



NBS MONOGRAPH **25—SECTION 19**

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

Standard X-ray Diffraction Powder Patterns

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

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CONTENTS

	Page	Page
Introduction	1	71
Experimental patterns:		
Aluminum yttrium oxide, AlY_3	7	73
Aluminum yttrium oxide, $\text{Al}_2\text{Y}_4\text{O}_9$	9	75
Aluminum yttrium oxide, $\text{Al}_5\text{Y}_3\text{O}_{12}$	11	
Ammonium cadmium phosphate hydrate, $\text{NH}_4\text{CdPO}_4 \cdot \text{H}_2\text{O}$	13	77
Barium aluminum titanium oxide, $\text{BaAl}_6\text{TiO}_{12}$	14	79
Barium aluminum titanium oxide, $\text{Ba}_3\text{Al}_{10}\text{TiO}_{20}$	16	81
Barium boride, BaB_6	18	83
Barium neodymium titanium oxide, $\text{BaNd}_2\text{Ti}_5\text{O}_{14}$	19	85
Barium tungsten oxide, Ba_3W_6	21	86
Beryllium carbide, Be_2C	23	
Cadmium iodide, $\alpha\text{-CdI}_2$	24	
Calcium aluminum oxide hydrate, $\text{Ca}_4\text{Al}_6\text{O}_{13} \cdot 3\text{H}_2\text{O}$	25	88
Calcium aluminum silicate hydrate, chabazite, $\text{Ca}_2\text{Al}_4\text{Si}_8\text{O}_{24} \cdot 12\text{H}_2\text{O}$	27	
Calcium silicate (larnite), $\beta\text{-Ca}_2\text{SiO}_4$	29	
Calcium silicon fluoride hydrate, $\text{CaSiF}_6 \cdot 2\text{H}_2\text{O}$	31	90
Cesium iodide, CsI_3	33	106
Cesium molybdenum oxide, $\text{Cs}_2\text{Mo}_3\text{O}_{10}$..	35	109
Chromium boride, CrB_2	37	
Chromium niobium oxide, CrNbO_4	38	112
Cobalt arsenate hydrate (erythrite), $\text{Co}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$	39	
Cobalt phosphate hydrate, $\text{Co}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$	40	
Erbium iron, ErFe_2	42	
Ethylenediamine Hydrochloride, $\text{C}_2\text{H}_8\text{N}_2 \cdot 2\text{HCl}$	43	
Ethylenediaminetetraacetic Acid, $\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_8$	45	
Hafnium nitride, HfN	46	
p-Iodobenzoic Acid, $\text{C}_7\text{H}_5\text{IO}_2$	47	
Iron aluminum oxide (hercynite), FeAl_2O_4	48	
Iron antimony oxide, FeSbO_4	49	
Iron chromium oxide (chromite), FeCr_2O_4	50	
Lithium zirconium oxide, Li_2ZrO_3	51	
Magnesium arsenate hydrate (hoernesite), $\text{Mg}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$	53	
Magnesium phosphate (farringtonite), $\text{Mg}_3(\text{PO}_4)_2$	55	
Manganese tartrate, $\text{C}_4\text{H}_4\text{MnO}_6$	57	
Molybdenum silicide, Mo_5Si_3	59	
Nickel arsenate hydrate (annabergite), $\text{Ni}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$	60	
Nickel molybdenum oxide, NiMoO_4	62	
Nickel phosphate hydrate, $\text{Ni}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$	64	
Nickel sulfate hydrate (nickel-hexa- hydrite), $\beta\text{-NiSO}_4 \cdot 6\text{H}_2\text{O}$	65	
Niobium, Nb	67	
Potassium barium phosphate, KBaPO_4	68	
Potassium calcium phosphate, KCaPO_4	70	
Calculated pattern:		
Phenobarbital hydrate, $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_3 \cdot \text{H}_2\text{O}$	21	88
Cumulative indices		
(Circular 539, Volumes 1-10 and Monograph 25, Sections 1-19 inclusive)	29	
1. Inorganic		90
2. Organic formula		106
3. Organic name		109
4. Mineral		112

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Publications Available

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

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

NBS Publication	Order Number	NBS Publication	Order Number
Circular 539, Volume 1.....	PB 178 902	Monograph 25, Section 1.....	PB 178 429
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		Section 11.....	COM 74-50183
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	<u>Catalog Number</u>	<u>Price</u>
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ERRATA

Circular 539

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

Monograph 25

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

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

p. 32: Z should be 4.

p. 34: Density should be 1.608.

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

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

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

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

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

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

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 19 --- Data for 51 Substances

by

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

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

INTRODUCTION

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

EXPERIMENTAL POWDER PATTERNS

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

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

¹JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081. This Pennsylvania non-profit corporation functions in co-operation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

²See previous page for other published volumes.

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

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

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

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

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

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

Table 1

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

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

Table 2

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

All data were collected at $25 \pm 1^\circ\text{C}$ on a diffractometer equipped with a focusing graphite crystal monochromator located between the sample

and the scintillation counter. Pulse height discrimination was used as well. The data were collected using copper radiation: $\lambda(\text{CuK}\alpha_1, \text{peak}) = 1.540598\text{\AA}$ [Deslattes and Henins, 1973].

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

Manual patterns were measured on a diffractometer equipped with a strip chart recorder. The readings of 2θ were taken at positions about 20% of the way down from the top, and in the center of the peak width. This avoided errors associated with aberrations at the very top of the peaks. The $\text{K}\alpha_2$ peaks were occasionally read to assist in establishing a $\text{K}\alpha_1$ peak position, but $\text{K}\alpha_2$ peaks are not reported.

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

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

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

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

At low angles, $\text{K}\alpha_1$ 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. For the manual patterns, if the internal standard correction varied along the length of the pattern, linear interpolations were used.

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

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

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

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

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

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

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

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

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

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

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

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

N , the number of observed reflections was chosen as 30, or as the maximum number of lines of the pattern if the pattern had fewer than 30 lines.

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

Intensity measurements. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentage of the strongest line. It has been found that samples which give satisfactory intensity patterns usually have an average particle size smaller than $10 \mu\text{m}$, 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, σ , in the relative intensity values was calculated from the values of the five strongest lines, excluding the line with $I^{rel}=100$.

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

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 σ_i was multiplied by the conversion factor

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

Reference intensity ratio, I/I_c corundum. The reference intensity ratio, I/I_c , has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the 113 (hexagonal) reflection of corundum (α -Al₂O₃) [Visser and de Wolff, 1964]. In this publication the ratios I/I_c are tabulated for copper K α_1 radiation, for a 1:1 mixture by weight of the sample and corundum. I/I_c was determined only for very common phases.

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

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

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

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

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

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

UNITS

In this publication the Ångström unit ($1\text{\AA} = 100 \text{ pm}$) 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 Å³ ($1\text{\AA}^3 = 1 \times 10^{-30} \text{ m}^3$). Densities are reported in g/cm³ ($1 \text{ gm/cm}^3 = 10^3 \text{ kg/m}^3$).

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REFERENCES

- Alexander, L., Klug, H. P., and Kummer, E. (1948). *J. Appl. Phys.*, 19, No. 8, 742.
- Chemical Abstracts Service Registry Handbook - Number Section (1974), (The American Chemical Society, Chemical Abstracts Service, The Ohio State Univ., Columbus, OH 43210).
- Crystal Data (1973). (3rd Ed. Published jointly by the U.S. Dept. of Commerce, Natl. Bur. of Stand., Washington, D.C. 20234, and the Joint Committee on Powder Diffraction Standards, 1601 Park Lane, Swarthmore, PA 19081).
- Daniels, R. W. (1978). An Introduction to Numerical Methods and Optimization Techniques, (Elsevier North-Holland Inc., New York), 78.
- Deslattes, R. D. and Henins, A. (1973). *Phys. Rev. Lett.* 31, 972.
- Deslattes, R. D., Henins, A., Bowman, H. A., Schoonover, R. M., Carroll, C. L., Barnes, I. L., Machlan, L. A., Moore, L. J., and Shields, W. R. (1974). *Phys. Rev. Lett.* 33, 463.
- Donnay, J. D. H. and Hennard, O. (1964). *Acta Crystallogr.* 17, 1337.
- Evans, H. T., Jr., Appleman, D. E., and Handwerker, D. S. (1963). Report #PB216188, U.S. Dept. of Commerce, National Technical Information Center, 5285 Port Royal Rd., Springfield, VA 22151, \$3.50.
- Groth, P. (1908). Chemische Kristallographie II, (Engelmann, Leipzig, Germany).
- Hartshorne, N. H. and Stuart, A. (1970). Crystals and the Polarizing Microscope, (Edward Arnold and Co., London, 4th Ed.).
- Hubbard, C. R. (1982a). *J. Appl. Cryst.* Accepted for Publication.
- Hubbard, C. R. (1982b). *J. Appl. Cryst.* Submitted for Publication.
- Hubbard, C. R. and Smith, D. K. (1977). Advances in X-ray Analysis, (Plenum Publishing Corporation, 227 West 17th St., New York, NY 10011), 20, 27.
- International Tables for X-ray Crystallography, I (1965), (The Kynoch Press, Birmingham, Eng.).
- International Union of Pure and Applied Chemistry (1979). *Pure Appl. Chem.* 51, No. 2, 407.
- ISCC-NBS Centroid Color Charts, SRM 2106 (1965), or Color Kit, SRM 2107 (1977) which contains both SRM 2106 and Color, an NBS Special Publication #SP 440. These can be obtained from the Natl. Bur. of Stand., Office of Standard Reference Materials, Washington, DC 20234. Current prices will be quoted on request.
- Mighell, A. D., Hubbard, C. R., and Stalick, J. K. (1981). NBS Technical Note 1141, U. S. Dept. of Commerce, Natl. Bur. Stand., Washington, DC 20234.
- Palache, C., Berman, H., and Frondel, C. (1944). Dana's System of Mineralogy I, (John Wiley and Sons, New York, 7th Ed.), 6.
- Savitzky, A. and Golay, M. J. E. (1964). *Anal. Chem.* 36, 1627.
- Smith, G. S. and Snyder, R. L. (1979). *J. Appl. Crystallogr.* 12, 60.
- Snyder, R. L., Hubbard, C. R., and Panagiotopoulos, N. C. (1981). Auto: A Real Time Diffractometer Control System Report, NBSIR 81-2229, U. S. Dept. of Commerce, Natl. Bur. Stand., Washington, DC 20234).
- Standard Reference Material 640a (1982), Silicon Powder X-ray Diffraction Standard, obtainable from the Natl. Bur. of Stand., Office of Standard Reference Materials, Washington, DC 20234. Current price will be quoted on request.
- Standard Reference Material 675 (1982), Fluorophlogopite Powder X-ray Diffraction Standard. To obtain, see procedure above for SRM 640a.
- Standard X-ray Diffraction Powder Patterns (1982), see page iv of this Monograph.
- Visser, J. W. (1969). *J. Appl. Crystallogr.* 2, 89.
- Visser, J. W. and de Wolff, P. M. (1964). "Absolute Intensities," Report 641.109, Technisch Physische Dienst, Delft, Netherlands.
- Wolff, de, P. M. (1968). *J. Appl. Crystallogr.* 1, 108.

Aluminum Yttrium Oxide, Al₂YO₅

Synonym

Yttrium aluminate

CAS registry no.

12003-86-0

Sample

The sample was prepared at NBS. Calculated amounts of Al₂O₃ and Y₂O₃ were mixed and heated at 1675 °C for 1 day. The composition was adjusted to approach the 1:1 phase, and the mixture was reheated at 1600 °C for 4 days and at 1675 °C for 3 days. The compound was ground daily during the process.

Color

Yellowish white

Structure

Orthorhombic, Pnma (62), Z = 4, isostructural with GdFeO₃ and YFeO₃ (Geller and Wood, 1956). The structure of GdFeO₃ was determined by Geller (1956). Coppens and Eibschütz (1965) refined the centric structure of GdFeO₃ and YFeO₃. The latter was refined also in the alternative non-centrosymmetric space group Pn2₁a (33), and that refinement showed small, possibly real, deviations from a centric structure.

Lattice constants of this sample

a = 5.3286(4) Å
b = 7.3706(5)
c = 5.1796(3)

a/b = 0.7230
c/b = 0.7027

Volume
203.43 Å³

Density
(calculated) 5.351 g/cm³

Polymorphism

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

Figure of merit

F₃₀ = 92.6(0.010,33)

Additional patterns

PDF card 11-662 (Roth, 1957)

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

Geller and Wood (1956)

Keith and Roy (1954). The pattern in table 4 labeled 3Y₂O₃·5Al₂O₃, YCrO₃ type, seems to be the phase reported here.

References

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

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

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

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

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

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

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

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

Aluminum Yttrium Oxide, Al₂Y₃O₁₂ - (continued)

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

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

Aluminum Yttrium Oxide, $\text{Al}_2\text{Y}_4\text{O}_9$

Synonym

Yttrium Aluminate

Sample

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

Color

Very pale yellowish white

Structure

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

Comment

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

Lattice constants of this sample

$a = 11.1156(16)\text{\AA}$
 $b = 10.4689(16)$
 $c = 7.3791(9)$
 $\beta = 108.61(1)^\circ$

$a/b = 1.0618$
 $c/b = 0.7049$

Volume
 813.79 \AA^3

Density

(calculated) 4.518 g/cm^3

Figure of merit

$F_{30} = 22.9(0.015, 86)$

Additional patterns

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

Warshaw and Roy (1959)

Abell et al. (1974)

References

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

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

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

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

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

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

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

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

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

Synonyms

Yttrium aluminate
Yttrogarnet

CAS registry no.
12005-21-9

Sample

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

Color

Colorless

Structure

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

Lattice constant of this sample

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

Volume
 1731.85 \AA^3

Density
(calculated) 4.552 g/cm^3

Polymorphism

Yoder and Keith (1951) reported that yttrium garnet inverts to a high temperature form, yttriumalumite, at $1970^\circ \pm 50$ °C.

Figure of merit

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

Additional patterns

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

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

References

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

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

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

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

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

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

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

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 5.8173(10) \text{\AA}$$

$$b = 8.8797(8)$$

$$c = 5.0134(8)$$

$$a/b = 0.6551$$

$$c/b = 0.5646$$

Volume cm^3
 258.97 \AA^3

Density

(calculated) 3.122 g/cm^3

Figure of merit

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

Additional patterns

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

Ropp and Mooney (1960)

References

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

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

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

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

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

Barium Aluminum Titanium Oxide, BaAl₆TiO₁₂

Synonym

Barium aluminum titanate

CAS registry no.

58834-02-9

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 7.1375(3) \text{ } \text{\AA}$$

$$b = 13.5978(8)$$

$$c = 4.8651(2)$$

$$a/b = 0.5249$$

$$c/b = 0.3578$$

Volume

$$472.18 \text{ } \text{\AA}^3$$

Density

$$(\text{calculated}) 3.792 \text{ g/cm}^3$$

Figure of merit

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

Additional pattern

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

References

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

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

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

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

Barium Aluminum Titanium Oxide, BaAl₆TiO₁₂ - (continued)

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

Barium Aluminum Titanium Oxide, $\text{Ba}_3\text{Al}_{10}\text{TiO}_{20}$

Synonym

Barium aluminum titanate

CAS registry no.

58834-01-8

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 14.8884(12)\text{\AA}$$

$$b = 11.3676(13)$$

$$c = 4.9781(5)$$

$$\beta = 90.84(1)^\circ$$

$$a/b = 1.3097$$

$$c/b = 0.4379$$

Volume
 842.43 \AA^3

Density

(calculated) 4.138 g/cm^3

Figure of merit

$$F_{30} = 53.24(0.010, 55)$$

Additional pattern

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

References

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

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

$\text{CuK}\alpha_1$ $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$				
Internal standard Ag, $a = 4.08651 \text{ \AA}$				
$d(\text{\AA})$	I^{rel}		hkl	$2\theta (^\circ)$
$\sigma = \pm 3$				
5.683	23	0 2 0		15.58
4.741	2	-1 0 1		18.70
4.560	34	0 1 1		19.45
3.912	1	-2 1 1		22.71
3.869	1	2 1 1		22.97

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

Barium Aluminum Titanium Oxide, Ba₃Al₁₀TiO₂₀ - (continued)

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

Barium Boride, BaB₆

Synonym

Barium hexaboride

Sample

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

Color

Very dark gray

Structure

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

Lattice constant of this sample

a = 4.2624(1) \AA

Volume
77.44 \AA^3

Density

(calculated) 4.336 g/cm³

Figure of merit

F₂₄ = 106.1(0.009, 24)

Additional pattern

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

References

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

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

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

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

Barium Neodymium Titanium Oxide, BaNd₂Ti₅O₁₄

Synonym

Barium neodymium titanate

Sample

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

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 12.1983(13)\text{\AA}$$

$$b = 22.347(3)$$

$$c = 3.8403(6)$$

$$a/b = 0.5459$$

$$c/b = 0.1718$$

Volume cm^3
1046.8 \AA^3

Density

(calculated) 5.643 g/cm³

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

Figure of merit

$$F_{30} = 50.1(0.012, 50)$$

Additional pattern

Kolar et al. (1981)

Reference

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

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

CuK α_1 $\lambda = 1.540598 \text{\AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$					
Internal standard Ag, $a = 4.08651 \text{\AA}$					
$d(\text{\AA})$	I^{rel}	hkl			$2\theta(\text{°})$
		$\sigma = \pm 4$			
11.20	12	0	2	0	7.89
10.73	5	1	1	0	8.23
8.25	1L	1	2	0	10.71
6.36	3	1	3	0	13.91
6.10	1	2	0	0	14.51

Barium Neodymium Titanium Oxide, BaNd₂Ti₅O₁₄ - (continued)

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

$d(\text{\AA})$	I^{rel}	hkl			$2\theta(^{\circ})$
$\sigma = \pm 4$					
1.4859	3	3	14	0	62.45
1.4741+	3	0	14	1	63.01
1.4741+		2	9	2	63.01
1.4686	3	4	12	1	63.27
1.4559+	1	0	10	2	63.89
1.4559+		6	9	1	63.89
1.4429	1L	8	5	0	64.53
1.4293	1	5	5	2	65.22
1.4235	1	3	9	2	65.52
1.3962M	2	0	16	0	66.97
1.3962M		6	0	2	66.97
1.3856M	8	3	14	1	67.55
1.3856M		6	2	2	67.55
1.3761	4	8	7	0	68.08
1.3722	6	6	3	2	68.30
1.3640	4	5	7	2	68.77

Barium Tungsten Oxide, Ba₃WO₆

Synonyms

Barium tungstate
Tribarium tungstate

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

a = 17.1765(5) Å

Comment

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

Volume
5067.6 Å³
Density
(calculated) 7.254 g/cm³ (based on 3:1 ratio)

Figure of merit
F₃₀ = 68.2(0.012,38)

Additional patterns

PDF card 25-82 (Kreidler, 1972)

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

Chang et al., (1966)

References

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

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

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

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

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

Barium Tungsten Oxide, Ba₃W₆O₁₃ - (continued)

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

Beryllium Carbide, Be₂C

CAS registry no.
506-66-1

Sample

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

Color

Grayish yellow brown

Structure

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

Lattice constant of this sample

a = 4.3422(1) Å

Volume
81.872 Å³

Density
(calculated) 2.437 g/cm³

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

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

References

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

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

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

Cadmium Iodide, α -CdI₂

CAS registry no.
7790-80-9

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 4.2481(3) \text{ \AA}$$

$$c = 13.7265(8)$$

$$c/a = 3.2312$$

Volume

$$214.53 \text{ \AA}^3$$

Density

$$(\text{calculated}) 5.669 \text{ g/cm}^3$$

Polymorphism

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

Figure of merit

$$F_{30} = 26.2(0.012, 92)$$

Additional patterns

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

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

Reference

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

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

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

Synonym

Tetracalcium trialuminate trihydrate

CAS registry no.

