel phosphide, Ni <sub>12</sub> P <sub>5</sub> .....  | 9m              | 83   | Potassium cadmium sulfate, K <sub>2</sub> Cd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> ....                                      | 7m              | 34   |
| Nickel silicon fluoride hydrate, NiSiF <sub>6</sub> ·6H <sub>2</sub> O .....                                     | 8               | 38   | Potassium calcium carbonate (fairchildite), K <sub>2</sub> Ca(CO <sub>3</sub> ) <sub>2</sub> ....                                   | 8m              | 48   |
| Nickel sulfate, NiSO <sub>4</sub> .....  | 2m              | 26   |   |                 |      |
| Nickel sulfate hydrate (retgersite), NiSO <sub>4</sub> ·6H <sub>2</sub> O (tetragonal) .....                     | 7               | 36   |   |                 |      |
| Nickel sulfate hydrate (nickel-hexahydrite), $\beta$ -NiSO <sub>4</sub> ·6H <sub>2</sub> O (monoclinic) .....    | 19m             | 65   |   |                 |      |

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| Potassium calcium chloride, $KCaCl_3$  | 7m              | 36   | Potassium lead selenate,<br>$K_2Pb(SeO_4)_2$ .....                                     | 15m             | 52   |
| Potassium calcium fluoride, $KCaF_3$   | 8m              | 49   | Potassium lead sulfate (palmierite),<br>$K_2Pb(SO_4)_2$ .....                          | 14m             | 30   |
| Potassium calcium magnesium sulfate,<br>$K_2CaMg(SO_4)_3$ .....                    | 7m              | 37   | Potassium magnesium chloride<br>hydrate (carnallite), $KMgCl_3 \cdot 6H_2O$            | 8m              | 50   |
| Potassium calcium nickel nitrite,<br>$K_2CaNi(NO_2)_6$ .....                       | 9m              | 33   | Potassium magnesium chromium oxide,<br>$K_2Mg_2(CrO_4)_3$ .....                        | 8m              | 52   |
| Potassium calcium sulfate,<br>$K_2Ca_2(SO_4)_3$ .....                              | 7m              | 39   | Potassium magnesium fluoride, $KMgF_3$   | 6m              | 42   |
| Potassium calcium sulfate hydrate<br>(syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$ ..... | 14m             | 25   | Potassium magnesium fluoride, $K_2MgF_4$   | 10m             | 42   |
| Potassium cerium fluoride, $\beta-KCeF_4$  | 12m             | 59   | Potassium magnesium selenate<br>hydrate, $K_2Mg(SeO_4)_2 \cdot 6H_2O$ .....            | 10m             | 43   |
| Potassium chlorate, $KClO_3$ .....   | 3m              | 42   | Potassium magnesium sulfate<br>(langbeinite), $K_2Mg_2(SO_4)_3$ .....                  | 6m              | 40   |
| Potassium chlorate, $KClO_4$ .....   | 6               | 43   | Potassium magnesium sulfate hydrate<br>(picromerite), $K_2Mg(SO_4)_2 \cdot 6H_2O$      | 8m              | 54   |
| Potassium chloride (sylvite), $KCl$  | 1               | 65   | Potassium manganese(II) fluoride,<br>$KMnF_3$ .....                                    | 6m              | 45   |
| Potassium chromium oxide, $K_3CrO_8$ ..  | 3m              | 44   | Potassium manganese oxide, $KMnO_4$  | 7               | 42   |
| Potassium chromium oxide (lopezite),<br>$K_2Cr_2O_7$ .....                         | 15m             | 47   | Potassium manganese(II) sulfate<br>(manganolangbeinite), $K_2Mn_2(SO_4)_3$             | 6m              | 43   |
| Potassium chromium oxide sulfate,<br>$K_2(CrO_4)_{.33}(SO_4)_{.67}$ .....          | 12m             | 28   | Potassium molybdenum oxide, $K_2MoO_4$   | 15m             | 53   |
| Potassium chromium oxide sulfate,<br>$K_2(CrO_4)_{.67}(SO_4)_{.33}$ .....          | 12m             | 27   | Potassium molybdenum oxide phos-<br>phate hydrate, $K_3(MoO_3)_{12}P_2O_7 \cdot 4H_2O$ | 8               | 43   |
| Potassium chromium sulfate,<br>$KCr(SO_4)_2$ .....                                 | 16m             | 58   | Potassium nickel fluoride, $KNiF_3$  | 7m              | 42   |
| Potassium chromium sulfate hydrate,<br>$KCr(SO_4)_2 \cdot 12H_2O$ .....            | 6               | 39   | Potassium nickel fluoride, $K_2NiF_4$  | 10m             | 45   |
| Potassium cobalt(II) fluoride,<br>$KCoF_3$ .....                                   | 6m              | 37   | Potassium nickel(II) sulfate,<br>$K_2Ni_2(SO_4)_3$ .....                               | 6m              | 46   |
| Potassium cobalt fluoride, $K_2CoF_4$  | 11m             | 46   | Potassium niobium fluoride, $K_2NbF_7$   | 8m              | 120  |
| Potassium cobalt nitrite,<br>$K_3Co(NO_2)_6$ .....                                 | 9               | 45   | Potassium niobium oxide, $KNbO_3$ .....  | 17m             | 62   |
| Potassium cobalt(II) sulfate,<br>$K_2Co_2(SO_4)_3$ .....                           | 6m              | 35   | Potassium nitrate (niter), $KNO_3$ .....   | 3               | 58   |
| Potassium copper chloride, $KCuCl_3$   | 7m              | 41   | Potassium nitrite, $KNO_2$ .....   | 9m              | 38   |
| Potassium copper chloride hydrate<br>(mitscherlichite), $K_2CuCl_4 \cdot 2H_2O$ .. | 9m              | 34   | Potassium nitrosyl ruthenium<br>chloride, $K_2NORuCl_5$ .....                          | 16m             | 61   |
| Potassium copper(II) fluoride,<br>$KCuF_3$ .....                                   | 6m              | 38   | Potassium oxide, $K_2O$ .....  | 10m             | 125  |
| Potassium cyanate, $KCNO$ .....  | 7               | 39   | Potassium platinum bromide, $K_2PtBr_6$  | 8               | 40   |
| Potassium cyanide, $KCN$ .....   | 1               | 77   | Potassium platinum chloride,<br>$K_2PtCl_6$ .....                                      | 13m             | 34   |
| Potassium fluoride, $KF$ .....   | 1               | 64   | Potassium platinum fluoride, $K_2PtF_6$  | 6               | 42   |
| Potassium fluoride hydrate, $KF \cdot 2H_2O$                                       | 18m             | 55   | Potassium rhenium chloride, $K_2ReCl_6$  | 2m              | 28   |
| Potassium germanium fluoride,<br>$K_2GeF_6$ .....                                  | 6               | 41   | Potassium rhenium oxide, $KReO_4$ .....  | 8               | 41   |
| Potassium hydrogen arsenate,<br>$KH_2AsO_4$ .....                                  | 1m              | 38   | Potassium rubidium chloride,<br>$K_{0.5}Rb_{0.5}Cl$ .....                              | 8m              | 76   |
| Potassium hydrogen iodate,<br>$KH(IO_3)_2$ .....                                   | 17m             | 58   | Potassium rubidium chromium oxide,<br>$KRbCrO_4$ .....                                 | 12m             | 29   |
| Potassium hydrogen phosphate,<br>$KH_2PO_4$ .....                                  | 3               | 69   | Potassium ruthenium chloride,<br>$K_2RuCl_6$ .....                                     | 10              | 46   |
| Potassium hydroxide, KOH at 300 °C   | 4m              | 66   | Potassium ruthenium oxide chloride<br>hydrate, $K_4Ru_2OCl_{10} \cdot H_2O$ .....      | 10              | 47   |
| Potassium iodate, $KIO_3$ .....  | 15m             | 48   | Potassium selenate, $K_2SeO_4$ .....   | 9m              | 41   |
| Potassium iodate, $KIO_4$ .....  | 7               | 41   | Potassium selenide, $K_2Se$ .....  | 10m             | 126  |
| Potassium iodide, $KI$ .....   | 1               | 68   | Potassium selenium bromide, $K_2SeBr_6$  | 8               | 41   |
| Potassium iron chloride hydrate<br>(erythrosiderite), $K_2FeCl_5 \cdot H_2O$ ..    | 14m             | 27   | Potassium silicon fluoride<br>(hieratite), $K_2SiF_6$ .....                            | 5               | 50   |
| Potassium iron cyanide, $K_3Fe(CN)_6$  | 9m              | 35   | Potassium silver cyanide, $KAg(CN)_2$  | 8m              | 78   |
| Potassium iron cyanide, $K_4Fe(CN)_6$  | 18m             | 56   | Potassium sodium aluminum fluoride<br>(elpasolite), $K_2NaAlF_6$ .....                 | 9m              | 43   |
| Potassium iron(II) fluoride, $KFeF_3$  | 6m              | 39   | Potassium sodium bromide,<br>$K_2Na_8Br$ .....   | 12m             | 62   |
| Potassium iron fluoride, $K_3FeF_6$ .....  | 9m              | 37   | Potassium sodium bromide,<br>$K_4Na_6Br$ .....   | 12m             | 62   |
| Potassium iron sulfate (yavapaiite),<br>$KFe(SO_4)_2$ .....                        | 16m             | 59   | Potassium sodium bromide,<br>$K_6Na_4Br$ .....   | 12m             | 62   |
| Potassium lead chloride, $KPb_2Cl_5$ ..  | 13m             | 33   | Potassium sodium bromide,<br>$K_8Na_2Br$ .....   | 12m             | 62   |
| Potassium lead chromium oxide,<br>$K_2Pb(CrO_4)_2$ .....                           | 14m             | 28   | Potassium sodium chloride,<br>$K_2Na_8Cl$ .....  | 12m             | 63   |
| Potassium lead molybdenum oxide,<br>$K_2Pb(MoO_4)_2$ .....                         | 14m             | 29   |  |                 |      |
| Potassium lead phosphate,<br>$K_2Pb(PO_3)_4$ .....                                 | 15m             | 50   |  |                 |      |