12355-68-9

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 12.422(3) \text{ Å}^{\circ}$$

$$b = 12.803(3)$$

$$c = 8.862(2)$$

$$a/b = 0.9702$$

$$c/b = 0.6922$$

Volume

$$1409.45 \text{ Å}^3$$

Density

$$(\text{calculated}) 2.753 \text{ g/cm}^3$$

Figure of merit

$$F_{30} = 52.8(0.014, 41)$$

Additional patterns

PDF card 14-464 (Pistorius, 1962)

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

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

Johnson and Thorvaldson, (1943)

References

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

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

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

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

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

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

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

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

Synonym

Calcium aluminosilicate hexahydrate

CAS registry no.

12251-32-0

Sample

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

Chemical Analysis (wt. %)

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

Color

Colorless to salmon pink

Structure

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

Lattice constants of this sample
Hexagonal axes

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

$c/a = 1.0877$
 $Z = 3$

Volume

2467.0 \AA^3

Density

(calculated) 2.045 g/cm³
(observed) 2.05(2) (Himes and Mighell, 1981)

Figure of merit

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

Additional pattern

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

References

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

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

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

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

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

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

Calcium Silicate (Larnite), $\beta\text{-Ca}_2\text{SiO}_4$

Synonyms

Beta dicalcium silicate
Belite

CAS registry no.
10034-77-2

Sample

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

Chemical analysis

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

Color

Colorless

Structure

Monoclinic, $P2_1/n$ (14), $Z = 4$. The structure of $\beta\text{-Ca}_2\text{SiO}_4$ was determined by Midgley (1952).

Lattice constants of this sample

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

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

Volume
 345.29 \AA^3

Density

(calculated) 3.313 g/cm^3

Polymorphism

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

Figure of merit

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

Additional patterns

PDF card 9-351 (Yannaquis, 1955)

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

Brownmiller and Bogue, (1930)

References

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

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

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

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

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

Calcium Silicate, (Larnite), $\beta\text{-Ca}_2\text{SiO}_4$ - (continued)

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

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

Synonym

Calcium fluorosilicate dihydrate

CAS registry no.

16961-80-1

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$a = 10.477(2)\text{\AA}$

$b = 9.1771(13)$

$c = 5.7281(13)$

$\beta = 98.98(2)^\circ$

$a/b = 1.1416$

$c/b = 0.6242$

Volume

543.99 \AA^3

Density

(calculated) 2.664 g/cm^3

Figure of merit

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

$M_{20} = 29.4$

Additional pattern

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

References

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

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

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

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

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

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

Cesium Iodide, CsI₃

Synonym

Cesium triiodide

CAS registry no.

12527-22-9

Sample

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

Color

Unground: dark purplish blue.

Ground: dark grayish reddish brown.

Structure

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

Lattice constants of this sample

a = 10.0289(9) Å

b = 11.0869(9)

c = 6.8457(8)

a/b = 0.9062

c/b = 0.6186

Volume °
761.17 Å³

Density

(calculated) 4.482 g/cm³

Figure of merit

F₃₀ = 83.5(0.007,50)

Reference

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

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

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

Cesium Iodide, CsI₃ - (continued)

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

Cesium Molybdenum Oxide, $\text{Cs}_2\text{Mo}_3\text{O}_{10}$

Synonyms

Cesium molybdate
Dicesium trimolybdate

Sample

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

Color

Colorless

Structure

Monoclinic, C2/c (15), Z = 4, isostructural with $\text{K}_2\text{Mo}_3\text{O}_{10}$. The structure of $\text{K}_2\text{Mo}_3\text{O}_{10}$ was determined by Gatehouse and Leverett (1968).

Lattice constants of this sample

$$a = 14.469(2) \text{\AA}$$

$$b = 8.4022(9)$$

$$c = 9.4609(14)$$

$$\beta = 97.73(1)^\circ$$

$$a/b = 1.7220$$

$$c/b = 1.1260$$

Volume

$$1139.7 \text{ \AA}^3$$

Density

$$(\text{calculated}) 4.159 \text{ g/cm}^3$$

Figure of merit

$$F_{30} = 94.2(0.008, 42)$$

Additional pattern

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

References

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

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

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

Cesium Molybdenum Oxide, $\text{Cs}_2\text{Mo}_3\text{O}_{10}$ - (continued)

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

$d(\text{\AA})$	I^{rel}	hkl			$2\theta(\text{\\circ})$
$\sigma = \pm 4$					
1.5476	5	-9	1	2	59.70
1.5385	6	-8	2	3	60.09
1.5332M	10	6	4	1	60.32
1.5332M		-3	3	5	60.32
1.5227+	5	-3	5	2	60.78
1.5227+		-3	1	6	60.78
1.5114	2	9	1	1	61.28
1.4982	1	8	2	2	61.88
1.4853	3	2	0	6	62.48
1.4816M	5	-1	5	3	62.65
1.4816M		3	5	2	62.65
1.4718M	1L	-2	2	6	63.12
1.4718M		6	2	4	63.12
1.4634M	4	-7	1	5	63.52
1.4634M		1	5	3	63.52
1.4612	4	-6	4	3	63.63
1.4496	1L	5	5	0	64.20
1.4398	1	-3	5	3	64.69

Chromium Boride, CrB₂

Synonym

Chromium diboride

CAS registry no.

12007-16-8

Sample

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

Color

Olive gray

Structure

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

Lattice constants of this sample
 $a = 2.9730(13)\text{\AA}$
 $c = 3.0709(2)$
 $c/a = 1.0329$
Volume
 23.506 \AA^3
Density

 (calculated) 5.200 g/cm³
Figure of merit
 $F_{20} = 94.4(0.011, 20)$

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

Additional pattern

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

Chromium Niobium Oxide, CrNbO₄

Synonyms

Niobium chromium oxide
Chromium niobate

CAS registry no.
58500-35-9

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

Color
Gray olive

Structure
Tetragonal, P4₂/mnm (136), Z = 1. Rutile structure (Brandt, 1943). The structure of CrNbO₄ is discussed by Khazai et al. (1981).

Lattice constants of this sample

$$a = 4.6443(2) \text{ Å}$$

$$c = 3.0125(3)$$

$$c/a = 0.6486$$

Volume A^3
64.977

Density
(calculated) 5.338 g/cm³

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

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

Additional patterns

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

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

References

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

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

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

$\text{CuK}\alpha_1$ $\lambda = 1.540598 \text{ Å}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$					
Internal standard W, $a = 3.16524 \text{ Å}$					
$d(\text{Å})$	I^{rel}	hkl		$2\theta (\text{°})$	
		$\sigma = \pm 1$			
3.283	100	1	1	0	27.14
2.528	65	1	0	1	35.48
2.322	15	2	0	0	38.75
2.220	11	1	1	1	40.60
2.077	4	2	1	0	43.54

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

Synonym

Cobalt orthoarsenate octahydrate

CAS registry no.

54496-59-2

Sample

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

Spectrographic analysis

Major impurities

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

Color

Medium purplish pink

Structure

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

Lattice constants of this sample

$$a = 10.118(5)\text{\AA}$$

$$b = 13.433(4)$$

$$c = 4.762(2)$$

$$\beta = 101.90(3)^\circ$$

$$a/b = 0.7532$$

$$c/b = 0.3545$$

Volume
 633.32 \AA^3

Density
(calculated) 3.140 g/cm^3

Comment

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

Figure of merit

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

Additional pattern

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

References

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

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

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

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

Synonym

Cobalt orthophosphate octahydrate

CAS registry no.

10294-50-5

Sample

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

Color

Unground: deep red

Ground: moderate pale red

Structure

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

Lattice constants of this sample

$a = 9.9265(14)\text{\AA}$

$b = 13.3360(14)$

$c = 4.6786(7)$

$\beta = 102.310(12)^\circ$

$a/b = 0.7443$

$c/b = 0.3508$

Volume

605.11 \AA^3

Density

(calculated) 2.804 g/cm^3

Figure of merit

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

Additional pattern

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

References

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

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

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ \text{C}$				
Internal standard Ag, $a = 4.08651 \text{ \AA}$				
$d(\text{\AA})$	I^{rel}	hkl	$2\theta (\circ)$	
$\sigma = \pm 3$				
7.852	23	1 1 0	11.26	
6.667	100	0 2 0	13.27	
4.849	25	2 0 0	18.28	
4.521	15	-1 0 1	19.62	
4.323	6	0 1 1	20.53	

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

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

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

Erbium Iron, ErFe₂

Synonym

Erbium diiron

CAS registry no.

12060-15-4

Sample

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

Color

Dark grayish olive

Structure

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

Lattice constant of this sample

a = 7.2777(2) Å

Volume

385.46 Å³

Density

(calculated) 9.614 g/cm³

Figure of merit

F₂₃ = 63.8(0.014,26)

Additional pattern

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

Reference

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

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

Ethylenediamine Hydrochloride, C₂H₈N₂·2HCl

Synonyms

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

CAS registry no.
20273-40-9

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

Color
Colorless

Structure
Monoclinic, P₂₁/a (14), Z = 2. The structure was determined by Ashida and Hirokawa (1963).

Lattice constants of this sample

a = 9.9683(13) Å
b = 6.8913(12)
c = 4.4293(6)
β = 91.311(12)°

a/b = 1.4465
c/b = 0.6427

Volume
304.19 Å³

Density
(calculated) 1.452 g/cm³

Figure of merit
F₃₀ = 57.8(0.011,49)

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

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

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

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

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

CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C				
Internal standard Si, a = 5.43088 Å				
d(Å)	I ^{rel}	h	k	l
5.669	1	1	1	0
4.427	5	0	0	1
3.725	15	0	1	1
3.466	100	1	1	1
3.350	89	-2	0	1
				25.68
				26.59

Ethylenediamine Hydrochloride, C₂H₈N₂·2HCl - (continued)

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

Ethylenediaminetetraacetic Acid, C₁₀H₁₆N₂O₈

Synonyms

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

CAS registry no.
60-00-4

Sample

The sample was prepared at NBS and recrystallized from water.

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 16.112(3)\text{\AA}$$

$$b = 5.5774(15)$$

$$c = 13.287(3)$$

$$\beta = 96.30(2)^\circ$$

$$a/b = 2.8890$$

$$c/b = 2.3825$$

Volume
1186.8 \AA^3

Density
(calculated) 1.636 g/cm³

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

Additional pattern

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

Reference

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

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{\AA}; \text{temp. } 25 \pm 1^\circ\text{C}$				
Internal standard Ag, $a = 4.08651 \text{\AA}$				
$d(\text{\AA})$	I^{rel}	hkl	$2\theta (\text{)}^\circ$	
$\sigma = \pm 4$				
8.01	17	2 0 0	11.04	
6.59	23	0 0 2	13.42	
5.394	13	-2 0 2	16.42	
5.142	12	0 1 1	17.23	
4.960	40	-1 1 1	17.87	
4.847M	4	2 0 2	18.29	
4.847M		1 1 1	18.29	
4.412	32	-2 1 1	20.11	
4.003	100	4 0 0	22.19	
3.783	12	-3 1 1	23.50	

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

Hafnium Nitride, HfN

Synonym

Hafnium mononitride

CAS registry no.

25817-87-2

Sample

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

Color

Dark olive brown

Structure

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

Lattice constant of this sample

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

Volume

92.67 \AA^3

Density

(calculated) 13.797 g/cm^3

Figure of merit

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

Additional pattern

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

Reference

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

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$				
Internal standard Ag, $a = 4.08651 \text{ \AA}$				
d(\AA)	I ^{rel}	hkl		2 θ ($^\circ$)
$\sigma = \pm 1$				
2.612	100	1	1	1
2.262	62	2	0	0
1.6002	37	2	2	0
1.3641	33	3	1	1
1.3061	9	2	2	2
1.1314	4	4	0	0
1.0379	8	3	3	1
1.0120	10	4	2	0
.9237	7	4	2	2
.8710	7	5	1	1
				124.36

p-Iodobenzoic Acid, C₇H₅IO₂

CAS registry no.
691-58-9

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 30.087(5) \text{ \AA}$$

$$b = 6.0346(12)$$

$$c = 4.1563(9)$$

$$\beta = 90.55(2)^\circ$$

$$a/b = 4.9857$$

$$c/b = 0.6887$$

Volume

$$754.60 \text{ \AA}^3$$

Density

$$(\text{calculated}) 2.183 \text{ g/cm}^3$$

Figure of merit

$$F_{30} = 42.1(0.010, 69)$$

Additional pattern

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

References

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

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

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$				
Internal standard W, $a = 3.16524 \text{ \AA}$				
d(\AA)	I ^{rel}	hkl	2 θ ($^\circ$)	
$\sigma = \pm 3$				
15.07	100	2 0 0	5.86	
7.53	8	4 0 0	11.75	
5.604	8	2 1 0	15.80	
5.175	3	3 1 0	17.12	
4.706	57	4 1 0	18.84	
4.261	4	5 1 0	20.83	
4.124	8	-1 0 1	21.53	
3.855M	61	6 1 0	23.05	
3.855M		-3 0 1	23.05	
3.764	7	8 0 0	23.62	

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

Iron Aluminum Oxide (Hercynite), FeAl_2O_4

Synonym

Iron aluminate

CAS registry no.

12068-49-4

Sample

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

Color

Greenish gray

Structure

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

Lattice constant of this sample

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

Volume
 542.03 \AA^3
Density

(calculated) 4.260 g/cm^3

Figure of merit

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

Additional patterns

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

Clark, et al. (1931)

Fischer and Hoffmann (1955)

Krause and Thiel (1932)

References

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

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

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

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

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

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

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

Iron Antimony Oxide, FeSbO₄

Synonym

Iron antimonate

Sample

The sample was prepared at NBS.

Chemical analysis

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

Color

Medium yellowish brown

Structure

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

Lattice constants of this sample

a = 4.6352(2) Å
c = 3.0733(2)

c/a = 0.6630

Volume
 66.030 Å³
Density
 (calculated) 6.076 g/cm³
Figure of merit

F₃₀ = 61.2(0.011,43)

Comment

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

References

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

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

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

Iron Chromium Oxide (Chromite), FeCr_2O_4

Synonym

Iron chromite

CAS registry no.

12068-77-8

Sample

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

Color

Dark reddish brown

Structure

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

Lattice constant of this sample

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

Volume

588.27 \AA^3

Density

(calculated) 5.055 g/cm^3

Polymorphism

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

Figure of merit

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

Additional patterns

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

Holgersson (1927)

Hilty, et al. (1955)

References

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

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

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

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

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

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

Lithium Zirconium Oxide, Li_2ZrO_3

Synonyms

Lithium zirconate
Dilithium zirconium trioxide

CAS registry no.
12031-83-3

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 5.4266(5)\text{\AA}$$

$$b = 9.0310(8)$$

$$c = 5.4227(7)$$

$$\beta = 112.720(8)^\circ$$

$$a/b = 0.6009$$

$$c/b = 0.6005$$

Volume
 245.13 \AA^3

Density
(calculated) 4.148 g/cm^3

Figure of merit

$$F_{30} = 62.6(0.011, 43)$$

Additional pattern

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

References

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

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

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

Lithium Zirconium Oxide, Li₂ZrO₃ - (continued)

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

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

Synonym

Magnesium arsenate octahydrate

CAS registry no.

37541-75-6

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 10.137(2)\text{\AA}$$

$$b = 13.455(2)$$

$$c = 4.7542(10)$$

$$\beta = 101.73(2)^\circ$$

$$a/b = 0.7530$$

$$c/b = 0.3533$$

Volume

$$634.9 \text{ \AA}^3$$

Density

$$(\text{calculated}) 2.589 \text{ g/cm}^3$$

Figure of merit

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

Additional pattern

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

References

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

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

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

$$CuK\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ C$$

$$\text{Internal standard Si, } a = 5.43088 \text{ \AA}$$

$d(\text{\AA})$	I^{rel}	hkl	$2\theta (^\circ)$
$\sigma = \pm 3$			
7.97	31	1 1 0	11.09
6.73	100	0 2 0	13.14
4.399	48	0 1 1	20.17
3.992	26	2 2 0	22.25
3.916	16	1 0 1	22.69

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

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

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

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

Synonyms

Magnesium orthophosphate
Trimagnesium biphenylate

CAS registry no.

10043-83-1

Sample

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

Color

Colorless

Structure

Monoclinic, $P2_1/n$ (14), $Z = 2$. The structure of $\text{Mg}_3(\text{PO}_4)_2$ was determined by Nord and Kierkegaard (1968).

Lattice constants of this sample

$a = 7.5995(8)$ Å

$b = 8.2355(8)$

$c = 5.0762(5)$

$\beta = 94.062(9)^\circ$

$a/b = 0.9228$

$c/b = 0.6164$

Volume

317.42 Å³

Density

(calculated) 2.750 g/cm³

Polymorphism

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

Figure of merit

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

Additional patterns

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

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

References

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

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

Geochim. Cosmochim. Acta 24, 198.

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

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

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

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

Manganese Tartrate, $C_4H_4MnO_6$

Sample

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

Color

Pale greenish yellow

Structure

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

Lattice constants of this sample

$$a = 9.4388(8)\text{\AA}$$

$$b = 11.6925(13)$$

$$c = 5.0706(4)$$

$$a/b = 0.8073$$

$$c/b = 0.4337$$

Volume

$$559.61 \text{ \AA}^3$$

Density

(calculated) 2.410 g/cm³, assuming Z = 4.

Figures of merit

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

$$M_{20} = 40.5$$

Additional pattern

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

References

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

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

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ\text{C}$				
Internal standard Si, $a = 5.430825 \text{ \AA}$				
$d(\text{\AA})$	I^{rel}	hkl	$2\theta (\text{)}^\circ$	
$\sigma = \pm 2$				
7.34	14	1 1 0	12.04	
5.843	65	0 2 0	15.15	
4.716	12	2 0 0	18.80	
4.653	53	0 1 1	19.06	
4.467	100	1 0 1	19.86	
3.673	57	2 2 0	24.21	
3.604	20	1 3 0	24.68	
3.549	98	1 2 1	25.07	
3.313	18	2 1 1	26.89	
3.092	3	0 3 1	28.85	

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

Manganese Tartrate, C₄H₄MnO₆ - (continued)

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

Molybdenum Silicide, Mo_5Si_3

CAS registry no.
12033-40-8

Sample

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

Color
Olive black

Structure

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

Lattice constants of this sample

$a = 9.6483(6)$ Å
 $c = 4.9135(5)$

$c/a = 0.5093$

Volume
457.40 Å³

Density
(calculated) 8.190 g/cm³

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

Additional patterns

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

Nowotny et al. (1956)

References

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

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

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

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

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

Synonym

Nickel orthoarsenate octahydrate

CAS registry no.

54469-74-1

Sample

The sample was prepared at NBS. A solution of 2 gms $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ in 1 liter H_2O was added dropwise to a solution of 2 gms Na_2HAsO_4 in 1½ liters of warm H_2O . The combined solution was held at 70 to 80 °C for 3 weeks. The crystals were filtered off and washed with H_2O and $\text{C}_2\text{H}_5\text{OH}$.

Color

Light yellow green

Structure

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

Lattice constants of this sample

$$a = 10.054(2) \text{ \AA}$$

$$b = 13.303(3)$$

$$c = 4.7159(10)$$

$$\beta = 102.10(2)^\circ$$

$$a/b = 0.7558$$

$$c/b = 0.3545$$

Volume

$$616.73 \text{ \AA}^3$$

Density

$$(\text{calculated}) 3.221 \text{ g/cm}^3$$

Figure of merit

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

Additional pattern

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

References

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

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

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

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

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

Nickel Molybdenum Oxide, NiMoO₄

Synonyms

Molybdenum nickel tetraoxide
Nickel molybdate

Sample

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

Color

Brilliant yellow green

Structure

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

Lattice constants of this sample

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

a/b = 1.0856
c/b = 0.8754

Volume

587.3 Å³

Density

(calculated) 4.946 g/cm³

Polymorphism

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

Figure of merit

F₃₀ = 27.7(0.017, 63)

Additional patterns

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

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

References

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

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

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

Nickel Molybdenum Oxide, NiMoO₄ - (continued)

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

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

Synonym

Nickel orthophosphate octahydrate

CAS registry no.

19033-89-7

Sample

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

Color

Very light yellowish green.

Structure

Monoclinic, $I2/m$ (12), $Z = 2$. Vivianite structure, from the similarity of cell size, space group and chemistry. The structure of vivianite, $\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$, is discussed by Mori and Ito (1950).

Lattice constants of this sample

$$a = 9.846(4) \text{ \AA}$$

$$b = 13.203(4)$$

$$c = 4.6342(15)$$

$$\beta = 102.27(3)^\circ$$

$$a/b = 0.7457$$

$$c/b = 0.3510$$

Volume

$$588.67 \text{ \AA}^3$$

Density

$$(\text{calculated}) 2.878 \text{ g/cm}^3$$

Figure of merit

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

Additional pattern

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

References

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

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

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

Nickel Sulfate Hydrate (Nickel-hexahydrite), $\beta\text{-NiSO}_4 \cdot 6\text{H}_2\text{O}$

Synonym

Nickel sulfate hexahydrate

CAS registry no.

10101-97-0

Sample

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

Color

Strong green

Structure

Monoclinic, $A2/a$ (15), $Z = 8$. Isostructural with other divalent hexahydrate sulfates (Sutor, 1959). The structure of $\text{MgSO}_4 \cdot 6\text{H}_2\text{O}$ was discussed by Ide (1938).

Lattice constants of this sample

$a = 24.188(5)\text{\AA}$

$b = 7.2410(14)$

$c = 9.895(2)$

$\beta = 98.41(2)^\circ$

$a/b = 3.3404$

$c/b = 1.3665$

Volume

1714.4 \AA^3

Density

(calculated) 2.037 g/cm^3

Polymorphism

$\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$ also occurs in a tetragonal form as the mineral retgersite.

Figure of merit

$F_{30} = 52.3(0.013, 45)$

Additional patterns

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

PDF card 26-1288 (Nawaz, 1973)

References

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

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

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

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

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

Nickel Sulfate Hydrate (Nickel-hexahydrite), $\beta\text{-NiSO}_4 \cdot 6\text{H}_2\text{O}$ - (continued)

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

Niobium, Nb

Synonym

Columbium

CAS registry no.

7440-03-1

Sample

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

Color

Dark gray

Structure

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

Lattice constant of this sample

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

Volume

36.046 \AA^3

Density

(calculated) 8.560 g/cm^3

Figure of merit

$F_g = 102.8(0.010, 8)$

Additional patterns

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

Nadler and Kempter (1959)

References

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

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

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

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

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

Potassium Barium Phosphate, KBaPO₄

Synonym

Potassium barium orthophosphate

CAS registry no.

25640-29-3

Sample

The sample was made by heating a 1:1 molar mixture of Ba(OH)₂ and KH₂PO₄ at 750 °C for 2 days, regrinding and heating to 900 °C for 1 hour.

Color.

Colorless

Structure

Orthorhombic, Pnam (62), Z = 4. (Struck and White, 1962). Isostructural with β-K₂SO₄, arcanite.

Lattice constants of this sample

$$a = 7.7084(5) \text{ Å}$$

$$b = 9.9783(8)$$

$$c = 5.6649(5)$$

$$a/b = 0.7725$$

$$c/b = 0.5677$$

Volume

$$435.73 \text{ Å}^3$$

Density

$$(\text{calculated}) 4.137 \text{ g/cm}^3$$

Polymorphism

KBaPO₄ is reported to have a high temperature form which is hexagonal (Klement and Uffelmann, 1941). This is questioned by Struck and White (1962).

Figure of merit

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

Additional patterns

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

Wanmaker and Spier (1962)

Majling, et al. (1979) calculated pattern

References

Klement, R. and Uffelmann, R. (1941).

Naturwissenschaften 29, 300.

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

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

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

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

Potassium Barium Phosphate, KBaPO_4 - (continued)

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

Potassium Calcium Phosphate, $KCaPO_4$

Synonym

Potassium calcium orthophosphate

CAS registry no.

18901-69-4

Sample

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

Color

Colorless

Structure

Hexagonal, $P\bar{3}m1$ (164), $Z = 2$. (Bredig, 1941)
Isostructural with aphthitalite, $(K,Na)_3Na(SO_4)_2$
The structure of aphthitalite was determined by Gossner (1928).

Lattice constants of this sample

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

$c/a = 1.3619$

Volume
197.14 \AA^3

Density
(calculated) 2.934 g/cm³

Polymorphism

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

Figure of merit

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

Additional patterns

PDF card 3-619 (Bredig, 1942)

Wanmaker and Spier (1962)

References

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

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

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

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

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

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

Potassium Strontium Phosphate, K₂StrPO₄

Synonym

Potassium strontium orthophosphate

CAS registry no.

53201-92-6

Sample

The sample was made at NBS by heating equimolar amounts of KH₂PO₄ and SrCO₃ at 900 °C for 1 hour; it was reground and heated to 1250 °C for 1 hour.

Color

Colorless

Structure

Orthorhombic, Pnam (62), Z = 4. Isostructural with arcanite, β-K₂SO₄. (Klement and Kresse, 1961) The structure of arcanite was determined by Robinson, (1958). This phase of K₂StrPO₄ can also be indexed on a hexagonal cell with a = 11.124 and c = 7.350, this being similar to the high form of K₂SO₄, but with a doubled α .

Lattice constants of this sample

$$a = 7.3507(7) \text{ Å}$$

$$b = 9.6340(9)$$

$$c = 5.5621(6)$$

$$a/b = 0.7630$$

$$c/b = 0.5773$$

Volume
393.89 Å³

Density
(calculated) 3.738 g/cm³

Polymorphism

K₂StrPO₄ is reported to have several other forms (Klement and Uffelmann, 1941).

Figure of merit

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

Additional patterns

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

Wanmaker and Spier, 1962

References

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

Klement, R. and Uffelmann, R. (1941).

Naturwissenschaften 29, 300.

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

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

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

Potassium Strontium Phosphate, K_2SrPO_4 - (continued)

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

Silver Telluride (Hessite), Ag_2Te

CAS registry no.
12002-98-1

Sample

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

Color

Unground: medium gray
Ground: dark gray

Structure

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

Lattice constants of this sample

$a = 8.1698(15)$ Å
 $b = 8.940(2)$
 $c = 8.0653(15)$
 $\beta = 112.793(15)$ °
 $a/b = 0.9138$
 $c/b = 0.9022$

Volume
543.07 Å³

Density
(calculated) 8.399 g/cm³

Polymorphism

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

Figure of merit

$F_{30} = 23.1(0.015, 89)$

Additional patterns

PDF card 12-695 (Thompson, 1949)

Frueh (1959)

Tokody (1932)

References

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

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

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

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

Silver Telluride (Hessite), Ag_2Te - (continued)

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

Sodium Barium Phosphate, NaBaPO₄

Synonym

Sodium barium orthophosphate

CAS registry no.

53201-91-5

Sample

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

Color

Colorless

Optical data

Low double refraction with an average value ~1.612.

Structure

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

Lattice constants of this sample

a = 5.6181(3) Å
c = 7.2636(5)

c/a = 1.2929

Volume

198.55 Å³

Density

(calculated) 4.270 g/cm³

Polymorphism

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

Figure of merit

F₃₀ = 82.1(0.010,38)

Additional patterns

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

Majling et al. (1979) (calculated pattern)

Comment

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

References

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

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

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

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

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

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

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

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

Sodium Barium Phosphate, NaBaPO₄ - (continued)

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

Sodium Strontium Phosphate, NaSrPO₄

Synonym

Sodium strontium orthophosphate

CAS registry no.

19553-80-1

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

$$a = 20.414(4)\text{\AA}$$

$$b = 5.429(11)$$

$$c = 17.246(3)$$

$$\beta = 101.76(2)^\circ$$

$$a/b = 3.7602$$

$$c/b = 3.1766$$

Volume

$$1871.21 \text{ \AA}^3$$

Density

$$(\text{calculated}) 2.919 \text{ g/cm}^3$$

Polymorphism

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

Figure of merit

$$F_{30} = 43.4(0.011, 63)$$

$$M_{20} = 20.6$$

Additional pattern

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

References

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

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

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

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

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

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

Sodium Strontium Phosphate, NaSrPO₄ - (continued)

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

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

Synonyms

Sodium titanium orthophosphate
NTP

CAS registry no.
22239-24-3

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

Hexagonal axes

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

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

Volume
1360.35 \AA^3

Density

(calculated) 2.957 g/cm³

Polymorphism

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

Figure of merit

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

Additional patterns

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

Chernorukov (1978)

References

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

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

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

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{\AA}; \text{temp. } 25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.430825 \text{\AA}$					
$d(\text{\AA})$	I^{rel}	hkl			$2\theta (^\circ)$
$\sigma = \pm 2$					
6.095	14	0	1	2	14.52
4.377	20	1	0	4	20.27
4.245	32	1	1	0	20.91
3.666	100	1	1	3	24.26
3.632	10	0	0	6	24.49
3.485	4	2	0	2	25.54
3.048	28	0	2	4	29.28
2.759M	64	1	1	6	32.42
2.759M		2	1	1	32.42
2.694	2	1	2	2	33.23
2.5532	1	0	1	8	35.12
2.4761	2	2	1	4	36.25
2.4520	16	3	0	0	36.62
2.1883	2	2	0	8	41.22
2.1032	7	1	1	9	42.97
2.0733	2	2	1	7	43.62
2.0378	5	2	2	3	44.42
2.0322M	6	3	0	6	44.55
2.0322M		1	3	1	44.55
2.0053	1	3	1	2	45.18
1.9455	15	1	2	8	46.65
1.9100	3	1	3	4	47.57
1.8740	2	0	2	10	48.54
1.8473	2	3	1	5	49.29
1.8330	16	2	2	6	49.70
1.8152	5	0	0	12	50.22
1.8128	6	0	4	2	50.29
1.7419	1L	4	0	4	52.49
1.7144	9	2	1	10	53.40
1.7058	7	1	3	7	53.69
1.6821	1L	3	2	1	54.51
1.6674	1	2	3	2	55.03
1.6328	6	3	1	8	56.30
1.6115	5	3	2	4	57.11
1.6048	11	4	1	0	57.37
1.5959	2	2	2	9	57.72
1.5733	2	2	3	5	58.63
1.5670	4	4	1	3	58.89
1.5236	5	0	4	8	60.74
1.4889	6	1	3	10	62.31
1.4678	6	4	1	6	63.31
1.4589	2	3	0	12	63.74
1.4331	5	2	0	14	65.03
1.4199	4	0	5	4	65.71
1.4153	3	3	3	0	65.95
1.4051	2	4	0	10	66.49
1.3890	1L	3	3	3	67.36
1.3798	1	2	2	12	67.87
1.3741	3	1	1	15	68.19
1.3583	3	1	2	14	69.10

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

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

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

Synonyms

Sodium zirconium orthophosphate
NZP

CAS registry no.
19527-81-2

Sample

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

Color

Colorless

Structure

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

Lattice constants of this sample

Hexagonal axes

$a = 8.8048(4)\text{\AA}$

$c = 22.7572(14)$

$c/a = 2.5846$

$Z = 6$

Volume

1527.88 \AA^3

Density

(calculated) 3.198 g/cm³

Figure of merit

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

Additional patterns

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

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

Majling, et al. (1979) calculated pattern

References

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

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

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

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

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

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

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

Yttrium Chromium Oxide, YCrO_3

Synonym

Yttrium orthochromite

Sample

The sample was prepared at NBS by T. Negas.

Color

Medium yellowish green

Structure

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

Lattice constants of this sample

$$a = 5.5237(3) \text{\AA}$$

$$b = 7.5343(5)$$

$$c = 5.2427(3)$$

$$a/b = 0.7331$$

$$c/b = 0.6958$$

Volume

$$218.19 \text{ \AA}^3$$

Density

$$(\text{calculated}) 5.751 \text{ g/cm}^3$$

Figure of merit

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

Additional patterns

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

Geller and Wood (1956)

Keith and Roy (1954)

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

References

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

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

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

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

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

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

Yttrium Chromium Oxide, YCrO_3 - (continued)

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

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

Synonyms

Zinc arsenate octahydrate
Zinc orthoarsenate octahydrate

Sample

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

Spectrographic analysis

Major impurities

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

Color

Colorless

Structure

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

Lattice constants of this sample

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

$a/b = 0.7533$	
$c/b = 0.3545$	

Volume
 633.37 \AA^3

Density

(calculated) 3.241 g/cm^3

Comment

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

Figure of merit

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

Additional pattern

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

References

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

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

$CuK\alpha_1$	$\lambda = 1.540598 \text{ \AA}$	$\text{temp. } 25 \pm 1 \text{ }^\circ\text{C}$
Internal standard Si, $a = 5.43088 \text{ \AA}$		

$d(\text{\AA})$	I^{rel}	hkl	$2\theta (\text{\\textdegree})$
$\sigma = \pm 2$			
7.97	24	1 1 0	11.09
6.72	100	0 2 0	13.17
4.951	10	2 0 0	17.90
4.595	5	-1 0 1	19.30
4.403	14	0 1 1	20.15

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

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

Synonym

Zinc sulfate monohydrate

CAS registry no.

7446-19-7

Sample

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

Color

Colorless

Structure

Monoclinic, $A2/a$ (15), $Z = 4$. Isostructural with kieserite ($\text{MgSO}_4 \cdot \text{H}_2\text{O}$), (Pistorius, 1961). The structure of kieserite was determined by Leonhardt and Weiss (1957).

Lattice constants of this sample

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

$$b = 7.5871(6)$$

$$c = 6.9355(6)$$

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

Volume

$$354.3 \text{ \AA}^3$$

Density

$$(\text{calculated}) 3.364 \text{ g/cm}^3$$

Figure of merit

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

Additional pattern

PDF card 12-781 (Pistorius)

References

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

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

$\text{CuK}\alpha_1$ $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$					
Internal standard Si, $a = 5.43088 \text{ \AA}$					
$d(\text{\AA})$	I^{rel}	hkl	$2\theta (\text{)}^\circ$	$\sigma = \pm 1$	
4.810	39	0 1 1	18.43		
4.759	39	-1 1 1	18.63		
3.794	11	0 2 0	23.43		
3.404	100	1 1 1	26.16		
3.348	23	-2 1 1	26.60		
3.307	28	1 2 0	26.94		
3.056	47	-2 0 2	29.20		
2.5595	16	-1 2 2	35.03		
2.5185	46	2 2 0	35.62		
2.4051	3	0 2 2	37.36		

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

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

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

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

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

Synonyms

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

CAS registry no.
 24486-13-3

Structure

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

Atom positions

All atoms were in general positions 8(c).

Lattice constants

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

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

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

Volume
 2402.7 \AA^3

Density

(calculated) 1.384 g/cm^3

Thermal parameters

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

Scattering factors

Zero ionization (International Tables, 1962)

Scale factors

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

Comment

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

Additional patterns

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

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

References

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

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

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

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

Williams, P. P. (1973). *Acta Crystallogr. B* 29, 1572.