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| Potassium sodium chloride,<br>K <sub>4</sub> Na <sub>6</sub> Cl .....  | 12m             | 63   | Rubidium cadmium chloride, high<br>form, RbCdCl <sub>3</sub> (tetragonal) .....   | 5m              | 43   |
| Potassium sodium chloride,<br>K <sub>6</sub> Na <sub>4</sub> Cl .....  | 12m             | 63   | Rubidium cadmium chloride,<br>low form, RbCdCl <sub>3</sub> (orthorhombic)  | 5m              | 41   |
| Potassium sodium chloride,<br>K <sub>8</sub> Na <sub>2</sub> Cl .....  | 12m             | 63   | Rubidium cadmium sulfate,<br>Rb <sub>2</sub> Cd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....                        | 7m              | 45   |
| Potassium sodium sulfate,<br>K <sub>67</sub> Na <sub>1.33</sub> SO <sub>4</sub> .....  | 6m              | 48   | Rubidium calcium chloride, RbCaCl <sub>3</sub> .....  | 7m              | 47   |
| Potassium sodium sulfate, KNaSO <sub>4</sub> ..  | 6m              | 50   | Rubidium calcium fluoride, RbCaF <sub>3</sub> .....   | 8m              | 57   |
| Potassium sodium sulfate<br>(aphthitalite), K <sub>3</sub> Na(SO <sub>4</sub> ) <sub>2</sub> .....                                 | 6m              | 52   | Rubidium calcium sulfate,<br>Rb <sub>2</sub> Ca <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....                        | 7m              | 48   |
| Potassium strontium chromium oxide,<br>K <sub>2</sub> Sr(CrO <sub>4</sub> ) <sub>2</sub> .....                                     | 15m             | 57   | Rubidium chlorate, RbClO <sub>3</sub> .....   | 8               | 47   |
| Potassium strontium niobium oxide,<br>KSr <sub>2</sub> (NbO <sub>3</sub> ) <sub>5</sub> .....                                      | 20m             | 74   | Rubidium chlorate, RbClO <sub>4</sub> .....   | 2m              | 30   |
| Potassium strontium phosphate,<br>KSrPO <sub>4</sub> .....   | 19m             | 71   | Rubidium chloride, RbCl .....   | 4               | 41   |
| Potassium strontium selenate,<br>K <sub>2</sub> Sr(SeO <sub>4</sub> ) <sub>2</sub> .....   | 15m             | 58   | Rubidium chromium oxide, Rb <sub>2</sub> CrO <sub>4</sub> ..  | 3m              | 46   |
| Potassium strontium sulfate<br>(kalistrontite), K <sub>2</sub> Sr(SO <sub>4</sub> ) <sub>2</sub> .....                             | 14m             | 31   | Rubidium chromium oxide, Rb <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> .....   | 15m             | 60   |
| Potassium sulfate, K <sub>2</sub> S <sub>2</sub> O <sub>7</sub> .....  | 9m              | 99   | Rubidium chromium sulfate hydrate,<br>RbCr(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....                       | 6               | 47   |
| Potassium sulfate, K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> .....  | 17m             | 64   | Rubidium cobalt(II) chloride,<br>RbCoCl <sub>3</sub> .....  | 6m              | 57   |
| Potassium sulfate (arcanite), K <sub>2</sub> SO <sub>4</sub>   | 3               | 62   | Rubidium cobalt fluoride, RbCoF <sub>3</sub> .....  | 8m              | 58   |
| Potassium sulfide, K <sub>2</sub> S .....  | 10m             | 127  | Rubidium cobalt sulfate,<br>Rb <sub>2</sub> Co <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....                         | 8m              | 59   |
| Potassium telluride, K <sub>2</sub> Te .....   | 10m             | 128  | Rubidium copper chloride hydrate,<br>Rb <sub>2</sub> CuCl <sub>4</sub> ·2H <sub>2</sub> O .....                           | 10m             | 47   |
| Potassium thiocyanate, KCNS .....  | 8               | 44   | Rubidium copper sulfate hydrate,<br>Rb <sub>2</sub> Cu(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....            | 8m              | 61   |
| Potassium tin chloride, K <sub>2</sub> SnCl <sub>6</sub> .....   | 6               | 38   | Rubidium fluoride, RbF .....  | 8m              | 63   |
| Potassium titanium fluoride, K <sub>2</sub> TiF <sub>6</sub>   | 7               | 40   | Rubidium hydrogen phosphate,<br>RbH <sub>2</sub> PO <sub>4</sub> .....  | 20m             | 79   |
| Potassium titanium phosphate,<br>KTi <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> .....  | 20m             | 76   | Rubidium iodate, RbIO <sub>3</sub> .....  | 15m             | 62   |
| Potassium tungsten oxide, K <sub>2</sub> WO <sub>4</sub> .....   | 11m             | 47   | Rubidium iodate, RbIO <sub>4</sub> .....  | 2m              | 31   |
| Potassium vanadium oxide, KV <sub>2</sub> O <sub>3</sub> .....   | 18m             | 57   | Rubidium iodide, RbI .....  | 4               | 43   |
| Potassium vanadium oxide, KV <sub>3</sub> O <sub>8</sub> .....   | 8m              | 56   | Rubidium iron chloride hydrate,<br>Rb <sub>2</sub> FeCl <sub>5</sub> ·H <sub>2</sub> O .....                              | 14m             | 33   |
| Potassium zinc bromide hydrate,<br>KZnBr <sub>3</sub> ·2H <sub>2</sub> O .....   | 11m             | 104  | Rubidium iron sulfate hydrate,<br>Rb <sub>2</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....              | 8m              | 64   |
| Potassium zinc fluoride, KZnF <sub>3</sub> .....   | 5               | 51   | Rubidium lead chromium oxide,<br>Rb <sub>2</sub> Pb(CrO <sub>4</sub> ) <sub>2</sub> .....                                 | 14m             | 34   |
| Potassium zinc fluoride, K <sub>2</sub> ZnF <sub>4</sub> .....   | 10m             | 46   | Rubidium lead molybdenum oxide,<br>Rb <sub>2</sub> Pb(MoO <sub>4</sub> ) <sub>2</sub> .....                               | 15m             | 63   |
| Potassium zinc iodide hydrate,<br>KZnI <sub>3</sub> ·2H <sub>2</sub> O .....   | 11m             | 107  | Rubidium magnesium chromium oxide,<br>Rb <sub>2</sub> Mg <sub>2</sub> (CrO <sub>4</sub> ) <sub>3</sub> .....              | 8m              | 66   |
| Potassium zinc phosphate, KZnPO <sub>4</sub> .....   | 20m             | 77   | Rubidium magnesium chromium oxide<br>hydrate, Rb <sub>2</sub> Mg(CrO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O ..... | 8m              | 68   |
| Potassium zinc sulfate, K <sub>2</sub> Zn <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>   | 6m              | 54   | Rubidium magnesium sulfate,<br>Rb <sub>2</sub> Mg <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....                      | 7m              | 50   |
| Potassium zinc sulfate hydrate,<br>K <sub>2</sub> Zn(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....                       | 7m              | 43   | Rubidium magnesium sulfate<br>hydrate, Rb <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....         | 8m              | 70   |
| Potassium zinc vanadium oxide<br>hydrate, K <sub>2</sub> Zn <sub>2</sub> V <sub>10</sub> O <sub>28</sub> ·16H <sub>2</sub> O ..... | 3m              | 45   | Rubidium manganese(II) fluoride,<br>RbMnF <sub>3</sub> .....  | 5m              | 44   |
| Potassium zirconium fluoride,<br>K <sub>3</sub> ZrF <sub>7</sub> .....   | 9               | 46   | Rubidium manganese sulfate,<br>Rb <sub>2</sub> Mn <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....                      | 7m              | 52   |
| Praseodymium arsenate, PrAsO <sub>4</sub> .....  | 4m              | 32   | Rubidium nickel(II) chloride,<br>RbNiCl <sub>3</sub> .....  | 6m              | 58   |
| Praseodymium arsenide, PrAs .....  | 4m              | 67   | Rubidium nickel sulfate,<br>Rb <sub>2</sub> Ni <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....                         | 8m              | 72   |
| Praseodymium chloride, PrCl <sub>3</sub> .....   | 1m              | 39   | Rubidium nickel sulfate hydrate,<br>Rb <sub>2</sub> Ni(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....            | 8m              | 74   |
| Praseodymium chloride oxide, PrOCl .....   | 9               | 47   | Rubidium nitrate, RbNO <sub>3</sub> (trigonal)  | 5m              | 45   |
| Praseodymium fluoride, PrF <sub>3</sub> .....  | 5               | 52   | Rubidium phosphate, RbPO <sub>3</sub> .....   | 20m             | 80   |
| Praseodymium sulfide, PrS .....  | 4m              | 67   | Rubidium platinum chloride,<br>Rb <sub>2</sub> PtCl <sub>6</sub> .....  | 5               | 53   |
| Praseodymium vanadium oxide, PrVO <sub>4</sub>   | 5m              | 40   | Rubidium platinum fluoride, Rb <sub>2</sub> PtF <sub>6</sub> .....  | 6               | 48   |
| Praseodymium zinc, PrZn .....  | 5m              | 72   | Rubidium selenate, Rb <sub>2</sub> SeO <sub>4</sub> .....   | 9m              | 44   |
| Rhenium, Re .....  | 2               | 13   | Rubidium silicon fluoride, Rb <sub>2</sub> SiF <sub>6</sub> .....   | 6               | 49   |
| Rhodium, Rh .....  | 3               | 9    | Rubidium strontium chloride,<br>RbSrCl <sub>3</sub> .....   | 7m              | 54   |
| Rhodium vanadium, RhV <sub>3</sub> .....   | 6m              | 56   | Rubidium strontium chromium oxide,<br>Rb <sub>2</sub> Sr(CrO <sub>4</sub> ) <sub>2</sub> .....                            | 15m             | 64   |
| Rubidium aluminum sulfate<br>hydrate, RbAl(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....                                | 6               | 44   |   |                 |      |
| Rubidium amide, RbNH <sub>2</sub> .....  | 5m              | 73   |   |                 |      |
| Rubidium barium chromium oxide,<br>Rb <sub>2</sub> Ba(CrO <sub>4</sub> ) <sub>2</sub> .....  | 14m             | 32   |   |                 |      |
| Rubidium barium molybdenum oxide,<br>Rb <sub>2</sub> Ba(MoO <sub>4</sub> ) <sub>2</sub> .....                                      | 15m             | 59   |   |                 |      |
| Rubidium bromate, RbBrO <sub>3</sub> .....   | 8               | 45   |   |                 |      |
| Rubidium bromide, RbBr .....   | 7               | 43   |   |                 |      |

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| Rubidium strontium niobium oxide,<br>RbSr <sub>2</sub> (NbO <sub>3</sub> ) <sub>5</sub> .....                | 20m             | 81   | Silver nitrite, AgNO <sub>2</sub> .....  | 5               | 60   |
| Rubidium strontium sulfate,<br>Rb <sub>2</sub> Sr(SO <sub>4</sub> ) <sub>2</sub> .....                       | 15m             | 65   | Silver oxide, Ag <sub>2</sub> O .....  | 1m              | 45   |
| Rubidium sulfate, Rb <sub>2</sub> SO <sub>4</sub> .....  | 8               | 48   | Silver(II) oxide nitrate, Ag <sub>7</sub> O <sub>8</sub> NO <sub>3</sub> .....   | 4               | 61   |
| Rubidium tellurium bromide,<br>Rb <sub>2</sub> TeBr <sub>6</sub> .....                                       | 8               | 46   | Silver phosphate, Ag <sub>3</sub> PO <sub>4</sub> .....  | 5               | 62   |
| Rubidium tellurium chloride,<br>Rb <sub>2</sub> TeCl <sub>6</sub> .....                                      | 8               | 48   | Silver rhenium oxide, AgReO <sub>4</sub> .....   | 8               | 53   |
| Rubidium tin chloride, Rb <sub>2</sub> SnCl <sub>6</sub> .....   | 6               | 46   | Silver selenate, Ag <sub>2</sub> SeO <sub>4</sub> .....  | 2m              | 32   |
| Rubidium zinc fluoride, RbZnF <sub>3</sub> .....   | 7m              | 57   | Silver sodium chloride,<br>Ag <sub>0.5</sub> Na <sub>0.5</sub> Cl .....  | 8m              | 79   |
| Rubidium zinc sulfate hydrate,<br>Rb <sub>2</sub> Zn(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O ..... | 7m              | 55   | Silver sulfate, Ag <sub>2</sub> SO <sub>4</sub> .....  | 13m             | 37   |
| Ruthenium, Ru .....  | 4               | 5    | Silver sulfide (acanthite), Ag <sub>2</sub> S .....  | 10              | 51   |
| Ruthenium titanium, RuTi .....   | 6m              | 86   | Silver telluride (hessite),<br>Ag <sub>2</sub> Te .....  | 19m             | 73   |
| Samarium arsenate, SmAsO <sub>4</sub> .....  | 4m              | 33   | Silver terbium, AgTb .....   | 5m              | 74   |
| Samarium arsenide, SmAs .....  | 4m              | 68   | Silver thiocyanate, AgCNS .....  | 16m             | 62   |
| Samarium chloride, SmCl <sub>3</sub> .....   | 1m              | 40   | Silver thulium, AgTm .....   | 5m              | 74   |
| Samarium chloride oxide, SmOCl .....   | 1m              | 43   | Silver yttrium, AgY .....  | 5m              | 75   |
| Samarium fluoride, SmF <sub>3</sub> .....  | 1m              | 41   | Sodium, Na .....   | 9m              | 105  |
| Samarium oxide, Sm <sub>2</sub> O <sub>3</sub> (cubic) .....   | 4m              | 34   | Sodium aluminum chloride silicate,<br>sodalite, Na <sub>8</sub> Al <sub>6</sub> Cl <sub>2</sub> (SiO <sub>4</sub> ) <sub>6</sub> .....   | 7m              | 158  |
| Samarium silver, SmAg .....  | 5m              | 73   | Sodium aluminum fluoride (chiolite),<br>Na <sub>5</sub> Al <sub>3</sub> F <sub>14</sub> .....  | 16m             | 63   |
| Samarium tin oxide, Sm <sub>2</sub> Sn <sub>2</sub> O <sub>7</sub> .....                                     | 8m              | 77   | Sodium aluminum oxide, β-NaAlO <sub>2</sub> .....  | 18m             | 62   |
| Samarium vanadium oxide, SmVO <sub>4</sub> .....   | 5m              | 47   | Sodium aluminum sulfate hydrate<br>(soda alum), NaAl(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....  | 15m             | 68   |
| Scandium arsenate, ScAsO <sub>4</sub> .....  | 4m              | 35   | Sodium antimony fluoride, NaSbF <sub>4</sub> .....   | 20m             | 82   |
| Scandium arsenide, ScAs .....  | 4m              | 68   | Sodium azide, α-NaN <sub>3</sub> , at -90 to<br>-100 °C .....  | 8m              | 129  |
| Scandium boride, ScB <sub>2</sub> .....  | 17m             | 66   | Sodium azide, β-NaN <sub>3</sub> .....   | 8m              | 130  |
| Scandium oxide, Sc <sub>2</sub> O <sub>3</sub> .....   | 3               | 27   | Sodium barium niobium oxide,<br>NaBa <sub>2</sub> (NbO <sub>3</sub> ) <sub>5</sub> .....   | 20m             | 83   |
| Scandium phosphate, ScPO <sub>4</sub> .....  | 8               | 50   | Sodium barium phosphate, NaBaPO <sub>4</sub> .....   | 19m             | 75   |
| Scandium silicate (thortveitite),<br>Sc <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> .....                    | 7m              | 58   | Sodium beryllium calcium aluminum<br>fluoride oxide silicate, meliphanite,<br>(Na <sub>0.63</sub> Ca <sub>1.37</sub> )Be(Al <sub>0.13</sub> Si <sub>1.87</sub> )<br>(F <sub>0.75</sub> O <sub>6.25</sub> ) ..... | 8m              | 135  |
| Selenium, Se .....   | 5               | 54   | Sodium beryllium calcium fluoride<br>silicate, leucophanite,<br>NaBeCaFSi <sub>2</sub> O <sub>6</sub> .....  | 8m              | 138  |
| Selenium oxide (selenolite), SeO <sub>2</sub> .....  | 7m              | 60   | Sodium borate, NaBO <sub>2</sub> .....   | 18m             | 63   |
| Silicon, Si .....  | 13m             | 35   | Sodium borate, Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> .....   | 16m             | 64   |
| Silicon, Si (reference standard) ..  | 12m             | 2    | Sodium borate, Na <sub>2</sub> B <sub>8</sub> O <sub>13</sub> .....  | 7m              | 160  |
| Silicon nitride, β-Si <sub>3</sub> N <sub>4</sub> .....  | 18m             | 59   | Sodium borate hydroxide hydrate<br>(borax), Na <sub>2</sub> B <sub>4</sub> O <sub>5</sub> (OH) <sub>4</sub> ·8H <sub>2</sub> O .....   | 16m             | 66   |
| Silicon nitride, β-Si <sub>3</sub> N <sub>4</sub><br>(calculated pattern) .....                              | 14m             | 116  | Sodium boron hydride, NaBH <sub>4</sub> .....  | 9               | 51   |
| Silicon oxide (α or low<br>cristobalite), SiO <sub>2</sub> (tetragonal)                                      | 10              | 48   | Sodium bromate, NaBrO <sub>3</sub> .....   | 5               | 65   |
| Silicon oxide (α or low<br>cristobalite), SiO <sub>2</sub> (tetragonal)<br>(calculated pattern) .....        | 15m             | 180  | Sodium bromide, NaBr .....   | 3               | 47   |
| Silicon oxide (quartz, low), α-SiO <sub>2</sub>  | 18m             | 61   | Sodium bromide chloride,<br>NaBr <sub>.33</sub> Cl <sub>.67</sub> .....  | 11m             | 49   |
| Silicon oxide (β or high<br>cristobalite), SiO <sub>2</sub> (cubic) .....                                    | 1               | 42   | Sodium bromide chloride,<br>NaBr <sub>.67</sub> Cl <sub>.33</sub> .....  | 11m             | 50   |
| Silver, Ag .....   | 1               | 23   | Sodium calcium aluminum fluoride<br>hydrate, thomsenolite,<br>Na <sub>2</sub> CaAlF <sub>6</sub> ·H <sub>2</sub> O .....   | 8m              | 132  |
| Silver, Ag (reference standard) ...  | 8m              | 2    | Sodium calcium carbonate hydrate,<br>pirssonite, Na <sub>2</sub> Ca(CO <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O .....  | 9m              | 106  |
| Silver arsenate, Ag <sub>3</sub> AsO <sub>4</sub> .....  | 5               | 56   | Sodium calcium phosphate, β-NaCaPO <sub>4</sub> .....  | 15m             | 69   |
| Silver arsenic sulfide,<br>xanthoconite, Ag <sub>3</sub> AsS <sub>3</sub> .....                              | 8m              | 126  | Sodium calcium silicate, Na <sub>2</sub> CaSiO <sub>4</sub> .....  | 10m             | 48   |
| Silver bromate, AgBrO <sub>3</sub> .....   | 5               | 57   | Sodium calcium sulfate (glauberite),<br>Na <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub> .....  | 6m              | 59   |
| Silver bromide (bromargyrite), AgBr .....  | 4               | 46   | Sodium carbonate hydrate (thermo-<br>natrite), Na <sub>2</sub> CO <sub>3</sub> ·H <sub>2</sub> O .....   | 8               | 54   |
| Silver carbonate, Ag <sub>2</sub> CO <sub>3</sub> .....  | 13m             | 36   | Sodium carbonate sulfate, Na <sub>4</sub> CO <sub>3</sub> SO <sub>4</sub> .....  | 11m             | 51   |
| Silver chlorate, AgClO <sub>3</sub> .....  | 7               | 44   | Sodium carbonate sulfate (burkeite),<br>Na <sub>6</sub> CO <sub>3</sub> (SO <sub>4</sub> ) <sub>2</sub> .....  | 11m             | 52   |
| Silver chloride (chlorargyrite),<br>AgCl .....   | 4               | 44   | Sodium carbonate sulfate, Na <sub>6</sub> CO <sub>3</sub> (SO <sub>4</sub> ) <sub>2</sub> .....  | 11m             | 53   |
| Silver chromium oxide, Ag <sub>2</sub> CrO <sub>4</sub> .....  | 12m             | 30   | Sodium carbonate sulfate,<br>Na <sub>6</sub> CO <sub>3</sub> (SO <sub>4</sub> ) <sub>2</sub> .....   | 11m             | 54   |
| Silver cyanide, AgCN .....   | 9m              | 48   | Sodium carbonate sulfate,<br>Na <sub>6</sub> (CO <sub>3</sub> ) <sub>2</sub> SO <sub>4</sub> .....   | 11m             | 54   |
| Silver fluoride, Ag <sub>2</sub> F .....   | 5m              | 53   |  |                 |      |
| Silver iodate, AgIO <sub>4</sub> .....   | 9               | 49   |  |                 |      |
| Silver iodide (iodargyrite), AgI<br>(hexagonal) .....  | 8               | 51   |  |                 |      |
| Silver iodide, γ-AgI (cubic) .....   | 9               | 48   |  |                 |      |
| Silver manganese oxide, AgMnO <sub>4</sub> .....   | 7m              | 155  |  |                 |      |
| Silver mercury iodide, β-Ag <sub>2</sub> HgI <sub>4</sub> .....  | 17m             | 67   |  |                 |      |
| Silver molybdenum oxide, Ag <sub>2</sub> MoO <sub>4</sub> .....  | 7               | 45   |  |                 |      |
| Silver nitrate, AgNO <sub>3</sub> .....  | 5               | 59   |  |                 |      |

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| Sodium chlorate, $\text{NaClO}_3$ .....  | 3            | 51         | Sodium nickel(II) sulfate hydrate,<br>$\text{Na}_2\text{Ni}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ .....             | 6m           | 68         |
| Sodium chlorate, $\text{NaClO}_4$<br>(orthorhombic) .....  | 7            | 49         | Sodium niobium oxide (lueshite),<br>$\text{NaNbO}_3$ .....  | 18m          | 64         |
| Sodium chlorate hydrate,<br>$\text{NaClO}_4 \cdot \text{H}_2\text{O}$ .....  | 17m          | 68         | Sodium nitrate (soda niter), $\text{NaNO}_3$ .....  | 6            | 50         |
| Sodium chloride (halite), $\text{NaCl}$ .....  | 2            | 41         | Sodium nitrite, $\text{NaNO}_2$ .....   | 4            | 62         |
| Sodium chromium oxide, $\text{Na}_2\text{CrO}_4$ .....   | 9m           | 48         | Sodium nitrosyl iron cyanide<br>hydrate, $\text{Na}_2(\text{NO})\text{Fe}(\text{CN})_5 \cdot 2\text{H}_2\text{O}$ ..... | 18m          | 66         |
| Sodium chromium oxide hydrate,<br>$\text{Na}_2\text{CrO}_4 \cdot 4\text{H}_2\text{O}$ .....  | 9m           | 50         | Sodium oxide, $\text{Na}_2\text{O}$ .....   | 10m          | 134        |
| Sodium chromium oxide hydrate,<br>$\text{Na}_2\text{Cr}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$ .....   | 7m           | 62         | Sodium phosphate, $\text{Na}_3\text{P}_3\text{O}_9$ .....   | 3m           | 49         |
| Sodium chromium oxide sulfate,<br>$\text{Na}_4(\text{CrO}_4)(\text{SO}_4)$ .....   | 11m          | 55         | Sodium phosphate hydrate,<br>$\alpha\text{-Na}_4\text{P}_4\text{O}_{12} \cdot 4\text{H}_2\text{O}$ (monoclinic) .....   | 13m          | 39         |
| Sodium cobalt nitrite, $\text{Na}_3\text{Co}(\text{NO}_2)_6$ .....   | 15m          | 70         | Sodium phosphate hydrate,<br>$\beta\text{-Na}_4\text{P}_4\text{O}_{12} \cdot 4\text{H}_2\text{O}$ (triclinic) .....     | 2m           | 35         |
| Sodium cobalt(II) sulfate hydrate,<br>$\text{Na}_2\text{Co}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ .....  | 6m           | 61         | Sodium phosphate hydrate,<br>$\text{Na}_6\text{P}_6\text{O}_{18} \cdot 6\text{H}_2\text{O}$ .....                       | 5m           | 54         |
| Sodium cyanate, $\text{NaCNO}$ .....   | 2m           | 33         | Sodium praseodymium fluoride<br>silicate, $(\text{Na}_2\text{Pr}_8)\text{F}_2(\text{SiO}_4)_6$ .....                    | 7m           | 68         |
| Sodium cyanide, $\text{NaCN}$ (cubic) .....  | 1            | 78         | Sodium selenate, $\text{Na}_2\text{SeO}_4$ .....  | 9m           | 55         |
| Sodium cyanide, $\text{NaCN}$ (orthorhombic)<br>at 6 °C .....  | 1            | 79         | Sodium selenide, $\text{Na}_2\text{Se}$ .....   | 10m          | 135        |
| Sodium fluoride (villiaumite), $\text{NaF}$ .....  | 1            | 63         | Sodium silicate, $\alpha\text{(III)}$ , $\text{Na}_2\text{Si}_2\text{O}_5$ .....  | 8m           | 141        |
| Sodium germanium phosphate,<br>$\text{NaGe}_2(\text{PO}_4)_3$ .....  | 20m          | 84         | Sodium silicate, $\beta\text{-Na}_2\text{Si}_2\text{O}_5$ .....   | 10m          | 136        |
| Sodium hydrogen carbonate hydrate,<br>trona, $\text{Na}_3\text{H}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$ .....                                  | 15m          | 71         | Sodium silicon fluoride<br>(malladrite), $\text{Na}_2\text{SiF}_6$ .....  | 16m          | 68         |
| Sodium hydrogen fluoride, $\text{NaHF}_2$ .....  | 5            | 63         | Sodium strontium niobium oxide,<br>$\text{NaSr}_2(\text{NbO}_3)_5$ .....  | 20m          | 89         |
| Sodium hydrogen phosphate,<br>$\text{Na}_3\text{H}(\text{PO}_3)_4$ .....   | 10m          | 130        | Sodium strontium phosphate,<br>$\text{NaSrPO}_4$ .....  | 19m          | 77         |
| Sodium hydrogen silicate hydrate,<br>$\text{Na}_2\text{H}_2\text{SiO}_4 \cdot 4\text{H}_2\text{O}$ .....   | 7m           | 163        | Sodium sulfate, $\text{Na}_2\text{SO}_4$ .....  | 11m          | 57         |
| Sodium hydrogen sulfate hydrate,<br>$\text{NaHSO}_4 \cdot \text{H}_2\text{O}$ .....  | 9m           | 52         | Sodium sulfate (thenardite), $\text{Na}_2\text{SO}_4$ .....   | 2            | 59         |
| Sodium hydroxide, $\text{NaOH}$ at 300 °C ..   | 4m           | 69         | Sodium sulfate hydrate,<br>$\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ .....                            | 17m          | 74         |
| Sodium iodate, $\text{NaIO}_3$ .....   | 7            | 47         | Sodium sulfide, $\text{Na}_2\text{S}$ .....   | 10m          | 140        |
| Sodium iodate, $\text{NaIO}_4$ .....   | 7            | 48         | Sodium sulfite, $\text{Na}_2\text{SO}_3$ .....  | 3            | 60         |
| Sodium iodate hydrate, $\text{NaIO}_3 \cdot \text{H}_2\text{O}$ ..   | 17m          | 73         | Sodium telluride, $\text{Na}_2\text{Te}$ .....  | 10m          | 141        |
| Sodium iodide, $\text{NaI}$ .....  | 4            | 31         | Sodium tin fluoride, $\text{NaSn}_2\text{F}_5$ .....  | 7m           | 166        |
| Sodium iron fluoride, $\text{Na}_3\text{FeF}_6$ .....  | 9m           | 54         | Sodium titanium oxide, $\text{Na}_2\text{Ti}_3\text{O}_7$ .....   | 16m          | 69         |
| Sodium iron silicate (acmite),<br>$\text{NaFe}(\text{SiO}_3)_2$ .....  | 20m          | 86         | Sodium titanium phosphate,<br>$\text{NaTi}_2(\text{PO}_4)_3$ .....  | 19m          | 79         |
| Sodium lanthanum fluoride silicate,<br>$(\text{Na}_2\text{La}_8)\text{F}_2(\text{SiO}_4)_6$ .....  | 7m           | 64         | Sodium tungsten oxide, $\text{Na}_2\text{WO}_4$ .....   | 1m           | 47         |
| Sodium lanthanum molybdenum oxide,<br>$\text{NaLa}(\text{MoO}_4)_2$ .....  | 10m          | 49         | Sodium tungsten(VI) oxide hydrate,<br>$\text{Na}_2\text{WO}_4 \cdot 2\text{H}_2\text{O}$ .....                          | 2m           | 33         |
| Sodium magnesium aluminum boron<br>hydroxide silicate, dravite,<br>$\text{NaMg}_3\text{Al}_6\text{B}_3(\text{OH})_4\text{Si}_6\text{O}_{27}$ ..... | 3m           | 47         | Sodium vanadium oxide, $\alpha\text{-NaVO}_3$ .....   | 18m          | 67         |
| Sodium magnesium carbonate<br>(eitelite), $\text{Na}_2\text{Mg}(\text{CO}_3)_2$ .....  | 11m          | 56         | Sodium vanadium oxide, $\beta\text{-NaVO}_3$ .....  | 18m          | 68         |
| Sodium magnesium sulfate<br>(vanthoffite), $\text{Na}_6\text{Mg}(\text{SO}_4)_4$ .....   | 15m          | 72         | Sodium zinc fluoride, $\text{NaZnF}_3$ .....  | 6m           | 74         |
| Sodium magnesium sulfate hydrate,<br>bloedite, $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ .....                               | 6m           | 63         | Sodium zinc sulfate hydrate,<br>$\text{Na}_2\text{Zn}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ .....                   | 6m           | 72         |
| Sodium magnesium sulfate hydrate<br>(Loeweite), $\text{Na}_{12}\text{Mg}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$ ..                        | 14m          | 35         | Sodium zirconium fluoride,<br>$\text{Na}_7\text{Zr}_6\text{F}_{31}$ .....   | 8m           | 144        |
| Sodium manganese(II) fluoride,<br>$\text{NaMnF}_3$ .....   | 6m           | 65         | Sodium zirconium phosphate,<br>$\text{NaZr}_2(\text{PO}_4)_3$ .....   | 19m          | 81         |
| Sodium manganese sulfate hydrate,<br>$\text{Na}_{12}\text{Mn}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$ .....                                | 14m          | 37         | Strontium aluminum hydroxide,<br>$\text{Sr}_3\text{Al}_2(\text{OH})_{12}$ .....   | 10m          | 50         |
| Sodium mercury(II) chloride hydrate,<br>$\text{NaHgCl}_3 \cdot 2\text{H}_2\text{O}$ .....  | 6m           | 66         | Strontium aluminum oxide, $\text{SrAl}_2\text{O}_4$ ..  | 20m          | 91         |
| Sodium molybdenum oxide, $\text{Na}_2\text{MoO}_4$ ..  | 1m           | 46         | Strontium aluminum oxide, $\text{Sr}_3\text{Al}_2\text{O}_6$ ..   | 10m          | 52         |
| Sodium molybdenum oxide, $\text{Na}_2\text{Mo}_2\text{O}_7$ ..   | 9m           | 110        | Strontium arsenate, $\text{Sr}_3(\text{AsO}_4)_2$ ..  | 2m           | 36         |
| Sodium molybdenum oxide hydrate,<br>$\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$ .....  | 20m          | 87         | Strontium azide, $\text{Sr}(\text{N}_3)_2$ .....  | 8m           | 146        |
| Sodium neodymium fluoride silicate,<br>$(\text{Na}_2\text{Nd}_8)\text{F}_2(\text{SiO}_4)_6$ .....  | 7m           | 66         | Strontium borate, $\text{SrB}_2\text{O}_4$ .....  | 3m           | 53         |