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

+ More than one hkl possible

Phenobarbital Hydrate, C₁₂H₁₂N₂O₃·H₂O - (continued)

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

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

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

INORGANIC NAMES

	Vol. or Sec.	Page		Vol. or Sec.	Page
Aluminum, Al	1	11	Ammonium aluminum fluoride, $(\text{NH}_4)_3\text{AlF}_6$	9m	5
Aluminum antimony, AlSb	4	72	Ammonium aluminum selenate hydrate, $\text{NH}_4\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$	9m	6
Aluminum bismuth oxide, $\text{Al}_4\text{Bi}_2\text{O}_9$	11m	5	Ammonium aluminum sulfate, $\text{NH}_4\text{Al}(\text{SO}_4)_2$	10m	5
Aluminum borate, $\text{Al}_{18}\text{B}_4\text{O}_{33}$	17m	5	Ammonium aluminum sulfate hydrate (tschermigite), $\text{NH}_4\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6	3
Aluminum chloride, AlCl_3	9m	61	Ammonium azide, NH_4N_3	9	4
Aluminum chloride hydrate (chloraluminite), $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$	7	3	Ammonium beryllium fluoride, $(\text{NH}_4)_2\text{BeF}_4$	3m	5
Aluminum copper, Al_4Cu_9	11m	79	Ammonium borate hydrate, $\text{NH}_4\text{B}_5\text{O}_8 \cdot 4\text{H}_2\text{O}$	17m	7
Aluminum fluoride hydroxide silicate, topaz, $\text{Al}_2(\text{F},\text{OH})_2\text{SiO}_4$	1m	4	Ammonium boron fluoride, NH_4BF_4	3m	6
Aluminum iron, AlFe	18m	5	Ammonium bromide, NH_4Br	2	49
Aluminum iron antimony oxide, bahianite, $\text{Al}_{5.66}\text{Fe}_{0.09}\text{Sb}_{2.95}\text{O}_{16}$	16m	87	Ammonium cadmium bromide, $(\text{NH}_4)_4\text{CdBr}_6$	15m	9
Aluminum iron oxide, AlFeO_3	15m	7	Ammonium cadmium chloride, NH_4CdCl_3	5m	6
Aluminum lithium, Al_4Li_9	10m	98	Ammonium cadmium phosphate hydrate, $\text{NH}_4\text{CdPO}_4 \cdot \text{H}_2\text{O}$	19m	13
Aluminum nickel, AlNi	6m	82	Ammonium cadmium sulfate, $(\text{NH}_4)_2\text{Cd}_2(\text{SO}_4)_3$	7m	5
Aluminum nitride, AlN	12m	5	Ammonium cadmium sulfate hydrate, $(\text{NH}_4)_2\text{Cd}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	8m	5
Aluminum nitrate hydrate, $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$	11m	6	Ammonium calcium sulfate, $(\text{NH}_4)_2\text{Ca}_2(\text{SO}_4)_3$	8m	7
Aluminum oxide (corundum), $\alpha\text{-Al}_2\text{O}_3$..	9	3	Ammonium cerium nitrate, $(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$	18m	6
Aluminum oxide hydrate (boehmite), $\alpha\text{-Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$	3	38	Ammonium chlorate, NH_4ClO_4 (orthorhombic)	7	6
Aluminum oxide hydrate, diaspore, $\beta\text{-Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$	3	41	Ammonium chloride (salammoniac), NH_4Cl	1	59
Aluminum phosphate, $\text{Al}(\text{PO}_3)_3$	2m	3	Ammonium chromium sulfate hydrate, $\text{NH}_4\text{Cr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6	7
Aluminum phosphate (berlinite), AlPO_4 (trigonal)	10	3	Ammonium cobalt (II) chloride, NH_4CoCl_3	6m	5
Aluminum phosphate, AlPO_4 (orthorhombic)	10	4	Ammonium cobalt fluoride, NH_4CoF_3	8m	9
Aluminum plutonium, Al_3Pu	15m	77	Ammonium copper bromide hydrate, $(\text{NH}_4)_2\text{CuBr}_4 \cdot 2\text{H}_2\text{O}$	10m	6
Aluminum rhenium, AlRe	15m	79	Ammonium copper chloride, NH_4CuCl_3	7m	7
Aluminum rhenium, Al_{12}Re	15m	80	Ammonium copper chloride hydrate, $(\text{NH}_4)_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$	12m	6
Aluminum rhodium, AlRh	15m	82	Ammonium copper fluoride, NH_4CuF_3	11m	8
Aluminum ruthenium, AlRu	15m	83	Ammonium gallium sulfate hydrate, $\text{NH}_4\text{Ga}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6	9
Aluminum ruthenium, Al_6Ru	15m	84	Ammonium germanium fluoride, $(\text{NH}_4)_2\text{GeF}_6$	6	8
Aluminum samarium, AlSm_2	15m	86	Ammonium hydrogen arsenate, $\text{NH}_4\text{H}_2\text{AsO}_4$	16m	9
Aluminum samarium, AlSm_3	15m	88	Ammonium hydrogen carbonate (teschemacherite), $(\text{NH}_4)\text{HCO}_3$	9	5
Aluminum samarium, Al_2Sm	15m	90	Ammonium hydrogen phosphate, $\text{NH}_4\text{H}_2\text{PO}_4$	4	64
Aluminum samarium, Al_3Sm	15m	91	Ammonium iodate, NH_4IO_3	10m	7
Aluminum silicate (mullite), $\text{Al}_6\text{Si}_2\text{O}_{13}$	3m	3	Ammonium iodide, NH_4I	4	56
Aluminum sulfate, $\text{Al}_2(\text{SO}_4)_3$	15m	8	Ammonium iridium chloride, $(\text{NH}_4)_2\text{IrCl}_6$	8	6
Aluminum technetium, Al_6Tc	15m	93	Ammonium iron chloride hydrate, $(\text{NH}_4)_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$	14m	7
Aluminum terbium, Al_2Tb	15m	95	Ammonium iron fluoride, $(\text{NH}_4)_3\text{FeF}_6$	9m	9
Aluminum terbium, Al_2Tb_3	15m	96	Ammonium iron sulfate, $\text{NH}_4\text{Fe}(\text{SO}_4)_2$	10m	8
Aluminum thorium uranium, Al_6ThU	15m	98	Ammonium iron sulfate hydrate, $\text{NH}_4\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6	10
Aluminum tungsten, Al_5W , δ -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, $\text{NH}_4\text{MgAlF}_6$	10m	9
Aluminum vanadium, Al_{10}V	15m	102			
Aluminum vanadium, $\text{Al}_{10.25}\text{V}$	15m	104			
Aluminum vanadium, Al_{23}V_4	15m	106			
Aluminum vanadium, Al_{45}V_7 , α' -phase ..	15m	108			
Aluminum ytterbium, Al_2Yb	15m	111			
Aluminum yttrium, Al_3Y	15m	112			
Aluminium yttrium oxide, AlYO_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.

	Vol. or Sec.	Page		Vol. or Sec.	Page
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 cobalt vanadium, CoSbV	15m	125
Ammonium magnesium phosphate hydrate (struvite), $\text{NH}_4\text{MgPO}_4 \cdot 6\text{H}_2\text{O}$	3m	41	Antimony dysprosium, DySb	4m	41
Ammonium manganese chloride hydrate, $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$	11m	11	Antimony erbium, ErSb	4m	41
Ammonium manganese(II) fluoride, NH_4MnF_3	5m	8	Antimony(III) fluoride, SbF_3	2m	4
Ammonium manganese sulfate, $(\text{NH}_4)_2\text{Mn}_2(\text{SO}_4)_3$	7m	8	Antimony gadolinium, GdSb	4m	42
Ammonium manganese sulfate hydrate, $(\text{NH}_4)_2\text{Mn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	8m	12	Antimony gallium, GaSb	6	30
Ammonium mercury chloride, NH_4HgCl_3	8m	14	Antimony gold (aurostibite), AuSb_2	7	18
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 indium, InSb	4	73
Ammonium nickel(II) chloride, NH_4NiCl_3	6m	6	Antimony(III) iodide, SbI_3	6	16
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 iron titanium oxide hydroxide, derbylite, $\text{SbFe}_4\text{Ti}_3\text{O}_{13}(\text{OH})$	16m	89
Ammonium nickel sulfate hydrate, $(\text{NH}_4)_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	17m	9	Antimony lanthanum, LaSb	4m	42
Ammonium nitrate (nitrammite), NH_4NO_3	7	4	Antimony neodymium, NdSb	4m	43
Ammonium osmium bromide, $(\text{NH}_4)_2\text{OsBr}_6$	3	71	Antimony(III) oxide (senarmontite), Sb_2O_3 (cubic)	3	31
Ammonium osmium chloride, $(\text{NH}_4)_2\text{OsCl}_6$	1m	6	Antimony(III) oxide, valentinite, Sb_2O_3 (orthorhombic)	10	6
Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_4$	6	6	Antimony(IV) oxide (cervantite), Sb_2O_4	10	8
Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_6$	8	7	Antimony oxide, Sb_6O_{13}	16m	14
Ammonium platinum bromide, $(\text{NH}_4)_2\text{PtBr}_6$	9	6	Antimony praseodymium, PrSb	4m	43
Ammonium platinum chloride, $(\text{NH}_4)_2\text{PtCl}_6$	5	3	Antimony scandium, SbSc	4m	44
Ammonium potassium iron chloride hydrate (kremersite), $(\text{NH}_4, \text{K})_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$	14m	8	Antimony selenide, Sb_2Se_3	3m	7
Ammonium rhenium oxide, NH_4ReO_4 ...	9	7	Antimony silver sulfide, AgSbS_2 (cubic)	5m	48
Ammonium selenium bromide, $(\text{NH}_4)_2\text{SeBr}_6$	8	4	Antimony silver sulfide (miargyrite), AgSbS_2 (monoclinic)	5m	49
Ammonium silicon fluoride (cryptothalite), $(\text{NH}_4)_2\text{SiF}_6$	5	5	Antimony silver sulfide (pyrargyrite), Ag_3SbS_3 (trigonal)	5m	51
Ammonium strontium chromium oxide, $(\text{NH}_4)_2\text{Sr}(\text{CrO}_4)_2$	14m	9	Antimony silver telluride, AgSbTe_2	3m	47
Ammonium strontium sulfate, $(\text{NH}_4)_2\text{Sr}(\text{SO}_4)_2$	15m	11	Antimony(III) sulfide (stibnite), Sb_2S_3	5	6
Ammonium sulfate (mascagnite), $(\text{NH}_4)_2\text{SO}_4$	9	8	Antimony telluride, Sb_2Te_3	3m	8
Ammonium sulfate, $(\text{NH}_4)_2\text{S}_2\text{O}_3$	17m	11	Antimony terbium, SbTb	5m	61
Ammonium sulfate, $(\text{NH}_4)_2\text{S}_2\text{O}_8$	17m	13	Antimony thorium, SbTh	4m	44
Ammonium tellurium bromide, $(\text{NH}_4)_2\text{TeBr}_6$	8	5	Antimony thulium, SbTm	4m	45
Ammonium tellurium chloride, $(\text{NH}_4)_2\text{TeCl}_6$	8	8	Antimony tin, SbSn	16m	15
Ammonium tin chloride, $(\text{NH}_4)_2\text{SnCl}_6$	5	4	Antimony ytterbium, SbYb	4m	45
Ammonium tin fluoride, NH_4SnF_3	18m	8	Antimony yttrium, SbY	4m	46
Ammonium titanium fluoride, $(\text{NH}_4)_2\text{TiF}_6$	16m	10	Arsenic, As	3	6
Ammonium vanadium oxide, NH_4VO_3 ...	8	9	Arsenic bromide, AsBr_3	18m	9
Ammonium zinc chloride, $(\text{NH}_4)_3\text{ZnCl}_5$	15m	12	Arsenic cerium, AsCe	4m	51
Ammonium zinc fluoride, NH_4ZnF_3 ...	8m	18	Arsenic(III) iodide, AsI_3	13m	7
Ammonium zirconium fluoride, $(\text{NH}_4)_3\text{ZrF}_7$	6	14	Arsenic oxide (arsenolite), As_2O_3 (cubic)	1	51
Antimony cobalt, CoSb	15m	121	Arsenic oxide, claudetite, As_2O_3 (monoclinic)	3m	9
Antimony cobalt, CoSb_2	15m	122	Barium, Ba	4	7
Antimony cobalt titanium, CoSbTi ..	15m	124	Barium aluminum oxide, BaAl_2O_4	5m	11
			Barium aluminum oxide, $\text{Ba}_3\text{Al}_2\text{O}_6$	12m	7
			Barium aluminum titanium oxide, $\text{BaAl}_6\text{TiO}_{12}$	19m	14
			Barium aluminum titanium oxide, $\text{Ba}_{1.23}\text{Al}_{2.46}\text{Ti}_{5.54}\text{O}_{16}$	18m	10
			Barium aluminum titanium oxide, $\text{Ba}_3\text{Al}_{10}\text{TiO}_{20}$	19m	16
			Barium arsenate, $\text{Ba}_3(\text{AsO}_4)_2$	2m	6
			Barium borate, BaB_4O_7	4m	6
			Barium borate, high form, BaB_2O_4 ..	4m	4
			Barium borate, $\text{BaB}_8\text{O}_{13}$	7m	10
			Barium boride, BaB_6	19m	18
			Barium bromate hydrate, $\text{Ba}(\text{BrO}_3)_2 \cdot \text{H}_2\text{O}$	8m	19
			Barium bromide, BaBr_2	10m	63

	Vol. or Sec.	Page		Vol. or Sec.	Page
Barium bromide fluoride, BaBrF	10m	10	Barium strontium nitrate,		
Barium bromide hydrate, BaBr ₂ ·H ₂ O	3m	10	Ba _{.50} Sr _{.50} (NO ₃) ₂	12m	42
Barium bromide hydrate, BaBr ₂ ·2H ₂ O	16m	16	Barium strontium nitrate,		
Barium cadmium chloride hydrate, BaCdCl ₄ ·4H ₂ O	15m	14	Ba _{.75} Sr _{.25} (NO ₃) ₂	12m	42
Barium calcium nitrate, Ba _{.25} Ca _{.75} (NO ₃) ₂	12m	38	Barium sulfate (baryte), BaSO ₄	10m	12
Barium calcium nitrate, Ba _{.50} Ca _{.50} (NO ₃) ₂	12m	38	Barium sulfide, BaS	7	8
Barium calcium nitrate, Ba _{.75} Ca _{.25} (NO ₃) ₂	12m	38	Barium thiosulfate hydrate, BaS ₂ O ₃ ·H ₂ O	16m	20
Barium calcium tungsten oxide, Ba ₂ CaWO ₆	9m	10	Barium tin oxide, BaSnO ₃	3m	11
Barium carbonate (witherite), BaCO ₃ (orthorhombic)	2	54	Barium titanium oxide, BaTiO ₃	3	45
Barium carbonate, BaCO ₃ (cubic) at 1075 °C	10	11	Barium titanium silicate (fresnoite), Ba ₂ TiSi ₂ O ₈	9m	14
Barium chlorate, Ba(ClO ₃) ₂	16m	17	Barium tungsten oxide, BaWO ₄	7	9
Barium chlorate hydrate, Ba(ClO ₃) ₂ ·H ₂ O	8m	21	Barium tungsten oxide, Ba ₂ WO ₅	12m	14
Barium chloride, BaCl ₂ , (cubic) ...	9m	13	Barium tungsten oxide, Ba ₃ WO ₆	19m	21
Barium chloride, BaCl ₂ , (orthorhombic)	9m	11	Barium vanadium oxide, Ba ₃ (VO ₄) ₂ ..	14m	10
Barium chloride fluoride, BaClF ...	10m	11	Barium zirconium oxide, BaZrO ₃	5	8
Barium chloride hydrate, BaCl ₂ ·2H ₂ O	12m	9	Beryllium, alpha, Be	9m	64
Barium chromium oxide, Ba ₃ (CrO ₄) ₂	15m	16	Beryllium aluminum oxide (chrysoberyl), BeAl ₂ O ₄	9	10
Barium fluoride, BaF ₂	1	70	Beryllium aluminum silicate, beryl, Be ₃ Al ₂ (SiO ₃) ₆	9	13
Barium hydroxide phosphate, Ba ₅ (OH)(PO ₄) ₃	11m	12	Beryllium calcium iron magnesium aluminum phosphate hydroxide hydrate, roscherite (monoclinic), Be ₂ Ca(Fe _{.3} Mg _{.7}) ₂ Al _{.67} (PO ₄) ₃ (OH) ₃ ·2H ₂ O	16m	96
Barium iodide, BaI ₂	10m	66	Beryllium calcium manganese aluminum iron phosphate hydroxide hydrate, roscherite (triclinic), Be ₄ Ca ₂ (Mn _{3.91} Mg _{.04} Ca _{.05})(Al _{.13} Fe _{.42} Mn _{.12})(PO ₄) ₆ (OH) ₄ ·6H ₂ O	16m	100
Barium iodide hydrate, BaI ₂ ·2H ₂ O ..	16m	18	Beryllium calcium oxide, Be ₁₇ Ca ₁₂ O ₂₉	7m	89
Barium lead chloride, BaPbCl ₄	11m	13	Beryllium carbide, Be ₂ C	19m	23
Barium lead nitrate, Ba _{.33} Pb _{.67} (NO ₃) ₂	12m	40	Beryllium chromium oxide, BeCr ₂ O ₄	10	12
Barium lead nitrate, Ba _{.67} Pb _{.33} (NO ₃) ₂	12m	40	Beryllium cobalt, BeCo	5m	62
Barium manganese oxide, BaMnO ₄	18m	11	Beryllium germanium oxide, Be ₂ GeO ₄	10	13
Barium manganese oxide, Ba(MnO ₄) ₂	15m	17	Beryllium lanthanum oxide, Be ₂ La ₂ O ₅	9m	65
Barium molybdenum oxide, BaMoO ₄ ...	7	7	Beryllium niobium, Be ₂ Nb	7m	92
Barium molybdenum oxide, Ba ₂ MoO ₅ ..	12m	10	Beryllium nitride, Be ₃ N ₂	18m	15
Barium neodymium titanium oxide, BaNd ₂ Ti ₃ O ₁₀	18m	12	Beryllium oxide (bromellite), BeO	1	36
Barium neodymium titanium oxide, BaNd ₂ Ti ₅ O ₁₄	19m	19	Beryllium palladium, BePd	5m	62
Barium nitrate (nitrobarite), Ba(NO ₃) ₂	11m	14	Beryllium silicate, phenakite, Be ₂ SiO ₄	8	11
Barium nitrite hydrate, Ba(NO ₂) ₂ ·H ₂ O	15m	18	Beryllium sulfate, BeSO ₄	15m	20
Barium oxide, BaO	9m	63	Bismuth, Bi	3	20
Barium oxide, BaO ₂	6	18	Bismuth bromide oxide, BiOBr	8	14
Barium phosphate, Ba ₂ P ₂ O ₇ , (high form)	16m	19	Bismuth cerium, BiCe	4m	46
Barium phosphate, Ba ₃ (PO ₄) ₂	12m	12	Bismuth chloride oxide (bismoclite), BiOCl	4	54
Barium selenide, BaSe	5m	61	Bismuth dysprosium, BiDy	4m	47
Barium silicate, β-BaSiO ₃	13m	8	Bismuth erbium, BiEr	4m	47
Barium silicate (sanbornite), β-BaSi ₂ O ₅	13m	10	Bismuth fluoride, BiF ₃	1m	7
Barium silicate, Ba ₂ SiO ₄	13m	12	Bismuth holmium, BiHo	4m	48
Barium silicate, Ba ₂ Si ₃ O ₈	13m	13	Bismuth(III) iodide, BiI ₃	6	20
Barium silicate, Ba ₃ SiO ₅	13m	15	Bismuth iodide oxide, BiOI	9	16
Barium silicate, Ba ₃ Si ₅ O ₁₃	13m	17	Bismuth lanthanum, BiLa	4m	48
Barium silicon fluoride, BaSiF ₆ ...	4m	7	Bismuth neodymium, BiNd	4m	49
Barium strontium nitrate, Ba _{.25} Sr _{.75} (NO ₃) ₂	12m	42	Bismuth oxide (bismite), α-Bi ₂ O ₃ ..	3m	17
			Bismuth phosphate, BiPO ₄ (monoclinic)	3m	11
			Bismuth phosphate, BiPO ₄ (trigonal)	3m	13
			Bismuth praseodymium, BiPr	4m	49
			Bismuth selenide (paraguanajuatite), Bi ₂ Se ₃	18m	16
			Bismuth sulfide (bismuthinite), Bi ₂ S ₃	5m	13

	Vol. or Sec.	Page		Vol. or Sec.	Page
Bismuth telluride, BiTe	4m	50	Calcium bromide, CaBr ₂	11m	70
Bismuth telluride (tellurobis-muthite), Bi ₂ Te ₃	3m	16	Calcium bromide hydrate, CaBr ₂ ·6H ₂ O	8	15
Bismuth vanadium oxide, high form, BiVO ₄ (monoclinic)	3m	14	Calcium carbonate (aragonite), CaCO ₃ (orthorhombic)	3	53
Bismuth vanadium oxide, low form, BiVO ₄ (tetragonal)	3m	14	Calcium carbonate (aragonite), CaCO ₃ (orthorhombic, calculated pattern)	14m	44
Boron oxide, B ₂ O ₃ , phase 1	10m	70	Calcium carbonate (calcite), CaCO ₃ (hexagonal)	2	51
Cadmium, Cd	3	10	Calcium chloride (hydrophilite), CaCl ₂	11m	18
Cadmium ammine chloride, Cd(NH ₃) ₂ Cl ₂	10m	14	Calcium chloride fluoride, CaClF	10m	17
Cadmium borate, CdB ₄ O ₇	16m	24	Calcium chloride hydrate, CaCl ₂ ·4H ₂ O	11m	73
Cadmium bromate hydrate, Cd(BrO ₃)·2H ₂ O	17m	14	Calcium chloride hydrate (antarcticite), CaCl ₂ ·6H ₂ O	12m	16
Cadmium bromide, CdBr ₂	9	17	Calcium chromium germanium oxide, Ca ₃ Cr ₂ (GeO ₄) ₃	10	16
Cadmium bromide chloride, CdBrCl ..	11m	15	Calcium chromium iron titanium oxide, loveringite, Ca _{.72} RE _{.33} (Y, Th, U, Pb) _{.05} Ti _{12.48} Fe _{3.38} Cr _{2.24} Mg _{.92} Zr _{.58} Al _{.39} V _{.21} Mn _{.04} O ₃₈	16m	106
Cadmium carbonate (otavite), CdCO ₃	7	11	Calcium chromium oxide (chromatite), CaCrO ₄	7	13
Cadmium cerium, CdCe	5m	63	Calcium chromium oxide, Ca ₃ (CrO ₄) ₂	15m	22
Cadmium chlorate hydrate, Cd(ClO ₄) ₂ ·6H ₂ O	3m	19	Calcium chromium silicate (uvarovite), Ca ₃ Cr ₂ (SiO ₄) ₃	10	17
Cadmium chloride, CdCl ₂	9	18	Calcium cyanamide, CaCN ₂	18m	19
Cadmium chromium oxide, CdCr ₂ O ₄	5m	16	Calcium fluoride (fluorite), CaF ₂	1	69
Cadmium copper, Cd ₈ Cu ₅	11m	81	Calcium fluoride phosphate (fluorapatite), Ca ₅ F(PO ₄) ₃	3m	22
Cadmium cyanide, Cd(CN) ₂	2m	8	Calcium fluoride phosphate hydrate, CaFPO ₃ ·2H ₂ O	15m	24
Cadmium fluoride, CdF ₂	10m	15	Calcium gallium germanium oxide, Ca ₃ Ga ₂ (GeO ₄) ₃	10	18
Cadmium iodide, α-CdI ₂	19m	24	Calcium hydrogen phosphate hydrate, Ca ₈ H ₂ (PO ₄) ₆ ·5H ₂ O	13m	21
Cadmium iron oxide, CdFe ₂ O ₄	9m	16	Calcium hydrogen phosphate sulfate hydrate, Ca ₂ HPO ₄ SO ₄ ·4H ₂ O	16m	109
Cadmium lanthanum, CdLa	5m	63	Calcium hydroxide (portlandite), Ca(OH) ₂	1	58
Cadmium manganese oxide, CdMn ₂ O ₄	10m	16	Calcium iodate (lautarite), Ca(IO ₃) ₂	14m	12
Cadmium molybdenum oxide, CdMoO ₄	6	21	Calcium iodate hydrate, Ca(IO ₃) ₂ ·6H ₂ O	14m	13
Cadmium nitrate hydrate, Cd(NO ₃) ₂ ·4H ₂ O	7m	93	Calcium iron germanium oxide, Ca ₃ Fe ₂ (GeO ₄) ₃	10	19
Cadmium oxide, CdO	2	27	Calcium iron oxide, CaFe ₂ O ₄	18m	20
Cadmium oxide, CdO (ref. standard)	8m	2	Calcium iron silicate (andradite), Ca ₃ Fe ₂ Si ₃ O ₁₂	9	22
Cadmium phosphate, Cd ₂ P ₂ O ₇	16m	26	Calcium iron silicate hydroxide, julgoldite, Ca ₂ Fe ₃ Si ₃ O ₁₀ (OH,O) ₂ (OH) ₂	10m	72
Cadmium phosphate, Cd ₃ (PO ₄) ₂	16m	27	Calcium lead nitrate, Ca _{.33} Pb _{.67} (NO ₃) ₂	12m	44
Cadmium praseodymium, CdPr	5m	64	Calcium lead nitrate, Ca _{.67} Pb _{.33} (NO ₃) ₂	12m	44
Cadmium selenide (cadmoselite), CdSe (hexagonal)	7	12	Calcium magnesium silicate (diopside), CaMg(SiO ₃) ₂	5m	17
Cadmium silicate, Cd ₂ SiO ₄	13m	19	Calcium molybdenum oxide (powellite), CaMoO ₄	6	22
Cadmium silicate, Cd ₃ SiO ₅	13m	20	Calcium nitrate, Ca(NO ₃) ₂	7	14
Cadmium sulfate, CdSO ₄	3m	20	Calcium oxide (lime), CaO	1	43
Cadmium sulfate hydrate, CdSO ₄ ·H ₂ O	6m	10	Calcium oxide (lime), CaO (calculated pattern)	14m	49
Cadmium sulfate hydrate, 3CdSO ₄ ·8H ₂ O	6m	8	Calcium oxide phosphate, Ca ₄ O(PO ₄) ₂	12m	17
Cadmium sulfide (greenockite), CdS	4	15	Calcium phosphate, β-Ca ₂ P ₂ O ₇	7m	95
Cadmium telluride, CdTe	3m	21	Calcium platinum oxide, Ca ₄ PtO ₆	10m	18
Cadmium titanium oxide, CdTiO ₃	15m	21			
Cadmium tungsten oxide, CdWO ₄	2m	8			
Calcium, Ca	9m	68			
Calcium aluminum germanium oxide, Ca ₃ Al ₂ (GeO ₄) ₃	10	15			
Calcium aluminum hydroxide, Ca ₃ Al ₂ (OH) ₁₂	11m	16			
Calcium aluminum iron oxide (brownmillerite), Ca ₄ Al ₂ Fe ₂ O ₁₀	16m	28			
Calcium aluminum oxide, Ca ₃ Al ₂ O ₆	5	10			
Calcium aluminum oxide (mayenite), Ca ₁₂ Al ₁₄ O ₃₃	9	20			
Calcium aluminum oxide hydrate, Ca ₄ Al ₆ O ₁₃ ·3H ₂ O	19m	25			
Calcium aluminum silicate hydrate, chabazite, Ca ₂ Al ₄ Si ₈ O ₂₄ ·12H ₂ O	19m	27			
Calcium aluminum sulfate hydrate (ettringite), Ca ₆ Al ₂ S ₃ O ₁₈ ·3H ₂ O	8	3			
Calcium borate, CaB ₂ O ₄	18m	17			
Calcium borate, CaB ₂ O ₄ (calculated pattern)	15m	136			
Calcium borate hydrate, hexahydroborite, Ca[B(OH) ₄] ₂ ·2H ₂ O	16m	104			
Calcium boride, CaB ₆	16m	29			

	Vol. or Sec.	Page		Vol. or Sec.	Page
Calcium selenide, CaSe	5m	64	Cesium chlorate, CsClO ₄ , (orthorhombic)	1m	10
Calcium silicate (larnite), β-Ca ₂ SiO ₄	19m	29	Cesium chloride, CsCl	2	44
Calcium silicon fluoride hydrate, CaSiF ₆ ·2H ₂ O	19m	31	Cesium chromium oxide, Cs ₂ CrO ₄	3m	25
Calcium strontium nitrate, Ca _{0.33} Sr _{0.67} (NO ₃) ₂	12m	46	Cesium chromium sulfate hydrate, CsCr(SO ₄) ₂ ·12H ₂ O	8	21
Calcium strontium nitrate, Ca _{0.67} Sr _{0.33} (NO ₃) ₂	12m	46	Cesium cobalt(II) chloride, CsCoCl ₃	6m	11
Calcium sulfate (anhydrite), CaSO ₄	4	65	Cesium cobalt chloride, Cs ₂ CoCl ₄	11m	19
Calcium sulfate hydrate (bassanite), CaSO ₄ ·0.5H ₂ O	18m	22	Cesium copper(II) chloride, CsCuCl ₃	5m	22
Calcium sulfate hydrate (gypsum), CaSO ₄ ·2H ₂ O	17m	16	Cesium copper chloride, Cs ₂ CuCl ₄	11m	20
Calcium sulfide (oldhamite), CaS	7	15	Cesium copper sulfate hydrate, Cs ₂ Cu(SO ₄) ₂ ·6H ₂ O	7m	14
Calcium telluride, CaTe	4m	50	Cesium fluoride, CsF	3m	26
Calcium tin oxide, CaSnO ₃	17m	18	Cesium gallium sulfate hydrate, CsGa(SO ₄) ₂ ·12H ₂ O	8	23
Calcium titanium oxide (perovskite), CaTiO ₃	9m	17	Cesium germanium fluoride, Cs ₂ GeF ₆	5	17
Calcium tungsten oxide, Ca ₃ WO ₆	9m	19	Cesium iodate, CsIO ₃	15m	26
Calcium tungsten oxide, scheelite, CaWO ₄	6	23	Cesium iodide, CsI	4	47
Carbon, diamond, C	2	5	Cesium iodide, CsI ₃	19m	33
Cerium arsenate, CeAsO ₄	4m	8	Cesium iodine bromide, CsI ₂ Br	7m	103
Cerium(III) chloride, CeCl ₃	1m	8	Cesium iodine chloride, CsICl ₂	3	50
Cerium cobalt, CeCo ₂	13m	50	Cesium iron chloride hydrate, Cs ₂ FeCl ₅ ·H ₂ O	14m	14
Cerium cobalt, Ce ₂₄ Co ₁₁	13m	51	Cesium iron sulfate hydrate, Cs ₂ Fe(SO ₄) ₂ ·6H ₂ O	7m	16
Cerium copper, CeCu ₆	7m	99	Cesium iron sulfate hydrate, CsFe(SO ₄) ₂ ·12H ₂ O	6	28
Cerium(III) fluoride, CeF ₃	8	17	Cesium lead(II) chloride, CsPbCl ₃ (tetragonal)	5m	24
Cerium gallium, CeGa ₂	13m	54	Cesium lead fluoride, CsPbF ₃	8m	26
Cerium magnesium, CeMg	5m	65	Cesium lithium cobalt cyanide, CsLiCo(CN) ₆	10m	79
Cerium magnesium, CeMg ₃	13m	56	Cesium lithium fluoride, CsLiF ₂	7m	105
Cerium nickel, CeNi ₂	13m	58	Cesium magnesium chromium oxide, Cs ₂ Mg ₂ (CrO ₄) ₃	8m	27
Cerium niobium oxide, CeNbO ₄	18m	25	Cesium magnesium chromium oxide hydrate, Cs ₂ Mg(CrO ₄) ₂ ·6H ₂ O	8m	29
Cerium niobium titanium oxide (aeschynite), CeNbTiO ₆	3m	24	Cesium magnesium sulfate hydrate, Cs ₂ Mg(SO ₄) ₂ ·6H ₂ O	7m	18
Cerium nitrate hydrate, Ce(NO ₃) ₃ ·6H ₂ O	17m	20	Cesium magnesium titanium oxide, Cs _{1.45} Mg _{0.724} Ti _{7.27} O ₁₆	18m	29
Cerium nitride, CeN	4m	51	Cesium manganese fluoride, CsMnF ₃	10m	21
Cerium(IV) oxide (cerianite), CeO ₂	1	56	Cesium manganese sulfate hydrate, Cs ₂ Mn(SO ₄) ₂ ·6H ₂ O	7m	20
Cerium phosphide, CeP	4m	52	Cesium mercury chloride, CsHgCl ₃	7m	22
Cerium tantalum oxide, CeTaO ₄	18m	27	Cesium molybdenum oxide, Cs ₂ Mo ₃ O ₁₀	19m	35
Cerium thallium, CeTl	13m	59	Cesium nickel(II) chloride, CsNiCl ₃	6m	12
Cerium thallium, CeTl ₃	13m	60	Cesium nickel sulfate hydrate, Cs ₂ Ni(SO ₄) ₂ ·6H ₂ O	7m	23
Cerium thallium, Ce ₃ Tl	13m	61	Cesium nitrate, CsNO ₃	9	25
Cerium(III) vanadium oxide, CeVO ₄	1m	9	Cesium osmium(IV) bromide, Cs ₂ O ₈ Br ₆	2m	10
Cerium zinc, CeZn	5m	65	Cesium osmium chloride, Cs ₂ O ₈ Cl ₆	2m	11
Cerium zinc, CeZn ₃	14m	50	Cesium platinum bromide, Cs ₂ PtBr ₆	8	19
Cerium zinc, CeZn ₅	14m	53	Cesium platinum chloride, Cs ₂ PtCl ₆	5	14
Cerium zinc, Ce ₂ Zn ₁₇	14m	55	Cesium platinum fluoride, Cs ₂ PtF ₆	6	27
Cesium aluminum sulfate hydrate, CsAl(SO ₄) ₂ ·12H ₂ O	6	25	Cesium selenium bromide, Cs ₂ SeBr ₆	8	20
Cesium antimony fluoride, CsSbF ₆	4m	9	Cesium silicon fluoride, Cs ₂ SiF ₆	5	19
Cesium beryllium fluoride, CsBeF ₃	9m	69	Cesium strontium chloride, CsSrCl ₃	6m	13
Cesium boron fluoride, CsBF ₄	8	22	Cesium sulfate, Cs ₂ SO ₄	7	17
Cesium bromate, CsBrO ₃	8	18	Cesium tellurium bromide, Cs ₂ TeBr ₆	9	24
Cesium bromide, CsBr	3	49	Cesium tin chloride, Cs ₂ SnCl ₆	5	16
Cesium cadmium bromide, CsCdBr ₃ (hexagonal)	10m	20	Cesium vanadium sulfate hydrate, CsV(SO ₄) ₂ ·12H ₂ O	1m	11
Cesium cadmium chloride, CsCdCl ₃ (hexagonal)	5m	19	Cesium zinc sulfate hydrate, Cs ₂ Zn(SO ₄) ₂ ·6H ₂ O	7m	25
Cesium calcium chloride, CsCaCl ₃	5m	21	Chromium, Cr	5	20
Cesium calcium fluoride, CsCaF ₃	8m	25	Chromium boride, ζ-CrB	17m	22
Cesium calcium sulfate, Cs ₂ Ca ₂ (SO ₄) ₃	7m	12			
Cesium cerium chloride, Cs ₂ CeCl ₆	14m	58			
Cesium chlorate, CsClO ₃	8	20			
Chromium, Cr	5	20			
Chromium boride, ζ-CrB	17m	22			

	Vol. or Sec.	Page		Vol. or Sec.	Page
Chromium boride, CrB ₂	19m	37	Cobalt germanium manganese,		
Chromium boride, Cr ₅ B ₃	18m	30	Co ₂ GeMn	13m	79
Chromium chloride, CrCl ₂	11m	77	Cobalt germanium niobium,		
Chromium chloride, CrCl ₃	17m	23	Co _{1.5} Ge _{0.5} Nb	15m	150
Chromium chloride hydrate, CrCl ₃ ·6H ₂ O	16m	31	Cobalt germanium niobium,		
Chromium cobalt niobium, CoCrNb ...	15m	140	Co ₁₆ Ge ₇ Nb ₆	14m	71
Chromium cobalt silicide,			Cobalt germanium oxide, Co ₂ GeO ₄ ...	10	27
Co ₉ Cr ₁₅ Si ₆	14m	62	Cobalt germanium tantalum,		
Chromium cobalt tantalum, CoCrTa ..	15m	142	Co _{1.5} Ge _{0.5} Ta	15m	152
Chromium fluoride, CrF ₂	10m	81	Cobalt germanium tantalum,		
Chromium fluoride, Cr ₂ F ₅	7m	108	Co ₁₆ Ge ₇ Ta ₆	14m	73
Chromium(III) fluoride hydrate, CrF ₃ ·3H ₂ O	5m	25	Cobalt germanium titanium, Co ₂ GeTi	13m	80
Chromium iridium, Cr ₃ Ir	6m	14	Cobalt hafnium tin, Co ₂ HfSn	14m	75
Chromium iron oxide, Cr _{1.3} Fe _{0.7} O ₃	17m	24	Cobalt holmium, Co ₂ Ho	14m	76
Chromium niobium oxide, CrNbO ₄	19m	38	Cobalt holmium, Co _{9.2} Ho ₁₂	15m	154
Chromium oxide, CrO ₃	17m	25	Cobalt hydroxide, β-Co(OH) ₂	15m	29
Chromium(III) oxide, Cr ₂ O ₃	5	22	Cobalt indium, CoIn ₃	13m	81
Chromium phosphate, α-CrPO ₄	2m	12	Cobalt iodide, CoI ₂	4m	52
Chromium phosphate, β-CrPO ₄	9	26	Cobalt iron arsenide (safflorite), CoFeAs ₄	10	28
Chromium phosphate hydrate, CrPO ₄ ·6H ₂ O	15m	27	Cobalt iron oxide, CoFe ₂ O ₄	9m	22
Chromium rhodium, Cr ₃ Rh	6m	15	Cobalt iron sulfide, Co ₈ FeS ₈	14m	77
Chromium silicide, Cr ₃ Si	6	29	Cobalt iron vanadium, Co _{4.35} Fe _{13.47} V _{12.18}	14m	79
Chromium sulfate, Cr ₂ (SO ₄) ₃	16m	33	Cobalt lanthanum, CoLa ₃	13m	83
Cobalt, Co (cubic)	4m	10	Cobalt lutetium, Co ₂ Lu	13m	86
Cobalt aluminum oxide, CoAl ₂ O ₄	9	27	Cobalt magnesium, Co ₂ Mg	15m	156
Cobalt ammine iodide, Co(NH ₃) ₆ I ₃ ..	10m	83	Cobalt manganese silicide, Co ₂ MnSi	14m	81
Cobalt antimony oxide, CoSb ₂ O ₆	5m	26	Cobalt mercury thiocyanate, Co Hg(CNS) ₄	2m	13
Cobalt arsenide, CoAs ₂	4m	10	Cobalt molybdenum, Co ₂ Mo	14m	82
Cobalt arsenide (skutterudite), CoAs ₃	10	21	Cobalt molybdenum, Co ₂ Mo ₃	15m	158
Cobalt borate, Co ₃ (BO ₃) ₂	12m	20	Cobalt molybdenum, Co ₇ Mo ₆	15m	160
Cobalt bromide hydrate, CoBr ₂ ·6H ₂ O	12m	21	Cobalt molybdenum silicide, Co ₃ Mo ₂ Si	15m	162
Cobalt(II) carbonate (sphaero- cobaltite), CoCO ₃	10	24	Cobalt neodymium, Co ₂ Nd	13m	87
Cobalt chlorate hydrate, Co(ClO ₄) ₂ ·6H ₂ O	3m	28	Cobalt nickel tin, Co _{.75} Ni _{.75} Sn _{.75}	13m	88
Cobalt chloride hydrate, CoCl ₂ ·2H ₂ O	11m	22	Cobalt niobium silicide, Co ₃ Nb ₄ Si ₇	15m	164
Cobalt chloride hydrate, CoCl ₂ ·6H ₂ O	11m	23	Cobalt niobium tin, Co ₂ NbSn	15m	166
Cobalt chromium oxide, CoCr ₂ O ₄	9m	21	Cobalt nitrate hydrate, α-Co(NO ₃) ₂ ·6H ₂ O	12m	22
Cobalt copper tin, CoCu ₂ Sn	14m	64	Cobalt(II) oxide, CoO	9	28
Cobalt dysprosium, Co ₂ Dy	13m	63	Cobalt(II,III) oxide, Co ₃ O ₄	9	29
Cobalt erbium, Co ₂ Er	13m	64	Cobalt phosphate, Co(PO ₃) ₂	13m	23
Cobalt erbium, Co ₇ Er ₂	13m	65	Cobalt phosphate hydrate, Co ₃ (PO ₄) ₂ ·8H ₂ O	19m	40
Cobalt fluoride, CoF ₂	18m	31	Cobalt phosphide, CoP	14m	83
Cobalt fluoride, CoF ₂ (calculated pattern)	10m	85	Cobalt phosphide, CoP ₃	14m	85
Cobalt fluoride hydrate, CoF ₂ ·4H ₂ O	11m	24	Cobalt phosphide, Co ₂ P	18m	32
Cobalt gadolinium, CoGd ₃	13m	68	Cobalt platinum, CoPt (disordered)	15m	167
Cobalt gadolinium, Co ₂ Gd	13m	71	Cobalt platinum, CoPt (ordered) ...	15m	168
Cobalt gadolinium, Co ₇ Gd ₂	13m	72	Cobalt platinum, CoPt ₃ (disordered)	15m	169
Cobalt gallium hafnium, Co ₂ GaHf ...	14m	65	Cobalt platinum, CoPt ₃ (ordered) ..	15m	170
Cobalt gallium manganese, Co ₂ GaMn	13m	75	Cobalt plutonium, CoPu ₂	14m	87
Cobalt gallium niobium, Co _{1.5} Ga _{0.5} Nb	15m	144	Cobalt plutonium, CoPu ₃	15m	171
Cobalt gallium niobium, Co ₂ GaNb ...	14m	66	Cobalt plutonium, CoPu ₆	14m	89
Cobalt gallium oxide, CoGa ₂ O ₄	10	27	Cobalt plutonium, Co ₂ Pu	14m	91
Cobalt gallium tantalum, Co _{1.5} Ga _{0.5} Ta	15m	146	Cobalt plutonium, Co ₃ Pu	14m	92
Cobalt gallium tantalum, Co ₂ GaTa	13m	76	Cobalt plutonium, Co ₁₇ Pu ₂	14m	94
Cobalt gallium titanium, Co ₂ GaTi ..	13m	77	Cobalt praseodymium, Co ₂ Pr	14m	97
Cobalt gallium vanadium, Co ₂ GaV ...	13m	78	Cobalt rhodium sulfide, Co ₂ RhS ₈ ...	14m	98
Cobalt germanium, Co ₃ Ge ₂	14m	67	Cobalt ruthenium sulfide, Co ₂ RuS ₈ ..	14m	100
Cobalt germanium, Co ₅ Ge ₇	15m	148	Cobalt samarium, Co ₂ Sm	15m	173
Cobalt germanium hafnium, Co ₁₆ Ge ₇ Hf ₆	14m	69	Cobalt samarium, Co ₅ Sm	13m	90
			Cobalt silicate, Co ₂ SiO ₄ (orthorhombic)	4m	11