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| Strontium chloride, $\text{SrCl}_2$ .....  | 4               | 40   | Terbium vanadium oxide, $\text{TbVO}_4$ .....  | 5m              | 56   |
| Strontium chloride fluoride, $\text{SrClF}$  | 10m             | 55   | Thallium, $\alpha\text{-Tl}$ .....   | 16m             | 73   |
| Strontium chloride hydrate,<br>$\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$ .....                           | 11m             | 58   | Thallium aluminum sulfate hydrate,<br>$\text{TlAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....          | 6               | 53   |
| Strontium chloride hydrate,<br>$\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ .....                           | 4               | 58   | Thallium(I) arsenate, $\text{Tl}_3\text{AsO}_4$ .....  | 2m              | 37   |
| Strontium chloride hydroxide<br>phosphate, $\text{Sr}_5\text{Cl}_{1.65}(\text{OH})_{.35}(\text{PO}_4)_3$ | 11m             | 60   | Thallium azide, $\text{TlN}_3$ .....   | 8m              | 82   |
| Strontium chromium oxide, $\text{SrCr}_2\text{O}_7$  | 17m             | 77   | Thallium(I) bromate, $\text{TlBrO}_3$ .....  | 8               | 60   |
| Strontium chromium oxide, $\text{Sr}_2\text{CrO}_4$  | 16m             | 71   | Thallium bromide, $\text{TlBr}$ .....  | 7               | 57   |
| Strontium chromium oxide hydrate,<br>$\text{SrCr}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$ .....           | 17m             | 79   | Thallium cadmium sulfate,<br>$\text{Tl}_2\text{Cd}_2(\text{SO}_4)_3$ .....                                   | 8m              | 83   |
| Strontium fluoride, $\text{SrF}_2$ .....   | 5               | 67   | Thallium(I) chlorate, $\text{TlClO}_4$ .....   | 2m              | 38   |
| Strontium hydroxide, $\text{Sr}(\text{OH})_2$ .....  | 13m             | 41   | Thallium(I) chlorate, $\text{TlClO}_3$ .....   | 8               | 61   |
| Strontium hydroxide hydrate,<br>$\text{Sr}(\text{OH})_2 \cdot \text{H}_2\text{O}$ .....                  | 13m             | 42   | Thallium(I) chloride, $\text{TlCl}$ .....  | 4               | 51   |
| Strontium hydroxide hydrate,<br>$\text{Sr}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ .....                 | 13m             | 43   | Thallium chromium oxide, $\text{Tl}_2\text{CrO}_4$ ..  | 3m              | 54   |
| Strontium indium hydroxide,<br>$\text{Sr}_3\text{In}_2(\text{OH})_{12}$ .....                            | 6m              | 76   | Thallium chromium sulfate hydrate,<br>$\text{TlCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....          | 6               | 55   |
| Strontium iodide hydrate,<br>$\text{SrI}_2 \cdot 6\text{H}_2\text{O}$ .....                              | 8               | 58   | Thallium cobalt sulfate,<br>$\text{Tl}_2\text{Co}_2(\text{SO}_4)_3$ .....                                    | 8m              | 85   |
| Strontium iron oxide, $\text{SrFe}_{12}\text{O}_{19}$ ...  | 18m             | 69   | Thallium cobalt sulfate hydrate,<br>$\text{Tl}_2\text{Co}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....    | 7m              | 70   |
| Strontium manganese oxide,<br>$\text{SrMnO}_3$ (cubic) .....   | 10m             | 56   | Thallium copper sulfate hydrate,<br>$\text{Tl}_2\text{Cu}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....    | 7m              | 72   |
| Strontium manganese oxide,<br>$\text{SrMnO}_3$ (hexagonal) .....   | 10m             | 58   | Thallium fluoride, $\text{TlF}$ .....  | 16m             | 74   |
| Strontium molybdenum oxide, $\text{SrMoO}_4$   | 7               | 50   | Thallium gallium sulfate hydrate,<br>$\text{TlGa}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ .....           | 6               | 57   |
| Strontium nitrate, $\text{Sr}(\text{NO}_3)_2$ .....  | 12m             | 31   | Thallium(I) iodate, $\text{TlIO}_3$ .....  | 8               | 62   |
| Strontium oxide, $\text{SrO}$ .....  | 5               | 68   | Thallium(I) iodide, $\text{TlI}$<br>(orthorhombic) .....   | 4               | 53   |
| Strontium oxide, $\text{SrO}_2$ .....  | 6               | 52   | Thallium iron sulfate hydrate,<br>$\text{Tl}_2\text{Fe}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....      | 8m              | 87   |
| Strontium oxide hydrate, $\text{SrO}_2 \cdot 8\text{H}_2\text{O}$  | 11m             | 61   | Thallium lead sulfate,<br>$\text{Tl}_2\text{Pb}(\text{SO}_4)_2$ .....  | 15m             | 74   |
| Strontium phosphate, $\alpha\text{-Sr}_2\text{P}_2\text{O}_7$ ....                                       | 11m             | 62   | Thallium magnesium chromium oxide,<br>$\text{Tl}_2\text{Mg}_2(\text{CrO}_4)_3$ .....                         | 8m              | 89   |
| Strontium phosphate, $\alpha\text{-Sr}_3(\text{PO}_4)_2$ ..  | 11m             | 64   | Thallium magnesium sulfate hydrate,<br>$\text{Tl}_2\text{Mg}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ ..... | 7m              | 74   |
| Strontium scandium oxide hydrate,<br>$\text{Sr}_3\text{Sc}_2\text{O}_6 \cdot 6\text{H}_2\text{O}$ .....  | 6m              | 78   | Thallium manganese sulfate,<br>$\text{Tl}_2\text{Mn}_2(\text{SO}_4)_3$ .....                                 | 7m              | 76   |
| Strontium silicate, $\alpha\text{-SrSiO}_3$ .....  | 20m             | 93   | Thallium nickel sulfate hydrate,<br>$\text{Tl}_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....    | 7m              | 78   |
| Strontium silicate, $\text{Sr}_3\text{SiO}_5$ .....  | 13m             | 44   | Thallium(I) nitrate, $\text{TlNO}_3$ .....   | 6               | 58   |
| Strontium sulfate (celestite), $\text{SrSO}_4$   | 2               | 61   | Thallium oxide (avicennite), $\text{Tl}_2\text{O}_3$ ..  | 16m             | 77   |
| Strontium sulfide, $\text{SrS}$ .....  | 7               | 52   | Thallium(III) oxide, $\text{Tl}_2\text{O}_3$ .....   | 2               | 28   |
| Strontium telluride, $\text{SrTe}$ .....   | 4m              | 69   | Thallium(I) phosphate, $\text{Tl}_3\text{PO}_4$ .....  | 7               | 58   |
| Strontium tin oxide, $\text{SrSnO}_3$ .....  | 8m              | 80   | Thallium(III) phosphate, $\text{TlPO}_4$ .....   | 7               | 59   |
| Strontium titanium oxide, $\text{SrTiO}_3$ ..  | 3               | 44   | Thallium platinum chloride,<br>$\text{Tl}_2\text{PtCl}_6$ .....  | 5               | 70   |
| Strontium tungsten oxide, $\text{SrW}_4$ ...   | 7               | 53   | Thallium silicon fluoride, $\text{Tl}_2\text{SiF}_6$   | 6               | 56   |
| Strontium tungsten oxide, $\text{Sr}_2\text{W}_5$ ..   | 12m             | 32   | Thallium strontium sulfate,<br>$\text{Tl}_2\text{Sr}(\text{SO}_4)_2$ .....                                   | 15m             | 75   |
| Strontium vanadium oxide, $\text{Sr}_3(\text{VO}_4)_2$   | 15m             | 73   | Thallium(I) sulfate, $\text{Tl}_2\text{SO}_4$ .....  | 6               | 59   |
| Strontium zirconium oxide, $\text{SrZrO}_3$ .  | 9               | 51   | Thallium(I) thiocyanate, $\text{TlCN}$ .....   | 8               | 63   |
| Strontium zirconium phosphate,<br>$\text{SrZr}_4(\text{PO}_4)_6$ .....                                   | 20m             | 94   | Thallium tin chloride, $\text{Tl}_2\text{SnCl}_6$ ...  | 6               | 54   |
| Sulfamic acid, $\text{H}_2\text{NSO}_3\text{H}$ .....  | 7               | 54   | Thallium(I) tungsten oxide, $\text{Tl}_2\text{WO}_4$   | 1m              | 48   |
| Sulfur, S (orthorhombic) .....   | 9               | 54   | Thallium zinc sulfate hydrate,<br>$\text{Tl}_2\text{Zn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ .....      | 7m              | 80   |
| Tantalum, Ta .....   | 1               | 29   | Thorium arsenide, $\text{ThAs}$ .....  | 4m              | 70   |
| Tantalum silicide, $\text{TaSi}_2$ .....   | 8               | 59   | Thorium carbide, $\text{ThC}$ .....  | 18m             | 71   |
| Tantalum tungsten oxide, $\text{Ta}_2\text{W}_8$ ...   | 20m             | 96   | Thorium molybdenum oxide,<br>$\alpha\text{-Th}(\text{MoO}_4)_2$ .....  | 20m             | 98   |
| Tellurium, Te .....  | 1               | 26   | Thorium molybdenum oxide,<br>$\beta\text{-Th}(\text{MoO}_4)_2$ .....   | 20m             | 100  |
| Tellurium(IV) oxide (paratellurite),<br>$\text{TeO}_2$ (tetragonal) .....                                | 7               | 56   | Thorium nitrate hydrate,<br>$\text{Th}(\text{NO}_3)_4 \cdot 5\text{H}_2\text{O}$ .....                       | 18m             | 72   |
| Tellurium(IV) oxide, paratellurite,<br>$\text{TeO}_2$ (tetragonal) .....                                 | 10              | 55   | Thorium oxide (thorianite), $\text{ThO}_2$ ..  | 1               | 57   |
| Tellurium(IV) oxide, tellurite,<br>$\text{TeO}_2$ (orthorhombic) .....                                   | 9               | 57   | Thorium silicate (huttonite),<br>$\beta\text{-ThSiO}_4$ .....  | 20m             | 102  |
| Terbium arsenate, $\text{TbAsO}_4$ .....   | 3m              | 54   | Thorium tantalum oxide, $\text{Th}_2\text{Ta}_2\text{O}_9$ ..  | 20m             | 104  |
| Terbium arsenide, $\text{TbAs}$ .....  | 5m              | 75   |  |                 |      |
| Terbium nitride, $\text{TbN}$ .....  | 4m              | 70   |  |                 |      |
| Terbium phosphide, $\text{TbP}$ .....  | 5m              | 76   |  |                 |      |
| Terbium selenide, $\text{TbSe}$ .....  | 5m              | 76   |  |                 |      |
| Terbium sulfide, $\text{TbS}$ .....  | 5m              | 77   |  |                 |      |
| Terbium telluride, $\text{TbTe}$ .....   | 5m              | 77   |  |                 |      |

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| Thorium tungsten oxide, $\alpha$ -Th(WO <sub>4</sub> ) <sub>2</sub>           | 20m          | 106        | Zinc antimony oxide, ZnSb <sub>2</sub> O <sub>4</sub> .....   | 4m           | 39         |
| Thulium arsenate, TmAsO <sub>4</sub> .....                                    | 3m           | 56         | Zinc Arsenate Hydrate (koettigite),<br>Zn <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O .....                        | 19m          | 85         |
| Thulium arsenide, TmAs .....  | 4m           | 71         | Zinc borate, Zn <sub>4</sub> B <sub>6</sub> O <sub>13</sub> .....   | 13m          | 48         |
| Thulium nitride, TmN .....  | 4m           | 71         | Zinc carbonate, smithsonite, ZnCO <sub>3</sub> .....  | 8            | 69         |
| Thulium oxide, Tm <sub>2</sub> O <sub>3</sub> .....                           | 9            | 58         | Zinc chlorate hydrate,<br>Zn(ClO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....   | 16m          | 79         |
| Thulium telluride, TmTe .....   | 4m           | 72         | Zinc chromium oxide, ZnCr <sub>2</sub> O <sub>4</sub> .....   | 9m           | 59         |
| Thulium vanadium oxide, TmVO <sub>4</sub> .....                               | 5m           | 57         | Zinc cobalt oxide, ZnCo <sub>2</sub> O <sub>4</sub> .....   | 10m          | 60         |
| Tin, $\alpha$ -Sn (cubic) .....   | 2            | 12         | Zinc cyanide, Zn(CN) <sub>2</sub> .....   | 5            | 73         |
| Tin, $\beta$ -Sn (tetragonal) .....   | 1            | 24         | Zinc fluoride, ZnF <sub>2</sub> .....   | 6            | 60         |
| Tin arsenide, SnAs .....  | 4m           | 37         | Zinc fluoride hydrate, ZnF <sub>2</sub> ·4H <sub>2</sub> O ..   | 11m          | 69         |
| Tin arsenide, Sn <sub>3.8</sub> As <sub>3</sub> .....                         | 15m          | 76         | Zinc germanium oxide, Zn <sub>2</sub> GeO <sub>4</sub> .....  | 10           | 56         |
| Tin chloride hydrate, SnCl <sub>2</sub> ·2H <sub>2</sub> O ..                 | 17m          | 84         | Zinc hydroxide silicate hydrate,<br>hemimorphite, Zn <sub>4</sub> (OH) <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> ·H <sub>2</sub> O .. | 2            | 62         |
| Tin(II) fluoride, SnF <sub>2</sub> .....                                      | 3m           | 51         | Zinc iodide, ZnI <sub>2</sub> .....   | 9            | 60         |
| Tin hydrogen phosphate, SnHPO <sub>4</sub> .....                              | 13m          | 46         | Zinc iron oxide (franklinite),<br>ZnFe <sub>2</sub> O <sub>4</sub> .....  | 9m           | 60         |
| Tin(IV) iodide, SnI <sub>4</sub> .....  | 5            | 71         | Zinc manganese oxide (hetaerolite),<br>ZnMn <sub>2</sub> O <sub>4</sub> .....   | 10m          | 61         |
| Tin(II) oxide (romarchite), SnO .....   | 4            | 28         | Zinc molybdenum oxide, Zn <sub>2</sub> Mo <sub>3</sub> O <sub>8</sub> ..  | 7m           | 173        |
| Tin(IV) oxide (cassiterite), SnO <sub>2</sub> .....                           | 1            | 54         | Zinc nitrate hydrate,<br>$\alpha$ -Zn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....   | 12m          | 36         |
| Tin sulfide (berndtite), $\beta$ -SnS <sub>2</sub> .....                      | 9m           | 57         | Zinc oxide (zincite), ZnO .....   | 2            | 25         |
| Tin(II) telluride, SnTe .....   | 7            | 61         | Zinc phosphate, $\alpha$ -Zn <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> .....   | 16m          | 80         |
| Titanium, Ti .....  | 3            | 4          | Zinc phosphate, $\beta$ -Zn <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> .....  | 16m          | 81         |
| Titanium carbide, TiC .....   | 18m          | 73         | Zinc phosphate, $\gamma$ -Zn <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> .....   | 16m          | 83         |
| Titanium(111) oxide, TiO <sub>1.515</sub> .....                               | 9            | 59         | Zinc phosphate hydrate (hopeite),<br>Zn <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> ·4H <sub>2</sub> O .....                           | 16m          | 85         |
| Titanium oxide (anatase), TiO <sub>2</sub> .....                              | 7m           | 82         | Zinc selenide, ZnSe .....   | 3            | 23         |
| Titanium oxide, brookite, TiO <sub>2</sub><br>(orthorhombic) .....            | 3m           | 57         | Zinc silicate (willemite), Zn <sub>2</sub> SiO <sub>4</sub> ..  | 7            | 62         |
| Titanium oxide (rutile), TiO <sub>2</sub> .....                               | 7m           | 83         | Zinc silicon fluoride hydrate,<br>ZnSiF <sub>6</sub> ·6H <sub>2</sub> O .....   | 8            | 70         |
| Titanium silicide, Ti <sub>5</sub> Si <sub>3</sub> .....                      | 8            | 64         | Zinc sulfate (zinkosite), ZnSO <sub>4</sub> ..  | 7            | 64         |
| Titanium sulfide, TiS <sub>2</sub> .....                                      | 4m           | 72         | Zinc sulfate hydrate (gunningite),<br>ZnSO <sub>4</sub> ·H <sub>2</sub> O .....   | 19m          | 86         |
| Titanium sulfide, Ti <sub>2</sub> S .....                                     | 8m           | 149        | Zinc sulfate hydrate (goslarite),<br>ZnSO <sub>4</sub> ·7H <sub>2</sub> O .....   | 8            | 71         |
| Tungsten, W .....   | 1            | 28         | Zinc sulfide (wurtzite), $\alpha$ -ZnS<br>(hexagonal) .....   | 2            | 14         |
| Tungsten, W (reference standard) ..   | 8m           | 2          | Zinc sulfide (sphaelerite), $\beta$ -ZnS<br>(cubic) .....   | 2            | 16         |
| Tungsten oxide, WO <sub>2</sub> .....   | 18m          | 74         | Zinc telluride, ZnTe .....  | 3m           | 58         |
| Tungsten sulfide (tungstenite), WS <sub>2</sub> .....                         | 8            | 65         | Zinc tin oxide, Zn <sub>2</sub> SnO <sub>4</sub> .....  | 10m          | 62         |
| Uranium nitride, UN .....   | 18m          | 75         | Zinc titanium oxide, ZnTiO <sub>3</sub> .....   | 13m          | 49         |
| Uranium oxide, UO .....   | 5m           | 78         | Zinc titanium oxide, Zn <sub>2</sub> TiO <sub>4</sub> .....   | 12m          | 37         |
| Uranium oxide (uraninite), UO <sub>2</sub> .....                              | 2            | 33         | Zinc tungsten oxide (sanmartinite),<br>ZnWO <sub>4</sub> .....  | 2m           | 40         |
| Uranium selenide, USe .....   | 5m           | 78         | Zinc vanadium oxide, Zn <sub>3</sub> (VO <sub>4</sub> ) <sub>2</sub> .....  | 20m          | 111        |
| Uranium telluride, UTe .....  | 4m           | 73         | Zirconium, $\alpha$ -Zr .....   | 2            | 11         |
| Vanadium, V .....   | 9m           | 58         | Zirconium boride, ZrB <sub>2</sub> .....  | 20m          | 113        |
| Vanadium oxide (karelianite), V <sub>2</sub> O <sub>3</sub> .....             | 20m          | 108        | Zirconium fluoride, ZrF <sub>4</sub> .....  | 18m          | 79         |
| Vanadium(V) oxide (shcherbinaite),<br>V <sub>2</sub> O <sub>5</sub> .....     | 8            | 66         | Zirconium hydride, ZrH <sub>2</sub> .....   | 5m           | 60         |
| Vanadium sulfide, $\alpha$ -V <sub>3</sub> S .....                            | 14m          | 118        | Zirconium hydrogen phosphate hydrate,<br>Zr(HPO <sub>4</sub> ) <sub>2</sub> ·H <sub>2</sub> O .....                                     | 20m          | 114        |
| Vanadium sulfide, $\beta$ -V <sub>3</sub> S .....                             | 14m          | 120        | Zirconium iodate, Zr(10 <sub>3</sub> ) <sub>4</sub> .....   | 1m           | 51         |
| Ytterbium arsenate, YbAsO <sub>4</sub> .....                                  | 4m           | 38         | Zirconium nitride, ZrN .....  | 5m           | 80         |
| Ytterbium arsenide, YbAs .....  | 4m           | 73         | Zirconium oxide, ZrO .....  | 5m           | 81         |
| Ytterbium fluoride, YbF <sub>3</sub> .....                                    | 20m          | 109        | Zirconium oxide chloride hydrate,<br>ZrOCl <sub>2</sub> ·8H <sub>2</sub> O .....  | 18m          | 81         |
| Ytterbium nitride, YbN .....  | 4m           | 74         | Zirconium phosphide, ZrP .....  | 4m           | 75         |
| Ytterbium oxide, Yb <sub>2</sub> O <sub>3</sub> .....                         | 6m           | 80         | Zirconium silicate, zircon, ZrSiO <sub>4</sub> ..   | 4            | 68         |
| Ytterbium selenide, YbSe .....  | 5m           | 79         | Zirconium silicide, ZrSi <sub>2</sub> .....   | 17m          | 86         |
| Ytterbium telluride, YbTe .....   | 5m           | 79         | Zirconium sulfate hydrate<br>(zirconosulfate), Zr(SO <sub>4</sub> ) <sub>2</sub> ·4H <sub>2</sub> O ..                                  | 7            | 66         |
| Ytterbium(III) vanadium oxide, YbVO <sub>4</sub> .....                        | 5m           | 58         | Zirconium titanium oxide, ZrTiO <sub>4</sub> ..   | 20m          | 115        |
| Yttrium, Y .....  | 18m          | 77         | Zirconium titanium oxide,<br>Zr <sub>5</sub> Ti <sub>7</sub> O <sub>24</sub> .....  | 20m          | 116        |
| Yttrium arsenate, YAsO <sub>4</sub> .....                                     | 2m           | 39         |   |              |            |
| Yttrium arsenide, YAs .....   | 4m           | 74         |   |              |            |
| Yttrium chloride oxide, YClO .....  | 1m           | 51         |   |              |            |
| Yttrium chromium oxide, YCrO <sub>3</sub> .....                               | 19m          | 83         |   |              |            |
| Yttrium oxide, Y <sub>2</sub> O <sub>3</sub> .....                            | 3            | 28         |   |              |            |
| Yttrium phosphate (xenotime), YPO <sub>4</sub> .....                          | 8            | 67         |   |              |            |
| Yttrium sulfide, YS .....   | 5m           | 80         |   |              |            |
| Yttrium telluride, YTe .....  | 4m           | 75         |   |              |            |
| Yttrium titanium oxide, Y <sub>2</sub> TiO <sub>5</sub> .....                 | 11m          | 113        |   |              |            |
| Yttrium vanadium oxide, YVO <sub>4</sub> .....                                | 5m           | 59         |   |              |            |
| Zinc, Zn .....  | 1            | 16         |   |              |            |
| Zinc aluminum oxide (gahnite),<br>ZnAl <sub>2</sub> O <sub>4</sub> .....      | 2            | 38         |   |              |            |
| Zinc ammine bromide, Zn(NH <sub>3</sub> ) <sub>2</sub> Br <sub>2</sub> .....  | 11m          | 68         |   |              |            |
| Zinc ammine chloride, Zn(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub> ..... | 10m          | 59         |   |              |            |

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| CHI <sub>3</sub>  | Iodoform   | 18m             | 34   |
| CH <sub>4</sub> N <sub>2</sub> O  | Urea   | 7               | 61   |
| CH <sub>4</sub> N <sub>2</sub> S  | Thiourea   | 17m             | 83   |
| CH <sub>5</sub> NO <sub>2</sub>   | Ammonium formate   | 11m             | 9    |
| CH <sub>5</sub> N <sub>3</sub> ·HCl   | Guanidinium chloride   | 17m             | 35   |
| CH <sub>5</sub> N <sub>3</sub> S  | Thiosemicarbazide  | 17m             | 81   |
| C <sub>2</sub> Ag <sub>2</sub> O <sub>4</sub>                                   | Silver oxalate   | 9m              | 47   |
| C <sub>2</sub> FeO <sub>4</sub> ·2H <sub>2</sub> O                              | Iron oxalate hydrate (humboldtine)   | 10m             | 24   |
| C <sub>2</sub> HNaO <sub>4</sub> ·H <sub>2</sub> O                              | Sodium hydrogen oxalate hydrate  | 17m             | 72   |
| C <sub>2</sub> H <sub>2</sub> CaO <sub>4</sub>                                  | Calcium formate  | 8               | 16   |
| C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> ·2H <sub>2</sub> O                 | Oxalic acid hydrate  | 16m             | 55   |
| C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> Pb                                 | Lead formate   | 8               | 30   |
| C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> Sr                                 | Strontium formate  | 8               | 55   |
| C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> Sr·2H <sub>2</sub> O               | Strontium formate hydrate (orthorhombic)                                       | 8               | 56   |
| C <sub>2</sub> H <sub>3</sub> KO <sub>4</sub>                                   | Potassium formate-formic acid complex  | 9m              | 93   |
| C <sub>2</sub> H <sub>3</sub> NaO <sub>2</sub> ·3H <sub>2</sub> O               | Sodium acetate hydrate   | 15m             | 66   |
| C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>                     | Glyoxime   | 8m              | 102  |
| C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>                                   | α-Glycine  | 17m             | 34   |
| C <sub>2</sub> H <sub>7</sub> NO <sub>2</sub>                                   | Ammonium acetate   | 8m              | 95   |
| C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> ·2HCl                              | Ethylenediamine Hydrochloride  | 19m             | 43   |
| C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O   | Ammonium oxalate hydrate (oxammite)  | 7               | 5    |
| C <sub>2</sub> K <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O                  | Potassium oxalate hydrate  | 9m              | 39   |
| C <sub>2</sub> Li <sub>2</sub> O <sub>4</sub>                                   | Lithium oxalate  | 10m             | 34   |
| C <sub>2</sub> Na <sub>2</sub> O <sub>4</sub>                                   | Sodium oxalate   | 6m              | 70   |
| C <sub>2</sub> O <sub>4</sub> Rb <sub>2</sub> ·H <sub>2</sub> O <sub>2</sub>    | Rubidium oxalate perhydrate  | 9m              | 102  |
| C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>                                   | L-Alanine  | 8m              | 93   |
| C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S                                 | L-Cysteine   | 11m             | 86   |
| C <sub>3</sub> H <sub>9</sub> N·HCl   | Trimethylammonium chloride   | 9m              | 113  |
| C <sub>4</sub> H <sub>3</sub> KO <sub>8</sub> ·2H <sub>2</sub> O                | Potassium hydrogen oxalate hydrate   | 17m             | 60   |
| C <sub>4</sub> H <sub>4</sub> CaO <sub>5</sub> ·2H <sub>2</sub> O               | Calcium malate hydrate   | 10m             | 76   |
| C <sub>4</sub> H <sub>4</sub> KNaO <sub>6</sub> ·4H <sub>2</sub> O              | Potassium sodium tartrate hydrate  | 15m             | 55   |
| C <sub>4</sub> H <sub>4</sub> MnO <sub>6</sub>                                  | Manganese Tartrate   | 19m             | 57   |
| C <sub>4</sub> H <sub>4</sub> NO <sub>8</sub> Y·H <sub>2</sub> O                | Ammonium yttrium oxalate hydrate   | 8m              | 97   |
| C <sub>4</sub> H <sub>4</sub> Na <sub>2</sub> O <sub>6</sub> ·2H <sub>2</sub> O | Sodium D-tartrate hydrate  | 11m             | 110  |
| C <sub>4</sub> H <sub>6</sub> CoO <sub>4</sub> ·4H <sub>2</sub> O               | Cobalt acetate hydrate   | 12m             | 19   |
| C <sub>4</sub> H <sub>6</sub> Hg <sub>2</sub> O <sub>4</sub>                    | Mercury acetate  | 17m             | 51   |
| C <sub>4</sub> H <sub>6</sub> NiO <sub>4</sub> ·4H <sub>2</sub> O               | Nickel acetate hydrate   | 13m             | 31   |
| C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> Zn·2H <sub>2</sub> O               | Zinc acetate hydrate   | 18m             | 78   |
| C <sub>4</sub> H <sub>6</sub> O <sub>6</sub>                                    | D-Tartaric acid  | 7m              | 168  |
| C <sub>4</sub> H <sub>6</sub> O <sub>6</sub> U·2H <sub>2</sub> O                | Uranyl acetate hydrate   | 18m             | 76   |
| C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O                                  | Creatinine   | 15m             | 31   |
| C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>                     | α-HMX  | 11m             | 100  |
| C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>                     | β-HMX  | 11m             | 102  |
| C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>                     | Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine, alpha-                       | 11m             | 100  |
| C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>                     | Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine, beta-bis-(o-Dodecacarborane) | 11m             | 102  |
| C <sub>4</sub> H <sub>22</sub> B <sub>2</sub> O                                 | Uric acid, phase 1 (calc. pattern)   | 6m              | 7    |
| C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>                     | Uric acid, phase 1   | 8m              | 154  |
| C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>                     | Copper glutamate hydrate   | 16m             | 78   |
| C <sub>5</sub> H <sub>7</sub> CuNO <sub>4</sub> ·2H <sub>2</sub> O              | Zinc glutamate hydrate   | 7m              | 110  |
| C <sub>5</sub> H <sub>7</sub> NO <sub>4</sub> Zn·2H <sub>2</sub> O              | Sodium glutamate hydrate   | 7m              | 170  |
| C <sub>5</sub> H <sub>8</sub> NNaO <sub>4</sub> ·H <sub>2</sub> O               | β-L-Glutamic acid  | 17m             | 70   |
| C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>                                   | Pentaerythritol  | 17m             | 32   |
| C <sub>5</sub> H <sub>12</sub> O <sub>4</sub>                                   | Picric acid  | 17m             | 55   |
| C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>7</sub>                     | Nicotinic acid   | 16m             | 56   |
| C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>                                   | γ-Hydroquinone   | 16m             | 54   |
| C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>                                    | Zinc diimidazole chloride  | 8m              | 107  |
| C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>4</sub> Zn                 | Phenylhydrazine hydrochloride  | 7m              | 123  |
| C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ·HCl                               | L-Ascorbic acid  | 17m             | 56   |
| C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>                                    | Hexamethylenetetramine   | 8m              | 99   |
| C <sub>6</sub> H <sub>12</sub> N <sub>4</sub>                                   | Dextrose   | 17m             | 37   |
| C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                                   |  | 11m             | 28   |