Cobalt silicon fluoride hydrate, $\text{CoSiF}_6 \cdot 6\text{H}_2\text{O}$	3m	27	Erbium phosphate, ErPO_4	9	31
Cobalt sulfate, $\beta\text{-CoSO}_4$	2m	14	Erbium silver, ErAg	5m	67
Cobalt tantalum silicide, $\text{Co}_{16}\text{Ta}_6\text{Si}_7$	14m	102	Erbium telluride, ErTe	4m	55
Cobalt thorium, $\text{Co}_{17}\text{Th}_2$	12m	64	Erbium vanadium oxide, ErVO_4	5m	29
Cobalt tin, Co_3Sn_2	13m	92	Europium arsenate, EuAsO_4	3m	32
Cobalt tin oxide, Co_2SnO_4	15m	30	Europium(III) chloride, EuCl_3	1m	13
Cobalt tin vanadium, Co_2SnV	15m	174	Europium chloride oxide, EuClO	1m	13
Cobalt tin zirconium, Co_2SnZr	15m	175	Europium gallium oxide, $\text{Eu}_3\text{Ga}_5\text{O}_{12}$	2m	17
Cobalt titanium oxide, CoTiO_3	4m	13	Europium nitride, EuN	4m	56
Cobalt titanium silicide, $\text{Co}_{16}\text{Ti}_6\text{Si}_7$	14m	104	Europium oxide, EuO	4m	56
Cobalt tungsten oxide, CoWO_4	4m	13	Europium phosphate, EuPO_4	11m	26
Cobalt vanadium silicide, Co_2VSi ..	15m	176	Europium(III) vanadium oxide, EuVO_4	4m	16
Copper, Cu	1	15	Gadolinium arsenate, GdAsO_4	4m	17
Copper ammine selenate, $\text{Cu}(\text{NH}_3)_4\text{SeO}_4$	10m	87	Gadolinium arsenide, GdAs	4m	57
Copper ammine sulfate hydrate, $\text{Cu}(\text{NH}_3)_4\text{SO}_4 \cdot \text{H}_2\text{O}$	10m	90	Gadolinium chloride hydrate, $\text{GdCl}_3 \cdot 6\text{H}_2\text{O}$	7m	118
Copper antimony oxide, CuSb_2O_6	5m	27	Gadolinium chloride oxide, GdClO ..	1m	17
Copper arsenate (trippkeite), CuAs_2O_4	16m	120	Gadolinium fluoride, GdF_3	1m	14
Copper(I) bromide, CuBr	4	36	Gadolinium gallium oxide, $\text{Gd}_3\text{Ga}_5\text{O}_{12}$	2m	18
Copper(I) chloride (nantokite), CuCl	4	35	Gadolinium indium, GdIn	5m	67
Copper chloride hydrate (eriochalcite), $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$	18m	33	Gadolinium nitride, GdN	4m	57
Copper fluoride hydrate, $\text{CuF}_2 \cdot 2\text{H}_2\text{O}$	11m	25	Gadolinium oxide, Gd_2O_3	1m	16
Copper hydrogen phosphite hydrate, $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$	11m	83	Gadolinium silver, GdAg	6m	87
Copper hydroxide carbonate, azurite, $\text{Cu}_3(\text{OH})_2(\text{CO}_3)_2$	10	30	Gadolinium titanium oxide, Gd_2TiO_5	8m	32
Copper hydroxide carbonate (malachite), $\text{Cu}_2(\text{OH})_2\text{CO}_3$	10	31	Gadolinium vanadium oxide, GdVO_4 ..	5m	30
Copper hydroxide phosphate (libethenite), $\text{Cu}_2(\text{OH})\text{PO}_4$	17m	30	Gallium, Ga	2	9
Copper(I) iodide (marshite), CuI ..	4	38	Gallium arsenide, GaAs	3m	33
Copper lead hydroxide sulfate, linarite, $\text{CuPb}(\text{OH})_2(\text{SO}_4)$	16m	34	Gallium lutetium oxide, $\text{Ga}_5\text{Lu}_3\text{O}_{12}$	2m	22
Copper(I) oxide (cuprite), Cu_2O ..	2	23	Gallium magnesium, Ga_2Mg	12m	48
Copper(II) oxide (tenorite), CuO ..	1	49	Gallium magnesium, Ga_5Mg_2	12m	51
Copper phosphate, $\text{Cu}(\text{PO}_3)_2$	14m	15	Gallium neodymium oxide, $\text{Ga}_5\text{Nd}_3\text{O}_{12}$	1m	34
Copper phosphate, $\alpha\text{-Cu}_2\text{P}_2\text{O}_7$	7m	113	Gallium oxide, $\alpha\text{-Ga}_2\text{O}_3$	4	25
Copper sulfate (chalcocyanite), CuSO_4	3m	29	Gallium phosphate (α -quartz type), GaPO_4	8	27
Copper(II) sulfide (covellite), CuS	4	13	Gallium phosphate hydrate, $\text{GaPO}_4 \cdot 2\text{H}_2\text{O}$	8m	34
Copper uranium oxide, CuUO_4	10m	93	Gallium samarium oxide, $\text{Ga}_5\text{Sm}_3\text{O}_{12}$	1m	42
Dichlorotetraaquochromium (III) chloride dihydrate, $\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2 \cdot \text{Cl} \cdot 2\text{H}_2\text{O}$	16m	31	Gallium ytterbium oxide, $\text{Ga}_5\text{Yb}_3\text{O}_{12}$	1m	49
Dysprosium arsenate, DyAsO_4	3m	30	Gallium yttrium oxide, $\text{Ga}_5\text{Y}_3\text{O}_{12}$..	1m	50
Dysprosium arsenide, DyAs	4m	53	Germanium, Ge	1	18
Dysprosium gallium oxide, $\text{Dy}_3\text{Ga}_5\text{O}_{12}$	2m	15	Germanium iodide, GeI_2	4m	58
Dysprosium gold, DyAu	5m	66	Germanium(IV) iodide, GeI_4	5	25
Dysprosium nitride, DyN	4m	53	Germanium oxide, GeO_2 (hexagonal) (low form)	1	51
Dysprosium oxide, Dy_2O_3	9	30	Germanium oxide, GeO_2 (tetragonal) (high form)	8	28
Dysprosium silver, DyAg	5m	66	Gold, Au	1	33
Dysprosium telluride, DyTe	4m	54	Gold chloride, AuCl	16m	37
Dysprosium vanadium oxide, DyVO_4 ..	4m	15	Gold(I) cyanide, AuCN	10	33
Erbium arsenate, ErAsO_4	3m	31	Gold holmium, AuHo	5m	68
Erbium arsenide, ErAs	4m	54	Gold magnesium, AuMg	6m	83
Erbium gallium oxide, $\text{Er}_3\text{Ga}_5\text{O}_{12}$..	1m	12	Gold niobium, AuNb_3	6m	16
Erbium iron, ErFe_2	19m	42	Gold potassium cyanide, $\text{AuK}(\text{CN})_2$..	8m	36
Erbium manganese oxide, ErMnO_3	2m	16	Gold tin, AuSn	7	19
Erbium nitride, ErN	4m	55	Gold titanium, AuTi_3	6m	17
Erbium oxide, Er_2O_3	8	25	Gold vanadium, AuV_3	6m	18
			Hafnium, Hf	3	18
			Hafnium nitride, HfN	19m	46
			Holmium arsenate, HoAsO_4	3m	34
			Holmium fluoride, HoF_3	10m	23
			Holmium nitride, HoN	4m	58
			Holmium oxide, Ho_2O_3	9	32
			Holmium selenide, HoSe	4m	59
			Holmium silver, HoAg	5m	68
			Holmium vanadium oxide, HoVO_4	4m	18
			Hydrazinium sulfate, $(\text{NH}_3)_2\text{SO}_4$	17m	38
			Hydrogen amidosulfate, $\text{H}_2\text{NSO}_3\text{H}$	7	54

	Vol. or Sec.	Page		Vol. or Sec.	Page
Hydrogen arsenate, $H_5As_3O_{10}$	7m	84	Lanthanum oxide, La_2O_3	3	33
Hydrogen borate, $\beta\text{-HBO}_2$ (monoclinic)	9m	71	Lanthanum phosphide, LaP	5m	69
Hydrogen borate (metaborite), HBO_2 (cubic)	4m	27	Lanthanum selenide, $LaSe$	4m	61
Hydrogen iodate, HIO_3	5	28	Lanthanum titanium oxide, $La_2Ti_2O_7$	15m	35
Hydrogen iodate, HI_3O_8	8m	104	Lanthanum zinc, $LaZn$	5m	70
Hydrogen phosphate hydrate, $H_3PO_4 \cdot 0.5H_2O$	12m	56	Lead, Pb	1	34
Hydrogen tellurate, H_6TeO_6	12m	34	Lead borate, PbB_4O_7	4m	19
Indium, In	3	12	Lead bromide, $PbBr_2$	17m	43
Indium arsenide, $InAs$	3m	35	Lead bromide chloride, $PbBrCl$	11m	33
Indium oxide, In_2O_3	5	26	Lead bromide fluoride, $PbBrF$	10m	25
Indium phosphate, $InPO_4$	8	29	Lead bromide hydroxide, $PbBr(OH)$..	16m	40
Indium sulfide, In_2S_3	11m	30	Lead bromide oxide, $Pb_3O_2Br_2$	5m	32
Iodine, I_2	3	16	Lead carbonate (cerussite), $PbCO_3$	2	56
Iridium, Ir	4	9	Lead chloride (cotunnite), $PbCl_2$..	12m	23
Iridium niobium, $IrNb_3$	6m	19	Lead chloride fluoride (matlockite), $PbClF$	13m	25
Iridium oxide, IrO_2	4m	19	Lead chromium oxide, Pb_2CrO_5	14m	16
Iridium titanium, $IrTi_3$	6m	20	Lead fluoride, $\alpha\text{-PbF}_2$ (orthorhombic)	5	31
Iridium vanadium, IrV_3	6m	21	Lead fluoride, $\beta\text{-PbF}_2$ (cubic)	5	33
Iron, $\alpha\text{-Fe}$	4	3	Lead fluoride iodide, $PbFI$	10m	26
Iron aluminum oxide (hercynite), $FeAl_2O_4$	19m	48	Lead hydrogen arsenate (schultenite), $PbHAsO_4$	14m	18
Iron antimony oxide, $FeSbO_4$	19m	49	Lead hydrogen phosphate, $PbHPO_4$	15m	37
Iron arsenide, $FeAs$	1m	19	Lead hydroxide phosphate, $Pb_5OH(Po_4)_3$	8	33
Iron arsenide (loellingite), $FeAs_2$	10	34	Lead iodate, $Pb(Io_3)_2$	17m	45
Iron boride, FeB	18m	35	Lead(II) iodide, PbI_2	5	34
Iron bromide, $FeBr_2$	4m	59	Lead molybdenum oxide (wulfenite), $PbMoO_4$	7	23
Iron carbonate, siderite, $FeCO_3$..	15m	32	Lead nitrate, $Pb(NO_3)_2$	5	36
Iron chloride hydrate (rokuhnite), $FeCl_2 \cdot 2H_2O$	11m	32	Lead oxide (litharge), PbO (red, tetragonal)	2	30
Iron chloride hydrate (hydromolysite), $FeCl_3 \cdot 6H_2O$	17m	40	Lead oxide (massicot), PbO (yellow, orthorhombic)	2	32
Iron chromium oxide (chromite), $FeCr_2O_4$	19m	50	Lead(II,III) oxide (minium), Pb_3O_4	8	32
Iron fluoride hydrate, $FeF_2 \cdot 4H_2O$	11m	90	Lead oxide sulfate, $Pb_5O_5S_4$	10m	27
Iron fluoride, FeF_3	18m	36	Lead selenide (clausthalite), $PbSe$	5	38
Iron fluoride hydrate, $\beta\text{-FeF}_3 \cdot 3H_2O$	17m	41	Lead strontium nitrate, $Pb_{.33}Sr_{.67}(NO_3)_2$	12m	53
Iron hydroxide sulfate hydrate, butlerite, $Fe(OH)SO_4 \cdot 2H_2O$	10m	95	Lead strontium nitrate, $Pb_{.67}Sr_{.33}(NO_3)_2$	12m	53
Iron iodide, FeI_2	4m	60	Lead sulfate (anglesite), $PbSO_4$	3	67
Iron oxide (hematite), $\alpha\text{-Fe}_2O_3$..	18m	37	Lead sulfide (galena), PbS	2	18
Iron(II,III) oxide (magnetite), Fe_3O_4	5m	31	Lead tin oxide, Pb_2SnO_4	10m	29
Iron phosphate, $FePO_4$	15m	33	Lead titanium oxide (macedonite), $PbTiO_3$	5	39
Iron phosphate hydrate (vivianite), $Fe_3(PO_4)_2 \cdot 8H_2O$	16m	38	Lead tungsten oxide (stolzite), $PbWO_4$ (tetragonal)	5m	34
Iron sulfate, $Fe_2(SO_4)_3$	16m	39	Lead uranium oxide, Pb_3UO_6	8m	109
Iron sulfate hydrate (melanterite), $FeSO_4 \cdot 7H_2O$	8m	38	Lithium aluminum fluoride, $\alpha\text{-Li}_3AlF_6$	8m	111
Iron sulfide (pyrite), FeS_2	5	29	Lithium arsenate, Li_3AsO_4	2m	19
Iron thorium, $Fe_{17}Th_2$	12m	67	Lithium azide, LiN_3	8m	113
Iron titanium oxide (ilmenite), $FeTiO_3$	15m	34	Lithium barium fluoride, $LiBaF_3$	5m	35
Iron yttrium oxide, $Fe_5Y_3O_{12}$	18m	38	Lithium beryllium fluoride, Li_2BeF_4	7m	126
Lanthanum arsenate, $LaAsO_4$	3m	36	Lithium borate, $Li_2B_4O_7$	8m	114
Lanthanum arsenide, $LaAs$	4m	60	Lithium bromide, $LiBr$	4	30
Lanthanum borate, $LaBO_3$	1m	20	Lithium calcium aluminum boron hydroxy silicate, liddicoatite, $Ca(Li,Al)_3Al_6B_3Si_6O_{27}(O,OH)_3(OH,F)$	16m	42
Lanthanum chloride, $LaCl_3$	1m	20	Lithium carbonate, Li_2CO_3	8m	42
Lanthanum chloride oxide, $LaClO$..	7	22	Lithium chlorate hydrate, $LiClO_4 \cdot 3H_2O$	8	34
Lanthanum fluoride, LaF_3	7	21	Lithium chloride, $LiCl$	1	62
Lanthanum magnesium, $LaMg$	5m	69	Lithium chromium oxide hydrate, $Li_2CrO_4 \cdot 2H_2O$	16m	44
Lanthanum nickel platinum, $LaNi_{0.25}Pt_{4.75}$	17m	42	Lithium fluoride, LiF	1	61
Lanthanum niobium titanium oxide, $LaNbTiO_6$	3m	37	Lithium gallium oxide, $LiGaO_2$	10m	31
Lanthanum nitrate hydrate, $La(NO_3)_3 \cdot 6H_2O$	8m	40			
Lanthanum nitride, LaN	4m	61			