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| C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                                      |                 |      |
| C <sub>6</sub> H <sub>15</sub> HoO <sub>12</sub> S <sub>3</sub> ·9H <sub>2</sub> O | 11m             | 28   |
| C <sub>6</sub> H <sub>15</sub> NdO <sub>12</sub> S <sub>3</sub> ·9H <sub>2</sub> O | 1m              | 18   |
| C <sub>7</sub> H <sub>5</sub> BrO <sub>2</sub>                                     | 9               | 41   |
| C <sub>7</sub> H <sub>5</sub> ClO <sub>2</sub>                                     | 16m             | 22   |
| C <sub>7</sub> H <sub>5</sub> FO <sub>2</sub>                                      | 16m             | 30   |
| C <sub>7</sub> H <sub>5</sub> IO <sub>2</sub>                                      | 16m             | 36   |
| C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub> S                                    | 19m             | 47   |
| C <sub>7</sub> H <sub>12</sub> O <sub>4</sub>                                      | 9m              | 78   |
| C <sub>8</sub> H <sub>4</sub> Hg <sub>2</sub> O <sub>4</sub>                       | 7m              | 153  |
| C <sub>8</sub> H <sub>5</sub> KO <sub>4</sub>                                      | 10m             | 113  |
| C <sub>8</sub> H <sub>5</sub> O <sub>4</sub> Tl                                    | 4m              | 30   |
| C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>7</sub>                        | 16m             | 75   |
| C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>                                       | 8m              | 152  |
| C <sub>8</sub> H <sub>9</sub> NO   | 16m             | 11   |
| C <sub>8</sub> H <sub>9</sub> NO   | 14m             | 38   |
| C <sub>8</sub> H <sub>11</sub> N <sub>2</sub> NaO <sub>3</sub>                     | 16m             | 7    |
| C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>                       | 16m             | 157  |
| C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>                       | 15m             | 126  |
| C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>                       | 15m             | 128  |
| C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>                       | 15m             | 130  |
| C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>                       | 15m             | 177  |
| C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>                      | 14m             | 41   |
| C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>8</sub>                      | 19m             | 45   |
| C <sub>10</sub> H <sub>15</sub> NO·HC1   | 16m             | 124  |
| C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>                      | 16m             | 162  |
| C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>                      | 15m             | 114  |
| C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>                      | 15m             | 117  |
| C <sub>12</sub> H <sub>10</sub> N <sub>2</sub>                                     | 7m              | 86   |
| C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> ·2HC1                               | 18m             | 14   |
| C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>                      | 16m             | 144  |
| C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> ·8H <sub>2</sub> O   | 19m             | 88   |
| C <sub>12</sub> H <sub>16</sub> Cl <sub>2</sub> CuN <sub>8</sub>                   | 8m              | 31   |
| C <sub>12</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>8</sub> Mi                  | 8m              | 44   |
| C <sub>12</sub> H <sub>16</sub> CuN <sub>10</sub> O <sub>6</sub>                   | 13m             | 24   |
| C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>                                     | 14m             | 109  |
| C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O                                   | 15m             | 133  |
| C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O                                   | 16m             | 152  |
| C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>                                    | 11m             | 66   |
| C <sub>12</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>                      | 7m              | 121  |
| C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> ·HC1                 | 16m             | 149  |
| C <sub>13</sub> H <sub>21</sub> N <sub>2</sub> O <sub>4</sub> P                    | 16m             | 154  |
| C <sub>14</sub> H <sub>11</sub> FO   | 8m              | 91   |
| C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> S·HC1                               | 14m             | 112  |
| C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O                                   | 18m             | 24   |
| C <sub>15</sub> H <sub>12</sub> O <sub>2</sub>                                     | 7m              | 115  |
| C <sub>16</sub> H <sub>13</sub> C1N <sub>2</sub> O                                 | 14m             | 106  |
| C <sub>16</sub> H <sub>13</sub> N  | 6m              | 29   |
| C <sub>17</sub> H <sub>19</sub> C1N <sub>2</sub> S                                 | 14m             | 60   |
| C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub> ·HC1·3H <sub>2</sub> O             | 16m             | 133  |
| C <sub>17</sub> H <sub>21</sub> NO <sub>4</sub> ·HC1                               | 16m             | 114  |
| C <sub>17</sub> H <sub>25</sub> N·HC1  | 16m             | 141  |
| C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub> ·HBr·2H <sub>2</sub> O             | 16m             | 117  |
| C <sub>18</sub> H <sub>24</sub> CdN <sub>14</sub> O <sub>6</sub>                   | 8m              | 23   |
| C <sub>18</sub> H <sub>24</sub> N <sub>14</sub> NiO <sub>6</sub>                   | 7m              | 27   |
| C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub> S                    | 15m             | 119  |
| C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub> ·HC1·2H <sub>2</sub> O             | 16m             | 136  |
| C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O                                   | 17m             | 26   |
| C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> ·HC1                                | 16m             | 129  |
| C <sub>20</sub> H <sub>25</sub> NO <sub>3</sub> ·HC1                               | 16m             | 92   |
| C <sub>20</sub> H <sub>34</sub>  |                 |      |
| C <sub>21</sub> H <sub>23</sub> C1FNO <sub>2</sub>                                 | 16m             | 122  |
| C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>                                     | 16m             | 127  |
| C <sub>22</sub> H <sub>25</sub> C1N <sub>2</sub> OS·2H <sub>2</sub> O              | 16m             | 111  |
| C <sub>22</sub> H <sub>30</sub> O <sub>4</sub>                                     | 17m             | 28   |
|  | 16m             | 160  |

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| C <sub>24</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub> Pd | Palladium bis-(N-isopropyl-3-ethylsalicylaldehyde)     | 7m | 144 |
| C <sub>25</sub> H <sub>15</sub> N <sub>6</sub>                   | N-Methylphenazinium-7,7,8,8-tetracyanoquinodimethanide | 7m | 146 |
| C <sub>33</sub> H <sub>40</sub> N <sub>2</sub> O <sub>9</sub>    | Reserpine  | 8m | 123 |

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| Acetanilide                                       | C <sub>8</sub> H <sub>9</sub> NO (calc. pattern)  | 14m             | 38   |
| Acetanilide                                       | C <sub>8</sub> H <sub>9</sub> NO  | 16m             | 7    |
| 4-Acetyl-2'-fluorodiphenyl                        | C <sub>14</sub> H <sub>11</sub> FO  | 8m              | 91   |
| Alanine, L-                                       | CH <sub>3</sub> CHNH <sub>2</sub> CO <sub>2</sub> H   | 8m              | 93   |
| Allobarbital                                      | C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>   | 14m             | 41   |
| Amobarbital, form I                               | C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>   | 15m             | 114  |
| Amobarbital, form II                              | C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>   | 15m             | 117  |
| Ammonium acetate                                  | NH <sub>4</sub> ·CH <sub>3</sub> CO <sub>2</sub>  | 8m              | 95   |
| Ammonium formate                                  | NH <sub>4</sub> HCO <sub>2</sub>  | 11m             | 9    |
| Ammonium oxalate hydrate (oxammite)               | (NH <sub>4</sub> ) <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O                                 | 7               | 5    |
| Ammonium yttrium oxalate hydrate                  | NH <sub>4</sub> Y(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> ·H <sub>2</sub> O                                | 8m              | 97   |
| Amphetamine sulfate, (+)-                         | C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub> S   | 15m             | 119  |
| p-Anisic acid                                     | C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>  | 16m             | 11   |
| Ascorbic acid, L-                                 | C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>  | 8m              | 99   |
| Azobenzene  | C <sub>6</sub> H <sub>5</sub> NNC <sub>6</sub> H <sub>5</sub>   | 7m              | 86   |
| Barbital, form I                                  | C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>  | 15m             | 126  |
| Barbital, form II                                 | C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>  | 15m             | 128  |
| Barbital, form IV                                 | C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>  | 15m             | 130  |
| Benactyzine hydrochloride                         | C <sub>20</sub> H <sub>25</sub> N <sub>2</sub> O <sub>3</sub> ·HCl  | 16m             | 92   |
| Benzidine hydrochloride                           | C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> ·2HCl  | 18m             | 14   |
| o-Bromobenzoic acid                               | C <sub>7</sub> H <sub>5</sub> BrO <sub>2</sub>  | 16m             | 22   |
| Bufofenine  | C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O  | 15m             | 133  |
| Cadmium hexaimidazole nitrate                     | Cd(C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>6</sub> (NO <sub>3</sub> ) <sub>2</sub>                  | 8m              | 23   |
| Calcium formate                                   | Ca(HCO <sub>2</sub> ) <sub>2</sub>  | 8               | 16   |
| Calcium malate hydrate                            | Ca(O <sub>2</sub> C) <sub>2</sub> (CH <sub>2</sub> CHOH)·2H <sub>2</sub> O                                      | 10m             | 76   |
| Cannabidiol                                       | C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>  | 16m             | 111  |
| Carbamazepine, β-                                 | C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O  | 18m             | 24   |
| m-Chlorobenzoic acid                              | C <sub>7</sub> H <sub>5</sub> ClO <sub>2</sub>  | 16m             | 30   |
| Chlorpromazine                                    | C <sub>17</sub> H <sub>19</sub> ClN <sub>2</sub> S  | 14m             | 60   |
| Cinchonine  | C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O  | 17m             | 26   |
| Clopenthixol hydrate                              | C <sub>22</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub> ·2H <sub>2</sub> O                              | 17m             | 28   |
| Cobalt acetate hydrate                            | Co(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> ·4H <sub>2</sub> O                               | 12m             | 19   |
| Cocaine hydrochloride, L-                         | C <sub>17</sub> H <sub>21</sub> NO <sub>4</sub> ·HCl  | 16m             | 114  |
| Codeine hydrobromide hydrate                      | C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub> ·HBr·2H <sub>2</sub> O  | 16m             | 117  |
| Copper glutamate hydrate                          | Cu(O <sub>2</sub> C) <sub>2</sub> (H <sub>2</sub> NCHCH <sub>2</sub> CH <sub>2</sub> )·2H <sub>2</sub> O        | 7m              | 110  |
| Copper tetraimidazole nitrate                     | Cu(C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub>                  | 13m             | 24   |
| Copper tetrapyrazole chloride                     | Cu(C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>4</sub> Cl <sub>2</sub>                                  | 8m              | 31   |
| Creatinine  | C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O  | 15m             | 31   |
| Cysteine, L-                                      | HSCH <sub>2</sub> ·CH(NH <sub>2</sub> )·COOH  | 11m             | 86   |
| Dextrose  | C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>   | 11m             | 28   |
| Diazepam  | C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O  | 14m             | 106  |
| Dibenzoylmethane                                  | (C <sub>6</sub> H <sub>5</sub> CO) <sub>2</sub> CH <sub>2</sub>   | 7m              | 115  |
| Dihydrophyllocladene, α-, hartite (or bombiccite) | C <sub>20</sub> H <sub>34</sub>   | 16m             | 122  |
| (N,N)-Dimethyltryptamine                          | C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>  | 14m             | 109  |
| bis-( <i>o</i> -Dodecacarborane)                  | C <sub>4</sub> B <sub>20</sub> H <sub>22</sub>  | 6m              | 7    |
| Ephedrine hydrochloride, (-)-                     | C <sub>10</sub> H <sub>15</sub> NO·HCl  | 16m             | 124  |
| Ethylenediamine hydrochloride                     | C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> ·2HCl  | 19m             | 43   |
| Ethylenediaminetetraacetic acid                   | C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>8</sub>   | 19m             | 45   |
| p-Fluorobenzoic acid                              | C <sub>7</sub> H <sub>5</sub> FO <sub>2</sub>   | 16m             | 36   |
| Glucose, α-D-                                     | C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>   | 11m             | 28   |
| Glutamic acid, β-L-                               | C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>   | 17m             | 32   |
| Glycine, α-                                       | C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>   | 17m             | 34   |
| Glyoxime  | H <sub>2</sub> C <sub>2</sub> (NOH) <sub>2</sub>  | 8m              | 102  |
| Guanidinium chloride                              | CH <sub>5</sub> N <sub>3</sub> ·HCl   | 17m             | 35   |
| Haloperidol                                       | C <sub>21</sub> H <sub>23</sub> ClFNO <sub>2</sub>  | 16m             | 127  |
| Hexamethylenediammonium adipate                   | (CH <sub>2</sub> ) <sub>4</sub> (CO <sub>2</sub> H <sub>3</sub> N) <sub>2</sub> (CH <sub>2</sub> ) <sub>6</sub> | 7m              | 121  |
| Hexamethylenetetramine                            | C <sub>6</sub> H <sub>12</sub> N <sub>4</sub>   | 17m             | 37   |
| HMX, α-   | C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>   | 11m             | 100  |
| HMX, β-   | C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>   | 11m             | 102  |
| Holmium ethylsulfate hydrate                      | Ho[(C <sub>2</sub> H <sub>5</sub> )SO <sub>4</sub> ] <sub>3</sub> ·9H <sub>2</sub> O                            | 1m              | 18   |
| Hydroquinone, γ-                                  | HOC <sub>6</sub> H <sub>4</sub> OH  | 8m              | 107  |

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| Imipramine hydrochloride  | C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> ·HCl  | 16m             | 129  |
| p-Iodobenzoic acid  | C <sub>7</sub> H <sub>5</sub> IO <sub>2</sub>  | 19m             | 47   |
| Iodoform  | CHI <sub>3</sub>   | 18m             | 34   |
| Iron oxalate hydrate (humboldtine)                                | FeC <sub>2</sub> O <sub>4</sub> ·2H <sub>2</sub> O   | 10m             | 24   |
| Lead formate  | Pb(HCO <sub>2</sub> ) <sub>2</sub>   | 8               | 30   |
| Lithium oxalate   | Li <sub>2</sub> C <sub>2</sub> O <sub>4</sub>  | 10m             | 34   |
| Manganese tartrate  | C <sub>4</sub> H <sub>4</sub> MnO <sub>6</sub>   | 19m             | 57   |
| Mercury acetate   | C <sub>4</sub> H <sub>6</sub> Hg <sub>2</sub> O <sub>4</sub>                                   | 17m             | 51   |
| Mercury o-phthalate   | C <sub>6</sub> H <sub>4</sub> (CO <sub>2</sub> Hg) <sub>2</sub>                                | 10m             | 113  |
| Methapyriene hydrochloride  | C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> S·HCl   | 14m             | 112  |
| Metharbital   | C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>                                   | 15m             | 177  |
| Methyl sulfonanilide  | C <sub>6</sub> H <sub>5</sub> NHSO <sub>2</sub> CH <sub>3</sub>                                | 9m              | 78   |
| N-Methylphenazinium-7,7,8,8-tetra-cyanoquinodimethanide           | C <sub>25</sub> H <sub>15</sub> N <sub>6</sub>   | 7m              | 146  |
| Morphine hydrochloride hydrate                                    | C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub> ·HCl·3H <sub>2</sub> O                         | 16m             | 133  |
| Naloxone hydrochloride hydrate                                    | C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub> ·HCl·2H <sub>2</sub> O                         | 16m             | 136  |
| 2-Naphthylamine, N-phenyl-  | C <sub>10</sub> H <sub>7</sub> NHC <sub>6</sub> H <sub>5</sub>                                 | 6m              | 29   |
| Neodymium ethylsulfate hydrate                                    | Nd[(C <sub>2</sub> H <sub>5</sub> )SO <sub>4</sub> ] <sub>3</sub> ·9H <sub>2</sub> O           | 9               | 41   |
| Nickel acetate hydrate  | Ni(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> ·4H <sub>2</sub> O              | 13m             | 31   |
| Nickel hexaimidazole nitrate                                      | Ni(C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>6</sub> (NO <sub>3</sub> ) <sub>2</sub> | 7m              | 27   |
| Nickel tetrapyrazole chloride                                     | Ni(C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>4</sub> Cl <sub>2</sub>                 | 8m              | 44   |
| Nicotinic acid  | C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>  | 16m             | 54   |
| Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine ( $\alpha$ -HMX) | C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>                                    | 11m             | 100  |
| Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine ( $\beta$ -HMX)  | C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>                                    | 11m             | 102  |
| Oxalic acid hydrate   | C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> ·2H <sub>2</sub> O                                | 16m             | 55   |
| Palladium bis-(N-isopropyl-3-ethylsalicylaldiminate)              | Pd(C <sub>12</sub> H <sub>16</sub> NO) <sub>2</sub>  | 7m              | 144  |
| Pentaerythritol   | C <sub>5</sub> H <sub>12</sub> O <sub>4</sub>  | 17m             | 55   |
| Phencyclidine hydrochloride                                       | C <sub>17</sub> H <sub>25</sub> N·HCl  | 16m             | 141  |
| Phenobarbital, form III   | C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>                                  | 16m             | 144  |
| Phenobarbital hydrate   | C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> ·H <sub>2</sub> O                | 19m             | 88   |
| Phenylhydrazine hydrochloride                                     | C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ·HCl  | 17m             | 56   |
| Picric acid   | C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>7</sub>                                    | 16m             | 56   |
| Pimelic acid  | (CH <sub>2</sub> ) <sub>5</sub> (CO <sub>2</sub> H) <sub>2</sub>                               | 7m              | 153  |
| Potassium formate-formic acid complex                             | KO <sub>2</sub> CH·HO <sub>2</sub> CH  | 9m              | 93   |
| Potassium hydrogen o-phthalate                                    | C <sub>6</sub> H <sub>4</sub> (COOH)(COOK)   | 4m              | 30   |
| Potassium hydrogen oxalate hydrate                                | C <sub>4</sub> H <sub>3</sub> KO <sub>8</sub> ·2H <sub>2</sub> O                               | 17m             | 60   |
| Potassium oxalate hydrate   | K <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O                                 | 9m              | 39   |
| Potassium oxalate perhydrate                                      | K <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O <sub>2</sub>                    | 9m              | 96   |
| Potassium sodium tartrate hydrate                                 | C <sub>4</sub> H <sub>4</sub> KNaO <sub>6</sub> ·4H <sub>2</sub> O                             | 15m             | 55   |
| Procaine hydrochloride  | C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> ·HCl                             | 16m             | 149  |
| Psilocin  | C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O   | 16m             | 152  |
| Psilocybin methanolate  | C <sub>13</sub> H <sub>21</sub> N <sub>2</sub> O <sub>4</sub> P                                | 16m             | 154  |
| Reserpine   | C <sub>33</sub> H <sub>40</sub> N <sub>2</sub> O <sub>9</sub>                                  | 8m              | 123  |
| Rubidium oxalate perhydrate                                       | Rb <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O <sub>2</sub>                   | 9m              | 102  |
| Silver oxalate  | Ag <sub>2</sub> C <sub>2</sub> O <sub>4</sub>  | 9m              | 47   |
| Sodium acetate hydrate  | C <sub>2</sub> H <sub>3</sub> NaO <sub>2</sub> ·3H <sub>2</sub> O                              | 15m             | 66   |
| Sodium barbital   | C <sub>8</sub> H <sub>11</sub> N <sub>2</sub> NaO <sub>3</sub>                                 | 16m             | 157  |
| Sodium glutamate hydrate  | C <sub>5</sub> H <sub>8</sub> NNaO <sub>4</sub> ·H <sub>2</sub> O                              | 17m             | 70   |
| Sodium hydrogen oxalate hydrate                                   | C <sub>2</sub> HNaO <sub>4</sub> ·H <sub>2</sub> O   | 17m             | 72   |
| Sodium oxalate  | Na <sub>2</sub> C <sub>2</sub> O <sub>4</sub>  | 6m              | 70   |
| Sodium D-tartrate hydrate   | (CHOH-CO <sub>2</sub> Na) <sub>2</sub> ·2H <sub>2</sub> O                                      | 11m             | 110  |
| Strontium formate   | Sr(CHO <sub>2</sub> ) <sub>2</sub>   | 8               | 55   |
| Strontium formate hydrate   | Sr(CHO <sub>2</sub> ) <sub>2</sub> ·2H <sub>2</sub> O (orthorhombic)                           | 8               | 56   |
| Sucrose   | C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>  | 11m             | 66   |
| Tartaric acid, D-   | (CHOHCO <sub>2</sub> H) <sub>2</sub>   | 7m              | 168  |
| $\Delta^9$ -Tetrahydrocannabinolic acid B                         | C <sub>22</sub> H <sub>30</sub> O <sub>4</sub>   | 16m             | 160  |
| Thallium hydrogen phthalate                                       | C <sub>8</sub> H <sub>5</sub> O <sub>4</sub> Tl  | 16m             | 75   |
| Thiosemicarbazide   | CH <sub>5</sub> N <sub>3</sub> S   | 17m             | 81   |
| Thiourea  | CH <sub>4</sub> N <sub>2</sub> S   | 17m             | 83   |
| Trimethylammonium chloride  | C <sub>3</sub> H <sub>9</sub> N·HCl  | 9m              | 113  |
| 2,4,6-Trinitrophenetole   | C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>7</sub>                                    | 8m              | 152  |
| Uranyl acetate hydrate  | C <sub>4</sub> H <sub>6</sub> O <sub>6</sub> U·2H <sub>2</sub> O                               | 18m             | 76   |
| Urea  | CO(NH <sub>2</sub> ) <sub>2</sub>  | 7               | 61   |
| Uric acid, phase 1, (calc. pattern)                               | C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>                                    | 8m              | 154  |
| Uric acid (phase 1)   | C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>                                    | 16m             | 78   |
| Vinbarbital, form I   | C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>                                  | 16m             | 162  |

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| Zinc acetate hydrate      | C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> · 2H <sub>2</sub> O   | 18m             | 78   |
| Zinc diimidazole chloride | Zn(C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub>                             | 7m              | 123  |
| Zinc glutamate hydrate,   | Zn(O <sub>2</sub> CCHNH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> ) · 2H <sub>2</sub> O | 7m              | 170  |

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| Borax, $\text{Na}_2\text{B}_4\text{O}_5(\text{OH})_4 \cdot 8\text{H}_2\text{O}$ .....         | 16m             | 66   | Franklinite, $\text{ZnFe}_2\text{O}_4$ .....  | 9m              | 60   |
| Bromargyrite, $\text{AgBr}$ .....   | 4               | 46   | Fresnoite, $\text{Ba}_2\text{TiSi}_2\text{O}_8$ .....   | 9m              | 14   |
| Bromellite, $\text{BeO}$ .....  | 1               | 36   | Gahnite, $\text{ZnAl}_2\text{O}_4$ .....  | 2               | 38   |
| *Brookite, $\text{TiO}_2$ .....   | 3m              | 57   | Galaxite, $\text{MnAl}_2\text{O}_4$ .....   | 9               | 35   |
| Brownmillerite, $\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$ .....                        | 16m             | 28   | Galena, $\text{PbS}$ .....  | 2               | 18   |
| Brucite, $\text{Mg}(\text{OH})_2$ .....   | 6               | 30   | Gaspeite, $\text{NiCO}_3$ .....   | 1m              | 36   |
| Bunsenite, $\text{NiO}$ .....   | 1               | 47   | Geikielite, $\text{MgTiO}_3$ .....  | 5               | 43   |
| Burkeite, $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$ .....                                       | 11m             | 52   | Gersdorffite, $\text{NiAsS}$ .....  | 1m              | 35   |
| *Butlerite, $\text{Fe}(\text{OH})\text{SO}_4 \cdot 2\text{H}_2\text{O}$ .....                 | 10m             | 95   | Glauberite, $\text{Na}_2\text{Ca}(\text{SO}_4)_2$ .....                                       | 6m              | 59   |
| Cadmoselite, $\text{CdSe}$ .....  | 7               | 12   | Gold, $\text{Au}$ .....   | 1               | 33   |
| Calcite, $\text{CaCO}_3$ .....  | 2               | 51   | Goslarite, $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$ .....                                    | 8               | 71   |
| Calomel, $\text{Hg}_2\text{Cl}_2$ .....   | 13m             | 30   | Greenockite, $\text{CdS}$ .....   | 4               | 15   |
| Carnallite, $\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$ .....                                  | 8m              | 50   | *Groutite, $\text{MnO}(\text{OH})$ .....  | 11m             | 97   |
| Carrobbiite, $\text{KF}$ .....  | 1               | 64   | Gunningite, $\text{ZnSO}_4 \cdot \text{H}_2\text{O}$ .....                                    | 19m             | 86   |
| Cassiterite, $\text{SnO}_2$ .....   | 1               | 54   | Gypsum, $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ .....                                       | 17m             | 16   |
| Celestite, $\text{SrSO}_4$ .....  | 2               | 61   | Halite, $\text{NaCl}$ .....   | 2               | 41   |
| Cerianite, $\text{CeO}_2$ .....   | 1               | 56   | *Hartite, $\text{C}_{20}\text{H}_{34}$ .....  | 16m             | 122  |
| Cerianite, $\text{CeO}_2$ .....   | 20m             | 38   | Hausmannite, $\text{Mn}_3\text{O}_4$ .....  | 10m             | 38   |
| Cerussite, $\text{PbCO}_3$ .....  | 2               | 56   | Hematite, $\alpha\text{-Fe}_2\text{O}_3$ .....  | 18m             | 37   |
| Cervantite, $\text{Sb}_2\text{O}_4$ .....   | 10              | 8    | *Hemimorphite, $\text{Zn}_4(\text{OH})_2\text{Si}_2\text{O}_7 \cdot \text{H}_2\text{O}$ ..... | 2               | 62   |
| *Chabazite, $\text{Ca}_2\text{Al}_4\text{Si}_8\text{O}_{24} \cdot 12\text{H}_2\text{O}$ ..... | 19m             | 27   | Hercynite, $\text{FeAl}_2\text{O}_4$ .....  | 19m             | 48   |
| Chalcocyanite, $\text{CuSO}_4$ .....  | 3m              | 29   | Hessite, $\text{Ag}_2\text{Te}$ .....   | 19m             | 73   |
| Chernovite, $\text{YAsO}_4$ .....   | 2m              | 39   | Hetaerolite, $\text{ZnMn}_2\text{O}_4$ .....  | 10m             | 61   |
| Chiolite, $\text{Na}_5\text{Al}_3\text{F}_{14}$ .....   | 16m             | 63   | *Hexahydroborite, $\text{Ca B}(\text{OH})_4 \cdot 2\text{H}_2\text{O}$ .....                  | 16m             | 104  |
| Chloraluminite, $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ .....                               | 7               | 3    | Hieratite, $\text{K}_2\text{SiF}_6$ .....   | 5               | 50   |
| Chlorargyrite, $\text{AgCl}$ .....  | 4               | 44   | Hoernesite, $\text{Mg}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$ .....                     | 19m             | 53   |
| Chloromagnesite, $\text{MgCl}_2$ .....  | 11m             | 94   | Hopeite, $\text{Zn}_3(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ .....                         | 16m             | 85   |
| Chromatite, $\text{CaCrO}_4$ .....  | 7               | 13   |   |                 |      |
| Chromite, $\text{FeCr}_2\text{O}_4$ .....   | 19m             | 50   |   |                 |      |
| Chrysoberyl, $\text{BeAl}_2\text{O}_4$ .....  | 9               | 10   |   |                 |      |