	Vol. or Sec.	Page		Vol. or Sec.	Page
Lithium hydroxide, LiOH	17m	46	Magnesium cerium nitrate hydrate, $Mg_3Ce_2(NO_3)_{12} \cdot 24H_2O$	10	20
Lithium hydroxide hydrate, LiOH·H ₂ O	11m	92	Magnesium chlorate hydrate, $Mg(ClO_4)_2 \cdot 6H_2O$	7m	30
Lithium iodate, LiIO ₃ (hexagonal)	7	26	Magnesium chloride (chloro- magnesite), MgCl ₂	11m	94
Lithium iodate, LiIO ₃ (tetragonal)	10m	33	Magnesium chloride hydrate, $MgCl_2 \cdot 12H_2O$	7m	135
Lithium iodide hydrate, LiI·3H ₂ O ..	18m	40	Magnesium chloride hydrate (bischofite), MgCl ₂ ·6H ₂ O	11m	37
Lithium molybdenum oxide, Li ₂ MoO ₄ (trigonal)	1m	23	Magnesium chromium oxide (magnesiochromite), MgCr ₂ O ₄	9	34
Lithium niobium oxide, LiNbO ₃	6m	22	Magnesium chromium oxide hydrate, $MgCrO_4 \cdot 5H_2O$	15m	39
Lithium nitrate, LiNO ₃	7	27	Magnesium fluoride (sellaite), MgF ₂	4	33
Lithium oxide, Li ₂ O	1m	25	Magnesium fluoride silicate (humite), Mg ₇ F ₂ Si ₃ O ₁₂	1m	30
Lithium phosphate, high form, Li ₃ PO ₄	3m	39	Magnesium fluoride silicate (norbergite), Mg ₃ F ₂ SiO ₄	10	39
Lithium phosphate, low form (lithiophosphate), Li ₃ PO ₄	4m	21	Magnesium gallium oxide, MgGa ₂ O ₄	10	36
Lithium phosphate hydrate, Li ₃ P ₃ O ₉ ·3H ₂ O	2m	20	Magnesium germanium oxide, Mg ₂ GeO ₄ (cubic)	10	37
Lithium potassium sulfate, KLiSO ₄	3m	43	Magnesium germanium oxide, Mg ₂ GeO ₄ (orthorhombic)	10	38
Lithium rubidium fluoride, LiRbF ₂	7m	128	Magnesium hydrogen phosphate hydrate, newberryite, MgHPO ₄ ·3H ₂ O	7m	139
Lithium selenide, Li ₂ Se	10m	100	Magnesium hydroxide (brucite), Mg(OH) ₂	6	30
Lithium silicate, Li ₂ SiO ₃	14m	19	Magnesium iodate hydrate, Mg(I ₀ 3) ₂ ·4H ₂ O	17m	48
Lithium silver bromide, Li ₂ Ag ₈ Br	12m	55	Magnesium iron hydroxide carbonate hydrate, pyroaurite, Mg ₆ Fe ₂ (OH) ₁₆ CO ₃ ·4H ₂ O (rhomb.)	10m	104
Lithium silver bromide, Li ₄ Ag ₆ Br	12m	55	Magnesium iron hydroxide carbonate hydrate, sjögrenite, Mg ₆ Fe ₂ (OH) ₁₆ CO ₃ ·4H ₂ O, (hexag.)	10m	103
Lithium silver bromide, Li ₆ Ag ₄ Br	12m	55	Magnesium lanthanum nitrate hydrate, Mg ₃ La ₂ (NO ₃) ₁₂ ·24H ₂ O	1m	22
Lithium silver bromide, Li ₈ Ag ₂ Br	12m	55	Magnesium manganese oxide, MgMn ₂ O ₄	10m	35
Lithium sodium aluminum fluoride, cryolithionite, Li ₃ Na ₃ Al ₂ F ₁₂	9m	23	Magnesium mercury, MgHg	6m	84
Lithium sodium sulfate, LiNaSO ₄	6m	24	Magnesium molybdenum oxide, MgMoO ₄	7m	28
Lithium sulfate, Li ₂ SO ₄	6m	26	Magnesium nickel oxide, MgNiO ₂	10m	36
Lithium sulfate hydrate, Li ₂ SO ₄ ·H ₂ O	4m	22	Magnesium oxide (periclase), MgO	1	37
Lithium sulfide, Li ₂ S	10m	101	Magnesium phosphate, Mg(PO ₃) ₂	13m	26
Lithium tantalum oxide, LiTaO ₃	14m	20	Magnesium phosphate, α-Mg ₂ P ₂ O ₇	18m	41
Lithium telluride, Li ₂ Te	10m	102	Magnesium phosphate (farringtonite), Mg ₃ (PO ₄) ₂	19m	55
Lithium tin oxide, Li ₂ SnO ₃	16m	45	Magnesium selenide, MgSe	5m	70
Lithium tungsten oxide, Li ₂ WO ₄ (trigonal)	1m	25	Magnesium selenite hydrate, MgSeO ₃ ·6H ₂ O	8m	116
Lithium tungsten oxide hydrate, Li ₂ WO ₄ ·0.5H ₂ O	2m	20	Magnesium silicate, enstatite, MgSiO ₃	6	32
Lithium uranium fluoride, LiUF ₅	7m	131	Magnesium silicate (forsterite), Mg ₂ SiO ₄	1	83
Lithium zirconium oxide, Li ₂ ZrO ₃	19m	51	Magnesium sulfate hydrate (kieserite), MgSO ₄ ·H ₂ O	16m	46
Lutetium arsenate, LuAsO ₄	5m	36	Magnesium sulfate hydrate (epsomite), MgSO ₄ ·7H ₂ O	7	30
Lutetium manganese oxide, LuMnO ₃	2m	23	Magnesium sulfide, MgS	7	31
Lutetium nitride, LuN	4m	62	Magnesium sulfite hydrate, MgSO ₃ ·6H ₂ O	9m	26
Lutetium oxide, Lu ₂ O ₃	1m	27	Magnesium tin, Mg ₂ Sn	5	41
Lutetium vanadium oxide, LuVO ₄	5m	37	Magnesium tin oxide, Mg ₂ SnO ₄	10m	37
Magnesium, Mg	1	10	Magnesium titanium oxide (geikielite), MgTiO ₃	5	43
Magnesium aluminum oxide (spinel), MgAl ₂ O ₄	9m	25	Magnesium titanium oxide, Mg ₂ TiO ₄	12m	25
Magnesium aluminum silicate (low cordierite), Mg ₂ Al ₄ Si ₅ O ₁₈ (orthorhombic)	1m	28	Magnesium tungsten oxide, MgW ₀ 4	13m	27
Magnesium aluminum silicate (indialite) Mg ₂ Al ₄ Si ₅ O ₁₈ (hexagonal)	1m	29	Manganese, α-Mn (calculated pattern)	7m	142
Magnesium aluminum silicate (pyrope), Mg ₃ Al ₂ (SiO ₄) ₂	4m	24	Manganese, α-Mn	17m	50
Magnesium arsenate hydrate (hoernesite), Mg ₃ (AsO ₄) ₂ ·8H ₂ O	19m	53			
Magnesium borate, MgB ₄ O ₇	17m	47			
Magnesium borate, Mg ₂ B ₂ O ₅ (triclinic)	4m	25			
Magnesium bromide, MgBr ₂	4m	62			
Magnesium bromide hydrate, MgBr ₂ ·6H ₂ O	11m	35			
Magnesium carbonate (magnesite), MgCO ₃	7	28			

	Vol. or Sec.	Page		Vol. or Sec.	Page
Manganese, β -Mn	18m	43	Molybdenum oxide (molybdite), MoO_3	3	30
Manganese aluminum oxide (galaxite), $MnAl_2O_4$	9	35	Molybdenum silicide, Mo_5Si_3	19m	59
Manganese bromide, $MnBr_2$	4m	63	Molybdenum sulfide (molybdenite), MoS_2	5	47
Manganese(II) carbonate (rhodochrosite), $MnCO_3$	7	32	Neodymium arsenate, $NdAsO_4$	4m	28
Manganese chloride (scacchite), $MnCl_2$	8m	43	Neodymium arsenide, $NdAs$	4m	64
Manganese chloride hydrate, $MnCl_2 \cdot 2H_2O$	11m	38	Neodymium borate, NdB_3O_3	1m	32
Manganese chloride hydrate, $MnCl_2 \cdot 4H_2O$	9m	28	Neodymium chloride, $NdCl_3$	1m	33
Manganese cobalt oxide, $MnCo_2O_4$	9m	30	Neodymium chloride oxide, $NdOCl$	8	37
Manganese fluoride, MnF_2	10m	105	Neodymium fluoride, NdF_3	8	36
Manganese iodide, MnI_2	4m	63	Neodymium oxide, Nd_2O_3	4	26
Manganese iron oxide (jacobsite), $MnFe_2O_4$	9	36	Neodymium phosphate, $NdPO_4$	11m	40
Manganese(II) oxide (manganosite), MnO	5	45	Neodymium selenide, $NdSe$	5m	71
Manganese oxide (pyrolusite), β - MnO_2	10m	39	Neodymium silver, $NdAg$	5m	71
Manganese oxide (bixbyite), α - Mn_2O_3	11m	95	Neodymium tantalum oxide, $NdTaO_4$	18m	46
Manganese oxide (hausmannite), Mn_3O_4	10m	38	Neodymium titanium oxide, Nd_2TiO_5	18m	48
Manganese oxide hydroxide, groutite, α - $MnOOH$	11m	97	Neodymium titanium oxide, $Nd_2Ti_2O_7$	18m	50
Manganese phosphate, $Mn(Po_3)_2$	14m	21	Neodymium titanium oxide, $Nd_4Ti_9O_{24}$	18m	52
Manganese phosphate, $Mn_2P_2O_7$	15m	41	Neodymium vanadium oxide, $NdVO_4$	4m	30
Manganese phosphate, $Mn_3(PO_4)_2$	16m	47	Neptunium nitride, NpN	4m	64
Manganese selenide, $MnSe$	10	41	Nickel, Ni	1	13
Manganese sulfate hydrate (szmkikite), $MnSO_4 \cdot H_2O$	16m	49	Nickel aluminum oxide, $NiAl_2O_4$	9	42
Manganese sulfide (alabandite), α - MnS	4	11	Nickel arsenate hydrate (annabergite), $Ni_3(AsO_4)_2 \cdot 8H_2O$	19m	60
Manganese titanium oxide (pyrophanite), $MnTiO_3$	15m	42	Nickel arsenide (rammelsbergite), $NiAs_2$	10	42
Manganese(II) tungsten oxide (huebnerite), $MnWO_4$	2m	24	Nickel arsenic sulfide (gersdorffite), $NiAsS$	1m	35
Manganese vanadium oxide, $Mn_2V_2O_7$	9m	75	Nickel bromide, $NiBr_2$	10m	119
Mercury amide chloride, $HgNH_2Cl$	10m	40	Nickel(II) carbonate, $NiCO_3$ (trigonal)	1m	36
Mercury amine chloride, $Hg(NH_3)_2Cl_2$	11m	39	Nickel chloride, $NiCl_2$	9m	81
Mercury bromate, $Hg(BrO_3)_2$	10m	107	Nickel chloride hydrate, $NiCl_2 \cdot 6H_2O$	11m	42
Mercury bromide, $HgBr_2$	10m	110	Nickel fluoride, NiF_2	10m	121
Mercury bromide, Hg_2Br_2	7	33	Nickel fluoride hydrate, $NiF_2 \cdot 4H_2O$	11m	43
Mercury chloride, $HgCl_2$	13m	29	Nickel gallium oxide, $NiGa_2O_4$	10	45
Mercury chloride (calomel), Hg_2Cl_2	13m	30	Nickel germanium oxide, Ni_2GeO_4	9	43
Mercury chloride sulfide, α - $Hg_3Cl_2S_2$	8m	118	Nickel iron oxide (trevorite), $NiFe_2O_4$	10	44
Mercury(II) cyanide, $Hg(CN)_2$	6	35	Nickel molybdenum oxide, $NiMoO_4$	19m	62
Mercury(II) fluoride, HgF_2	2m	25	Nickel nitrate hydrate, $Ni(NO_3)_2 \cdot 6H_2O$	12m	26
Mercury hydroxide nitrate, $Hg(OH)NO_3$	17m	52	Nickel(II) oxide (bunsenite), NiO	1	47
Mercury(I) iodide, HgI	4	49	Nickel phosphate, $Ni(Po_3)_2$	14m	22
Mercury(II) iodide, HgI_2 (tetragonal)	7m	32	Nickel phosphate hydrate, $Ni_3(PO_4)_2 \cdot 8H_2O$	19m	64
Mercury(II) oxide (montroydite), HgO	9	39	Nickel phosphide, $Ni_{12}P_5$	9m	83
Mercury(II) selenide (tiemannite), $HgSe$	7	35	Nickel silicon fluoride hydrate, $NiSiF_6 \cdot 6H_2O$	8	38
Mercury sulfate, $HgSO_4$	16m	50	Nickel sulfate, $NiSO_4$	2m	26
Mercury sulfate, Hg_2SO_4	16m	52	Nickel sulfate hydrate (retgersite), $NiSO_4 \cdot 6H_2O$ (tetragonal)	7	36
Mercury(II) sulfide (cinnabar), HgS (hexagonal)	4	17	Nickel sulfate hydrate (nickel-hexahydrite), β - $NiSO_4 \cdot 6H_2O$ (monoclinic)	19m	65
Mercury(II) sulfide (metacinnabar), HgS (cubic)	4	21	Nickel sulfide, millerite, NiS	1m	37
Molybdenum, Mo	1	20	Nickel titanium oxide, $NiTiO_3$	18m	54
Molybdenum arsenide, Mo_2As_3	10m	115	Nickel tungsten oxide, $NiWO_4$	2m	27
Molybdenum osmium, Mo_3Os	6m	28	Nickel yttrium, Ni_3Y	10m	123
Molybdenum oxide, MoO_2	18m	44	Niobium, Nb (monoclinic)	19m	67
			Niobium boride, ζ - NbB	17m	54
			Niobium chloride oxide, $NbCl_3O$	7m	148
			Niobium osmium, Nb_3Os	6m	30
			Niobium platinum, Nb_3Pt	6m	31
			Niobium silicide, $NbSi_2$	8	39
			Niobium silicide, α - Nb_5Si_3	15m	43
			Niobium silicide, β - Nb_5Si_3	15m	44
			Osmium, Os	4	8

	Vol. or Sec.	Page		Vol. or Sec.	Page
Osmium titanium, OsTi	6m	85	Potassium chromium oxide sulfate, $K_2(CrO_4)_{.33}(SO_4)_{.67}$	12m	28
Palladium, Pd	1	21	Potassium chromium oxide sulfate, $K_2(CrO_4)_{.67}(SO_4)_{.33}$	12m	27
Palladium hydride, $PdH_{0.706}$	5m	72	Potassium chromium sulfate, $KCr(SO_4)_2$	16m	58
Palladium oxide, PdO	4	27	Potassium chromium sulfate hydrate, $KCr(SO_4)_2 \cdot 12H_2O$	6	39
Palladium selenium (palladseite), $Pd_{17}Se_{15}$	16m	139	Potassium cobalt(II) fluoride, $KCoF_3$	6m	37
Palladium vanadium, PdV_3	6m	32	Potassium cobalt fluoride, K_2CoF_4	11m	46
Phosphorus bromide, PBr_7	7m	150	Potassium cobalt nitrite, $K_3Co(NO_2)_6$	9	45
Phosphorus oxide (stable form I), P_2O_5 (orthorhombic)	9m	86	Potassium cobalt(II) sulfate, $K_2Co_2(SO_4)_3$	6m	35
Phosphorus oxide (stable form II), P_2O_5 (orthorhombic)	9m	88	Potassium copper chloride, $KCuCl_3$	7m	41
Phosphorus oxide (metastable form), P_4O_{10} (rhombohedral)	9m	91	Potassium copper chloride hydrate (mitscherlichite), $K_2CuCl_4 \cdot 2H_2O$..	9m	34
Platinum, Pt	1	31	Potassium copper(II) fluoride, $KCuF_3$	6m	38
Platinum titanium, $PtTi_3$	6m	33	Potassium cyanate, $KCNO$	7	39
Platinum vanadium, PtV_3	6m	34	Potassium cyanide, KCN	1	77
Plutonium arsenide, $PuAs$	4m	65	Potassium fluoride, KF	1	64
Plutonium phosphide, PuP	4m	65	Potassium fluoride hydrate, $KF \cdot 2H_2O$..	18m	55
Plutonium telluride, $PuTe$	4m	66	Potassium germanium fluoride, K_2GeF_6	6	41
Potassium aluminum sulfate, $KAl(SO_4)_2$	9m	31	Potassium hydrogen arsenate, KH_2AsO_4	1m	38
Potassium aluminum sulfate hydrate (potash alum), $KAl(SO_4)_2 \cdot 12H_2O$..	6	36	Potassium hydrogen iodate, $KH(IO_3)_2$	17m	58
Potassium arsenic fluoride, $KAsF_6$	17m	57	Potassium hydrogen phosphate, KH_2PO_4	3	69
Potassium barium chromium oxide, $K_2Ba(CrO_4)_2$	14m	23	Potassium hydroxide, KOH at $300^{\circ}C$..	4m	66
Potassium barium iron titanium oxide, $K_{1.16}Ba_{0.72}Fe_{0.36}Ti_{5.58}O_{13}$..	16m	147	Potassium iodate, KIO_3	15m	48
Potassium barium molybdenum oxide, $K_2Ba(MoO_4)_2$	14m	24	Potassium iodate, KIO_4	7	41
Potassium barium nickel nitrite, $K_2BaNi(NO_2)_6$	9m	32	Potassium iodide, KI	1	68
Potassium barium phosphate, $KBaPO_4$	19m	68	Potassium iron chloride hydrate (erythrosiderite), $K_2FeCl_5 \cdot H_2O$..	14m	27
Potassium borate hydroxide hydrate, $K_2B_4O_5(OH)_4 \cdot 2H_2O$	15m	46	Potassium iron cyanide, $K_3Fe(CN)_6$..	9m	35
Potassium calcium phosphate, $KCaPO_4$	19m	70	Potassium iron cyanide, $K_4Fe(CN)_6$..	18m	56
Potassium boron hydride, KBH_4	9	44	Potassium iron(II) fluoride, $KFeF_3$..	6m	39
Potassium bromate, $KBrO_3$	7	38	Potassium iron fluoride, K_3FeF_6 ..	9m	37
Potassium bromide, KBr	1	66	Potassium iron sulfate (yavapaiite), $KFe(SO_4)_2$	16m	59
Potassium bromide chloride, $KBr_{0.5}Cl_{0.5}$	8m	46	Potassium lead chloride, KPb_2Cl_5 ..	13m	33
Potassium bromide iodide, $KBr_{.33}I_{.67}$	11m	44	Potassium lead chromium oxide, $K_2Pb(CrO_4)_2$	14m	28
Potassium bromide iodide, $KBr_{.67}I_{.33}$..	11m	45	Potassium lead molybdenum oxide, $K_2Pb(MoO_4)_2$	14m	29
Potassium cadmium fluoride, $KCdF_3$	8m	47	Potassium lead phosphate, $K_2Pb(PO_3)_4$	15m	50
Potassium cadmium sulfate, $K_2Cd_2(SO_4)_3$	7m	34	Potassium lead selenate, $K_2Pb(SeO_4)_2$	15m	52
Potassium calcium carbonate (fairchildite), $K_2Ca(CO_3)_2$	8m	48	Potassium lead sulfate (palmierite), $K_2Pb(SO_4)_2$	14m	30
Potassium calcium chloride, $KCaCl_3$	7m	36	Potassium magnesium chloride hydrate (carnallite), $KMgCl_3 \cdot 6H_2O$..	8m	50
Potassium calcium fluoride, $KCaF_3$	8m	49	Potassium magnesium chromium oxide, $K_2Mg_2(CrO_4)_3$	8m	52
Potassium calcium magnesium sulfate, $K_2CaMg(SO_4)_3$	7m	37	Potassium magnesium fluoride, $KMgF_3$..	6m	42
Potassium calcium nickel nitrite, $K_2CaNi(NO_2)_6$	9m	33	Potassium magnesium fluoride, K_2MgF_4 ..	10m	42
Potassium calcium sulfate, $K_2Ca_2(SO_4)_3$	7m	39	Potassium magnesium selenate hydrate, $K_2Mg(SeO_4)_2 \cdot 6H_2O$	10m	43
Potassium calcium sulfate hydrate (syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$	14m	25	Potassium magnesium sulfate (langbeinite), $K_2Mg_2(SO_4)_3$	6m	40
Potassium cerium fluoride, $\beta-KCeF_4$	12m	59	Potassium magnesium sulfate hydrate (picromerite), $K_2Mg(SO_4)_2 \cdot 6H_2O$..	8m	54
Potassium chlorate, $KClO_3$	3m	42	Potassium manganese(II) fluoride, $KMnF_3$	6m	45
Potassium chlorate, $KClO_4$	6	43			
Potassium chloride (sylvite), KCl	1	65			
Potassium chromium oxide, K_3CrO_8 ..	3m	44			
Potassium chromium oxide (lopezite), $K_2Cr_2O_7$	15m	47			