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| Huebnerite, MnWO <sub>4</sub> .....  | 2m              | 24   | Monteponite, CdO .....   | 2               | 27   |
| Humboldtine, FeC <sub>2</sub> O <sub>4</sub> ·2H <sub>2</sub> O .....  | 10m             | 24   | Monticellite, CaMgSiO <sub>4</sub> .....   | 20m             | 30   |
| Humite, Mg <sub>7</sub> F <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> .....   | 1m              | 30   | Montroydite, HgO .....   | 9               | 39   |
| Huttonite, β-ThSiO <sub>4</sub> .....  | 20m             | 102  | Mullite, Al <sub>6</sub> Si <sub>2</sub> O <sub>13</sub> .....   | 3m              | 3    |
| Hydromolyosite, FeCl <sub>3</sub> ·6H <sub>2</sub> O .....   | 17m             | 40   | Nantokite, CuCl .....  | 4               | 35   |
| Hydrophilite, CaCl <sub>2</sub> .....  | 11m             | 18   | *Newberryite, MgHPO <sub>4</sub> ·3H <sub>2</sub> O .....  | 7m              | 139  |
| Ilmenite, FeTiO <sub>3</sub> .....   | 15m             | 34   | Nickel-hexahydrite, β-NiSO <sub>4</sub> ·6H <sub>2</sub> O .....   | 19m             | 65   |
| Indialite, Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub> .....   | 1m              | 29   | Niter, KNO <sub>3</sub> .....  | 3               | 58   |
| Iodargyrite, AgI .....   | 8               | 51   | Nitrammite, NH <sub>4</sub> NO <sub>3</sub> .....  | 7               | 4    |
| Iron, α-Fe .....   | 4               | 3    | Nitrobarite, Ba(NO <sub>3</sub> ) <sub>2</sub> .....   | 11m             | 14   |
| Jacobsite, MnFe <sub>2</sub> O <sub>4</sub> .....  | 9               | 36   | Norbergite, Mg <sub>3</sub> F <sub>2</sub> SiO <sub>4</sub> .....  | 10              | 39   |
| *Julgoldite, Ca <sub>2</sub> Fe <sub>3</sub> Si <sub>3</sub> O <sub>10</sub> (OH, <sub>0</sub> ) <sub>2</sub> (OH) <sub>2</sub>  | 10m             | 72   | Oldhamite, CaS .....   | 7               | 15   |
| Kalistrontite, K <sub>2</sub> Sr(SO <sub>4</sub> ) <sub>2</sub> .....  | 14m             | 31   | Otavite, CdCO <sub>3</sub> .....   | 7               | 11   |
| Karelianite, V <sub>2</sub> O <sub>3</sub> .....   | 20m             | 108  | Oxammite, (NH <sub>4</sub> ) <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O .....  | 7               | 5    |
| Kieserite, MgSO <sub>4</sub> ·H <sub>2</sub> O .....   | 16m             | 46   | Palladium, Pd .....  | 1               | 21   |
| Kirschsteinite, CaFeSiO <sub>4</sub> .....   | 20m             | 28   | Palladseite, Pd <sub>17</sub> Se <sub>15</sub> .....   | 16m             | 139  |
| Koettigite, Zn <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O .....  | 19m             | 85   | Palmierite, K <sub>2</sub> Pb(SO <sub>4</sub> ) <sub>2</sub> .....   | 14m             | 30   |
| Kremersite, (NH <sub>4</sub> ,K) <sub>2</sub> FeCl <sub>5</sub> ·H <sub>2</sub> O .....  | 14m             | 8    | Paraguanajuatite, Bi <sub>2</sub> Se <sub>3</sub> .....  | 18m             | 16   |
| Langbeinite, K <sub>2</sub> Mg <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....  | 6m              | 40   | *Paratellurite, TeO <sub>2</sub> .....   | 10              | 55   |
| Larnite, β-Ca <sub>2</sub> SiO <sub>4</sub> .....  | 19m             | 29   | Paratellurite, TeO <sub>2</sub> .....  | 7               | 56   |
| Lautarite, Ca(I <sub>0</sub> 3) <sub>2</sub> .....   | 14m             | 12   | Periclase, MgO .....   | 1               | 37   |
| Lead, Pb .....   | 1               | 34   | Perovskite, CaTiO <sub>3</sub> .....   | 9m              | 17   |
| *Leucophanite, NaCaBeFSi <sub>2</sub> O <sub>6</sub> .....   | 8m              | 138  | *Phenakite, Be <sub>2</sub> SiO <sub>4</sub> .....   | 8               | 11   |
| Libethenite, Cu <sub>2</sub> (OH)PO <sub>4</sub> .....   | 17m             | 30   | Picromerite, K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....   | 8m              | 54   |
| *Liddicoatite, Ca(Li,Al) <sub>3</sub> Al <sub>6</sub> B <sub>3</sub> Si <sub>6</sub> O <sub>27</sub><br>(O,OH) <sub>3</sub> (OH,F) .....   | 16m             | 42   | *Pirssonite, Na <sub>2</sub> Ca(CO <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O .....  | 9m              | 106  |
| Lime, CaO .....  | 1               | 43   | Platinum, Pt .....   | 1               | 31   |
| Lime, CaO (calculated pattern) .....   | 14m             | 49   | Portlandite, Ca(OH) <sub>2</sub> .....   | 1               | 58   |
| *Linarite, CuPb(OH) <sub>2</sub> (SO <sub>4</sub> ) .....  | 16m             | 34   | Potash alum, KAl(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....  | 6               | 36   |
| Litharge, PbO (red) .....  | 2               | 30   | Powellite, CaMoO <sub>4</sub> .....  | 6               | 22   |
| Lithiophosphate, Li <sub>3</sub> PO <sub>4</sub> .....   | 4m              | 21   | Pyrargyrite, Ag <sub>3</sub> SbS <sub>3</sub> .....  | 5m              | 51   |
| Loellingite, FeAs <sub>2</sub> .....   | 10              | 34   | Pyrite, FeS <sub>2</sub> .....   | 5               | 29   |
| Loeweite, Na <sub>12</sub> Mg <sub>7</sub> (SO <sub>4</sub> ) <sub>13</sub> ·15H <sub>2</sub> O .....  | 14m             | 35   | *Pyroaurite, Mg <sub>6</sub> Fe <sub>2</sub> CO <sub>3</sub> (OH) <sub>16</sub> ·4H <sub>2</sub> O .....   | 10m             | 104  |
| Lopezite, K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> .....  | 15m             | 47   | Pyrolusite, β-MnO <sub>2</sub> .....   | 10m             | 39   |
| *Loveringite, Ca. <sub>.72</sub> RE. <sub>.33</sub> (Y,Th,U,<br>Pb). <sub>.05</sub> Ti <sub>.12</sub> . <sub>.48</sub> Fe <sub>.33</sub> . <sub>.38</sub> Cr <sub>.24</sub> Mg. <sub>.92</sub><br>Zr. <sub>.58</sub> Al. <sub>.39</sub> V. <sub>.21</sub> Mn. <sub>.04</sub> O. <sub>.38</sub> ..... | 16m             | 106  | Pyrope, Mg <sub>3</sub> Al <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub> .....   | 4m              | 24   |
| Lueshite, NaNbO <sub>3</sub> .....   | 18m             | 64   | Pyrophanite, MnTiO <sub>3</sub> .....  | 15m             | 42   |
| Macedonite, PbTiO <sub>3</sub> .....   | 5               | 39   | *Quartz, SiO <sub>2</sub> (α or low) .....   | 3               | 24   |
| Magnesiochromite, MgCr <sub>2</sub> O <sub>4</sub> .....   | 9               | 34   | Quartz, low, α-SiO <sub>2</sub> .....  | 18m             | 61   |
| Magnesite, MgCO <sub>3</sub> .....   | 7               | 28   | Rammelsbergite, NiAs <sub>2</sub> .....  | 10              | 42   |
| Magnetite, Fe <sub>3</sub> O <sub>4</sub> .....  | 5m              | 31   | Retgersite, NiSO <sub>4</sub> ·6H <sub>2</sub> O .....   | 7               | 36   |
| Malachite, Cu <sub>2</sub> (OH) <sub>2</sub> CO <sub>3</sub> .....   | 10              | 31   | Rhodochrosite, MnCO <sub>3</sub> .....   | 7               | 32   |
| Malladrite, Na <sub>2</sub> SiF <sub>6</sub> .....   | 16m             | 68   | Rokuhnite, FeCl <sub>2</sub> ·2H <sub>2</sub> O .....  | 11m             | 32   |
| Manganolangbeinite, K <sub>2</sub> Mn <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....   | 6m              | 43   | Romarchite, SnO .....  | 4               | 28   |
| Manganosite, MnO .....   | 5               | 45   | *Roscherite, (monoclinic),<br>Be <sub>2</sub> Ca(Fe. <sub>.3</sub> Mg. <sub>.7</sub> ) <sub>2</sub> Al. <sub>.67</sub> (PO <sub>4</sub> ) <sub>3</sub> (OH) <sub>3</sub> ·<br>2H <sub>2</sub> O .....  | 16m             | 96   |
| Marshite, CuI .....  | 4               | 38   | *Roscherite, (triclinic), Be <sub>4</sub> Ca <sub>2</sub><br>(Mn <sub>.3</sub> . <sub>.91</sub> Mg. <sub>.04</sub> Ca. <sub>.05</sub> )(Al. <sub>.13</sub> Fe. <sub>.42</sub> Mn. <sub>.12</sub> )<br>(PO <sub>4</sub> ) <sub>6</sub> (OH) <sub>4</sub> ·6H <sub>2</sub> O ..... | 16m             | 100  |
| Mascagnite, (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> .....  | 9               | 8    | Rutile, TiO <sub>2</sub> .....   | 7m              | 83   |
| Massicot, PbO (yellow) .....   | 2               | 32   | Safflorite, CoFeAs <sub>4</sub> .....  | 10              | 28   |
| Matlockite, PbFCl .....  | 13m             | 25   | Salammoniac, NH <sub>4</sub> Cl .....  | 1               | 59   |
| Matteuccite, NaHSO <sub>4</sub> ·H <sub>2</sub> O .....  | 9m              | 52   | Sanbornite, β-BaSi <sub>2</sub> O <sub>5</sub> .....   | 13m             | 10   |
| Mayenite, Ca <sub>12</sub> Al <sub>14</sub> O <sub>33</sub> .....  | 9               | 20   | Sanmartinitite, ZnWO <sub>4</sub> .....  | 2m              | 40   |
| Melanterite, FeSO <sub>4</sub> ·7H <sub>2</sub> O .....  | 8m              | 38   | Scacchite, MnCl <sub>2</sub> .....   | 8m              | 43   |
| *Melpianite,<br>Na. <sub>.63</sub> Ca <sub>1.37</sub> BeAl. <sub>.13</sub> Si <sub>1.87</sub> O <sub>6.25</sub> F. <sub>.75</sub>  | 8m              | 135  | *Scheelite, CaWO <sub>4</sub> .....  | 6               | 23   |
| Merwinite, Ca <sub>3</sub> Mg(SiO <sub>4</sub> ) <sub>2</sub> .....  | 20m             | 34   | Schultenite, PbHASO <sub>4</sub> .....   | 14m             | 18   |
| Metaborite, HBO <sub>2</sub> .....   | 4m              | 27   | Selenium, Se .....   | 5               | 54   |
| Metacinnabar, HgS .....  | 4               | 21   | Selenolite, SeO <sub>2</sub> .....   | 7m              | 60   |
| Miargyrite, AgSbS <sub>2</sub> .....   | 5m              | 49   | Sellaite, MgF <sub>2</sub> .....   | 4               | 33   |
| *Millerite, NiS .....  | 1m              | 37   | Senarmontite, Sb <sub>2</sub> O <sub>3</sub> .....   | 3               | 31   |
| Minium, Pb <sub>3</sub> O <sub>4</sub> .....   | 8               | 32   | Shcherbinaite, V <sub>2</sub> O <sub>5</sub> .....   | 8               | 66   |
| Mitscherlichite, K <sub>2</sub> CuCl <sub>4</sub> ·2H <sub>2</sub> O .....   | 9m              | 34   | *Siderite, FeCO <sub>3</sub> .....   | 15m             | 32   |
| Molybdenite, MoS <sub>2</sub> .....  | 5               | 47   | Silver, Ag .....   | 1               | 23   |
| Molybdite, MoO <sub>3</sub> .....  | 3               | 30   | Silver, Ag (reference standard) .....  | 8m              | 2    |
| Molybdite, MoO <sub>3</sub> (calculated<br>pattern) .....  | 20m             | 118  | *Sjögrenite, Mg <sub>6</sub> Fe <sub>2</sub> CO <sub>3</sub> (OH) <sub>16</sub> ·4H <sub>2</sub> O .....   | 10m             | 103  |
|  |                 |      | Skutterudite, CoAs <sub>3</sub> .....  | 10              | 21   |

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| *Smithsonite, ZnCO <sub>3</sub> .....  | 8               | 69   |
| Soda alum, NaAl(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....   | 15m             | 68   |
| *Sodalite, Na <sub>8</sub> Si <sub>6</sub> Al <sub>6</sub> O <sub>24</sub> Cl <sub>2</sub> .....                   | 7m              | 158  |
| Soda niter, NaNO <sub>3</sub> .....  | 6               | 50   |
| Sphaerocobaltite, CoCO <sub>3</sub> .....  | 10              | 24   |
| Sphalerite, ZnS .....  | 2               | 16   |
| Spinel, MgAl <sub>2</sub> O <sub>4</sub> .....   | 9m              | 25   |
| Stibnite, Sb <sub>2</sub> S <sub>3</sub> .....   | 5               | 6    |
| Stilleite, ZnSe .....  | 3               | 23   |
| Stolzite, PbWO <sub>4</sub> .....  | 5m              | 34   |
| Strontianite, SrCO <sub>3</sub> .....  | 3               | 56   |
| Struvite, MgNH <sub>4</sub> PO <sub>4</sub> ·6H <sub>2</sub> O .....   | 3m              | 41   |
| Sulfur, S (orthorhombic) .....   | 9               | 54   |
| Sylvite, KCl .....   | 1               | 65   |
| Syngenite, K <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub> ·H <sub>2</sub> O .....                                | 14m             | 25   |
| Szmikite, MnSO <sub>4</sub> ·H <sub>2</sub> O .....  | 16m             | 49   |
| Tellurantimony, Sb <sub>2</sub> Te <sub>3</sub> .....  | 3m              | 8    |
| *Tellurite, TeO <sub>2</sub> .....   | 9               | 57   |
| Tellurium, Te .....  | 1               | 26   |
| Tellurobismuthite, Bi <sub>2</sub> Te <sub>3</sub> .....   | 3m              | 16   |
| Tenorite, CuO .....  | 1               | 49   |
| Teschemacherite, NH <sub>4</sub> HCO <sub>3</sub> .....  | 9               | 5    |
| Thenardite, Na <sub>2</sub> SO <sub>4</sub> .....  | 2               | 59   |
| Thermonatrite, Na <sub>2</sub> CO <sub>3</sub> ·H <sub>2</sub> O .....   | 8               | 54   |
| *Thomsenolite, NaCaAlF <sub>6</sub> ·H <sub>2</sub> O .....  | 8m              | 132  |
| Thorianite, ThO <sub>2</sub> .....   | 1               | 57   |
| Thortveitite, Sc <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> .....   | 7m              | 58   |
| Tiemannite, HgSe .....   | 7               | 35   |
| Tin, α-Sn (cubic) .....  | 2               | 12   |
| Tin, β-Sn (tetragonal) .....   | 1               | 24   |
| *Topaz, Al <sub>2</sub> SiO <sub>4</sub> (F,OH) <sub>2</sub> .....   | 1m              | 4    |
| Trevorite, NiFe <sub>2</sub> O <sub>4</sub> .....  | 10              | 44   |
| Trippkeite, CuAs <sub>2</sub> O <sub>4</sub> .....   | 16m             | 120  |
| *Trona, Na <sub>3</sub> H(CO <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O .....                                  | 15m             | 71   |
| Tschermigite, NH <sub>4</sub> Al(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O ...                            | 6               | 3    |
| Tungstenite, WS <sub>2</sub> .....   | 8               | 65   |
| Ulvöspinel, Fe <sub>2</sub> TiO <sub>4</sub> .....   | 20m             | 61   |
| Unnamed mineral,<br>K <sub>1.16</sub> Ba <sub>.72</sub> Fe <sub>.36</sub> Ti <sub>5.58</sub> O <sub>13</sub> ..... | 16m             | 147  |
| Uraninite, UO <sub>2</sub> .....   | 2               | 33   |
| Uvarovite, Ca <sub>3</sub> Cr <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub> .....                                  | 10              | 17   |
| *Valentinite, Sb <sub>2</sub> O <sub>3</sub> .....   | 10              | 6    |
| Vanthoffite, Na <sub>6</sub> Mg(SO <sub>4</sub> ) <sub>4</sub> .....   | 15m             | 72   |
| Villiaumite, NaF .....   | 1               | 63   |
| Vivianite, Fe <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O .....                                | 16m             | 38   |
| Wakefieldite, YVO <sub>4</sub> .....   | 5m              | 59   |
| Willemite, Zn <sub>2</sub> SiO <sub>4</sub> .....  | 7               | 62   |
| Witherite, BaCO <sub>3</sub> .....   | 2               | 54   |
| Wulfenite, PbMoO <sub>4</sub> .....  | 7               | 23   |
| Wurtzite, ZnS .....  | 2               | 14   |
| *Xanthoconite, Ag <sub>3</sub> AsS <sub>3</sub> .....  | 8m              | 126  |
| Xenotime, YPO <sub>4</sub> .....   | 8               | 67   |
| Yavapaiite, KFe(SO <sub>4</sub> ) <sub>2</sub> .....   | 16m             | 59   |
| Zinc, Zn .....   | 1               | 16   |
| Zincite, ZnO .....   | 2               | 25   |
| *Zincobotryogen, (Zn,Mg,Mn)Fe(SO <sub>4</sub> ) <sub>2</sub><br>(OH)·7H <sub>2</sub> O .....                       | 20m             | 67   |
| Zinkosite, ZnSO <sub>4</sub> .....   | 7               | 64   |
| *Zircon, ZrSiO <sub>4</sub> .....  | 4               | 68   |
| Zircosulfate, Zr(SO <sub>4</sub> ) <sub>2</sub> ·4H <sub>2</sub> O .....   | 7               | 66   |



|  |  |   |  |   |
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| <b>12. KEY WORDS</b> (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)<br>crystal structure; densities; lattice constants; powder patterns; reference intensities; standard; x-ray diffraction.  |  |   |  |   |
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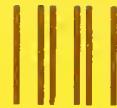
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