	Vol. or Sec.	Page		Vol. or Sec.	Page
Potassium manganese oxide, $KMnO_4$	7	42	Potassium sulfate, $K_2S_2O_8$	17m	64
Potassium manganese(II) sulfate (manganolangbeinite), $K_2Mn_2(SO_4)_3$	6m	43	Potassium sulfate (arcanite), K_2SO_4	3	62
Potassium molybdenum oxide, K_2MoO_4	15m	53	Potassium sulfide, K_2S	10m	127
Potassium molybdenum oxide phos- phate hydrate, $K_3(MoO_3)_{12}PO_4 \cdot 4H_2O$	8	43	Potassium telluride, K_2Te	10m	128
Potassium nickel fluoride, $KNiF_3$	7m	42	Potassium thiocyanate, $KCNS$	8	44
Potassium nickel fluoride, K_2NiF_4	10m	45	Potassium tin chloride, K_2SnCl_6	6	38
Potassium nickel(II) sulfate, $K_2Ni_2(SO_4)_3$	6m	46	Potassium titanium fluoride, K_2TiF_6	7	40
Potassium niobium fluoride, K_2NbF_7	8m	120	Potassium tungsten oxide, K_2WO_4	11m	47
Potassium niobium oxide, $KNbO_3$	17m	62	Potassium vanadium oxide, KVO_3	18m	57
Potassium nitrate (niter), KNO_3 ...	3	58	Potassium vanadium oxide, KV_3O_8	8m	56
Potassium nitrite, KNO_2	9m	38	Potassium zinc bromide hydrate, $KZnBr_3 \cdot 2H_2O$	11m	104
Potassium nitrosyl ruthenium chloride, $K_2NORuCl_5$	16m	61	Potassium zinc fluoride, $KZnF_3$	5	51
Potassium oxide, K_2O	10m	125	Potassium zinc fluoride, K_2ZnF_4	10m	46
Potassium platinum bromide, K_2PtBr_6	8	40	Potassium zinc iodide hydrate, $KZnI_3 \cdot 2H_2O$	11m	107
Potassium platinum chloride, K_2PtCl_6	13m	34	Potassium zinc sulfate, $K_2Zn_2(SO_4)_3$	6m	54
Potassium platinum fluoride, K_2PtF_6	6	42	Potassium zinc sulfate hydrate, $K_2Zn(SO_4)_2 \cdot 6H_2O$	7m	43
Potassium rhenium chloride, K_2ReCl_6	2m	28	Potassium zinc vanadium oxide hydrate, $K_2Zn_2V_{10}O_{28} \cdot 16H_2O$	3m	45
Potassium rhenium oxide, $KReO_4$	8	41	Potassium zirconium fluoride, K_3ZrF_7	9	46
Potassium rubidium chloride, $K_{0.5}Rb_{0.5}Cl$	8m	76	Praseodymium arsenate, $PrAsO_4$	4m	32
Potassium rubidium chromium oxide, $KRbCrO_4$	12m	29	Praseodymium arsenide, $PrAs$	4m	67
Potassium ruthenium chloride, K_2RuCl_6	10	46	Praseodymium chloride, $PrCl_3$	1m	39
Potassium ruthenium oxide chloride hydrate, $K_4Ru_2OCl_{10} \cdot H_2O$	10	47	Praseodymium chloride oxide, $PrOCl$	9	47
Potassium selenate, K_2SeO_4	9m	41	Praseodymium fluoride, PrF_3	5	52
Potassium selenide, K_2Se	10m	126	Praseodymium sulfide, PrS	4m	67
Potassium selenium bromide, K_2SeBr_6	8	41	Praseodymium vanadium oxide, $PrVO_4$	5m	40
Potassium silicon fluoride (hieratite), K_2SiF_6	5	50	Praseodymium zinc, $PrZn$	5m	72
Potassium silver cyanide, $KAg(CN)_2$	8m	78	Rhenium, Re	2	13
Potassium sodium aluminum fluoride (elpasolite), K_2NaAlF_6	9m	43	Rhodium, Rh	3	9
Potassium sodium bromide, $K_{2.8}Na_{.8}Br$	12m	62	Rhodium vanadium, RhV_3	6m	56
Potassium sodium bromide, $K_{4.6}Na_{.6}Br$	12m	62	Rubidium aluminum sulfate hydrate, $RbAl(SO_4)_2 \cdot 12H_2O$	6	44
Potassium sodium bromide, $K_{6.4}Na_{.4}Br$	12m	62	Rubidium amide, $RbNH_2$	5m	73
Potassium sodium bromide, $K_{.8}Na_{.2}Br$	12m	62	Rubidium barium chromium oxide, $Rb_2Ba(CrO_4)_2$	14m	32
Potassium sodium chloride, $K_{.2}Na_{.8}Cl$	12m	63	Rubidium barium molybdenum oxide, $Rb_2Ba(MoO_4)_2$	15m	59
Potassium sodium chloride, $K_{.4}Na_{.6}Cl$	12m	63	Rubidium bromate, $RbBrO_3$	8	45
Potassium sodium chloride, $K_{.6}Na_{.4}Cl$	12m	63	Rubidium bromide, $RbBr$	7	43
Potassium sodium chloride, $K_{.8}Na_{.2}Cl$	12m	63	Rubidium cadmium chloride, high form, $RbCdCl_3$ (tetragonal)	5m	43
Potassium sodium sulfate, $K_{.67}Na_{1.33}SO_4$	6m	48	Rubidium cadmium chloride, low form, $RbCdCl_3$ (orthorhombic)	5m	41
Potassium sodium sulfate, $KNaSO_4$..	6m	50	Rubidium cadmium sulfate, $Rb_2Cd_2(SO_4)_3$	7m	45
Potassium sodium sulfate (aphthitalite), $K_3Na(SO_4)_2$	6m	52	Rubidium calcium chloride, $RbCaCl_3$	7m	47
Potassium strontium chromium oxide, $K_2Sr(CrO_4)_2$	15m	57	Rubidium calcium fluoride, $RbCaF_3$	8m	57
Potassium strontium phosphate, $KSrPO_4$	19m	71	Rubidium calcium sulfate, $Rb_2Ca_2(SO_4)_3$	7m	48
Potassium strontium selenate, $K_2Sr(SeO_4)_2$	15m	58	Rubidium chlorate, $RbClO_3$	8	47
Potassium strontium sulfate (kalistrontite), $K_2Sr(SO_4)_2$	14m	31	Rubidium chlorate, $RbClO_4$	2m	30
Potassium sulfate, $K_2S_2O_7$	9m	99	Rubidium chloride, $RbCl$	4	41

	Vol. or Sec.	Page		Vol. or Sec.	Page
Rubidium fluoride, RbF	8m	63	Selenium, Se	5	54
Rubidium iodate, RbIO ₃	15m	62	Selenium oxide (selenolite), SeO ₂	7m	60
Rubidium iodate, RbIO ₄	2m	31	Silicon, Si	13m	35
Rubidium iodide, RbI	4	43	Silicon, Si (reference standard)	12m	2
Rubidium iron chloride hydrate, Rb ₂ FeCl ₅ ·H ₂ O	14m	33	Silicon nitride, β-Si ₃ N ₄	18m	59
Rubidium iron sulfate hydrate, Rb ₂ Fe(SO ₄) ₂ ·6H ₂ O	8m	64	Silicon nitride, β-Si ₃ N ₄ (calculated pattern)	14m	116
Rubidium lead chromium oxide, Rb ₂ Pb(CrO ₄) ₂	14m	34	Silicon oxide (α or low cristobalite), SiO ₂ (tetragonal)	10	48
Rubidium lead molybdenum oxide, Rb ₂ Pb(MoO ₄) ₂	15m	63	Silicon oxide (α or low cristobalite), SiO ₂ (tetragonal) (calculated pattern)	15m	180
Rubidium magnesium chromium oxide, Rb ₂ Mg ₂ (CrO ₄) ₃	8m	66	Silicon oxide (quartz, low), α-SiO ₂	18m	61
Rubidium magnesium chromium oxide hydrate, Rb ₂ Mg(CrO ₄) ₂ ·6H ₂ O	8m	68	Silicon oxide (β or high cristobalite), SiO ₂ (cubic)	1	42
Rubidium magnesium sulfate, Rb ₂ Mg ₂ (SO ₄) ₃	7m	50	Silver, Ag	1	23
Rubidium magnesium sulfate hydrate, Rb ₂ Mg(SO ₄) ₂ ·6H ₂ O	8m	70	Silver, Ag (reference standard)	8m	2
Rubidium manganese(II) fluoride, RbMnF ₃	5m	44	Silver arsenate, Ag ₃ AsO ₄	5	56
Rubidium manganese sulfate, Rb ₂ Mn ₂ (SO ₄) ₃	7m	52	Silver arsenic sulfide, xanthoconite, Ag ₃ AsS ₃	8m	126
Rubidium nickel(II) chloride, RbNiCl ₃	6m	58	Silver bromate, AgBrO ₃	5	57
Rubidium nickel sulfate, Rb ₂ Ni ₂ (SO ₄) ₃	8m	72	Silver bromide (bromargyrite), AgBr	4	46
Rubidium nickel sulfate hydrate, Rb ₂ Ni(SO ₄) ₂ ·6H ₂ O	8m	74	Silver carbonate, Ag ₂ CO ₃	13m	36
Rubidium nitrate, RbNO ₃ (trigonal)	5m	45	Silver chlorate, AgClO ₃	7	44
Rubidium platinum chloride, Rb ₂ PtCl ₆	5	53	Silver chloride (chlorargyrite), AgCl	4	44
Rubidium platinum fluoride, Rb ₂ PtF ₆	6	48	Silver chromium oxide, Ag ₂ CrO ₄	12m	30
Rubidium selenate, Rb ₂ SeO ₄	9m	44	Silver cyanide, AgCN	9m	48
Rubidium silicon fluoride, Rb ₂ SiF ₆	6	49	Silver fluoride, Ag ₂ F	5m	53
Rubidium strontium chloride, RbSrCl ₃	7m	54	Silver iodate, AgIO ₄	9	49
Rubidium strontium chromium oxide, Rb ₂ Sr(CrO ₄) ₂	15m	64	Silver iodide (iodargyrite), AgI (hexagonal)	8	51
Rubidium strontium sulfate, Rb ₂ Sr(SO ₄) ₂	15m	65	Silver iodide, γ-AgI (cubic)	9	48
Rubidium sulfate, Rb ₂ SO ₄	8	48	Silver manganese oxide, AgMnO ₄	7m	155
Rubidium tellurium bromide, Rb ₂ TeBr ₆	8	46	Silver mercury iodide, β-Ag ₂ HgI ₄	17m	67
Rubidium tellurium chloride, Rb ₂ TeCl ₆	8	48	Silver molybdenum oxide, Ag ₂ MoO ₄	7	45
Rubidium tin chloride, Rb ₂ SnCl ₆	6	46	Silver nitrate, AgNO ₃	5	59
Rubidium zinc fluoride, RbZnF ₃	7m	57	Silver nitrite, AgNO ₂	5	60
Rubidium zinc sulfate hydrate, Rb ₂ Zn(SO ₄) ₂ ·6H ₂ O	7m	55	Silver oxide, Ag ₂ O	1m	45
Ruthenium, Ru	4	5	Silver(II) oxide nitrate, Ag ₇ O ₈ NO ₃	4	61
Ruthenium titanium, RuTi	6m	86	Silver phosphate, Ag ₃ PO ₄	5	62
Samarium arsenate, SmAsO ₄	4m	33	Silver rhenium oxide, AgReO ₄	8	53
Samarium arsenide, SmAs	4m	68	Silver selenate, Ag ₂ SeO ₄	2m	32
Samarium chloride, SmCl ₃	1m	40	Silver sodium chloride, Ag _{0.5} Na _{0.5} Cl	8m	79
Samarium chloride oxide, SmOCl	1m	43	Silver sulfate, Ag ₂ SO ₄	13m	37
Samarium fluoride, SmF ₃	1m	41	Silver sulfide (acanthite), Ag ₂ S	10	51
Samarium oxide, Sm ₂ O ₃ (cubic)	4m	34	Silver telluride (hessite), Ag ₂ Te	19m	73
Samarium silver, SmAg	5m	73	Silver terbium, AgTb	5m	74
Samarium tin oxide, Sm ₂ Sn ₂ O ₇	8m	77	Silver thiocyanate, AgCNS	16m	62
Samarium vanadium oxide, SmVO ₄	5m	47	Silver thulium, AgTm	5m	74
Scandium arsenate, ScAsO ₄	4m	35	Silver yttrium, AgY	5m	75
Scandium arsenide, ScAs	4m	68	Sodium, Na	9m	105
Scandium boride, ScB ₂	17m	66	Sodium aluminum chloride silicate, sodalite, Na ₈ Al ₆ Cl ₂ (SiO ₄) ₆	7m	158
Scandium oxide, Sc ₂ O ₃	3	27	Sodium aluminum fluoride (chiolite), Na ₅ Al ₃ F ₁₄	16m	63
Scandium phosphate, ScPO ₄	8	50	Sodium aluminum oxide, β-NaAlO ₂	18m	62
Scandium silicate (thortveitite), Sc ₂ Si ₂ O ₇	7m	58	Sodium aluminum sulfate hydrate (soda alum), NaAl(SO ₄) ₂ ·12H ₂ O	15m	68
			Sodium azide, α-NaN ₃ , at -90 to -100 °C	8m	129
			Sodium azide, β-NaN ₃	8m	130
			Sodium barium phosphate, NaBaPO ₄	19m	75
			Sodium beryllium calcium aluminum fluoride oxide silicate, meliphanite, (Na _{0.63} Ca _{1.37})Be(Al _{0.13} Si _{1.87}) (F _{0.75} O _{6.25})	8m	135

Sodium beryllium calcium fluoride silicate, leucophanite, $\text{NaBeCaFSi}_2\text{O}_6$	8m	138	Sodium lanthanum fluoride silicate, $(\text{Na}_2\text{La}_8)\text{F}_2(\text{SiO}_4)_6$	7m	64
Sodium borate, NaBO_2	18m	63	Sodium lanthanum molybdenum oxide, $\text{NaLa}(\text{MoO}_4)_2$	10m	49
Sodium borate, $\text{Na}_2\text{B}_4\text{O}_7$	16m	64	Sodium magnesium aluminum boron hydroxide silicate, dravite, $\text{NaMg}_3\text{Al}_6\text{B}_3(\text{OH})_4\text{Si}_6\text{O}_{27}$	3m	47
Sodium borate, $\text{Na}_2\text{B}_8\text{O}_{13}$	7m	160	Sodium magnesium carbonate (eitelite), $\text{Na}_2\text{Mg}(\text{CO}_3)_2$	11m	56
Sodium borate hydroxide hydrate (borax), $\text{Na}_2\text{B}_4\text{O}_5(\text{OH})_4 \cdot 8\text{H}_2\text{O}$	16m	66	Sodium magnesium sulfate (vanthoffite), $\text{Na}_6\text{Mg}(\text{SO}_4)_4$	15m	72
Sodium boron hydride, NaBH_4	9	51	Sodium magnesium sulfate hydrate, bloedite, $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$	6m	63
Sodium bromate, NaBrO_3	5	65	Sodium magnesium sulfate hydrate (loeweite), $\text{Na}_{12}\text{Mg}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$	14m	35
Sodium bromide, NaBr	3	47	Sodium manganese(II) fluoride, NaMnF_3	6m	65
Sodium bromide chloride, $\text{NaBr}_{.33}\text{Cl}_{.67}$	11m	49	Sodium manganese sulfate hydrate, $\text{Na}_{12}\text{Mn}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$	14m	37
Sodium bromide chloride, $\text{NaBr}_{.67}\text{Cl}_{.33}$	11m	50	Sodium mercury(II) chloride hydrate, $\text{NaHgCl}_3 \cdot 2\text{H}_2\text{O}$	6m	66
Sodium calcium aluminum fluoride hydrate, thomsenolite, $\text{NaCaAlF}_6 \cdot \text{H}_2\text{O}$	8m	132	Sodium molybdenum oxide, Na_2MoO_4	1m	46
Sodium calcium carbonate hydrate, pirssonite, $\text{Na}_2\text{Ca}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$	9m	106	Sodium molybdenum oxide, $\text{Na}_2\text{Mo}_2\text{O}_7$	9m	110
Sodium calcium phosphate, $\beta\text{-NaCaPO}_4$	15m	69	Sodium neodymium fluoride silicate, $(\text{Na}_2\text{Nd}_8)\text{F}_2(\text{SiO}_4)_6$	7m	66
Sodium calcium silicate, $\text{Na}_2\text{CaSiO}_4$	10m	48	Sodium nickel(II) sulfate hydrate, $\text{Na}_2\text{Ni}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$	6m	68
Sodium calcium sulfate (glauberite), $\text{Na}_2\text{Ca}(\text{SO}_4)_2$	6m	59	Sodium niobium oxide (lueshite), NaNbO_3	18m	64
Sodium carbonate hydrate (thermor- natrite), $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O}$	8	54	Sodium nitrate (soda niter), NaNO_3	6	50
Sodium carbonate sulfate, $\text{Na}_4\text{CO}_3\text{SO}_4$	11m	51	Sodium nitrite, NaNO_2	4	62
Sodium carbonate sulfate (burkeite), $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$	11m	52	Sodium nitrosyl iron cyanide hydrate, $\text{Na}_2(\text{NO})\text{Fe}(\text{CN})_5 \cdot 2\text{H}_2\text{O}$	18m	66
Sodium carbonate sulfate, $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$	11m	53	Sodium oxide, Na_2O	10m	134
Sodium carbonate sulfate, $\text{Na}_6(\text{CO}_3)_2\text{SO}_4$	11m	54	Sodium phosphate, $\text{Na}_3\text{P}_3\text{O}_9$	3m	49
Sodium chlorate, NaClO_3	3	51	Sodium phosphate hydrate, $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$	3m	50
Sodium chlorate, NaClO_4 (orthorhombic)	7	49	Sodium phosphate hydrate, $\alpha\text{-Na}_4\text{P}_4\text{O}_{12} \cdot 4\text{H}_2\text{O}$ (monoclinic)	13m	39
Sodium chlorate hydrate, $\text{NaClO}_4 \cdot \text{H}_2\text{O}$	17m	68	Sodium phosphate hydrate, $\beta\text{-Na}_4\text{P}_4\text{O}_{12} \cdot 4\text{H}_2\text{O}$ (triclinic)	2m	35
Sodium chloride (halite), NaCl	2	41	Sodium phosphate hydrate, $\text{Na}_6\text{P}_6\text{O}_{18} \cdot 6\text{H}_2\text{O}$	5m	54
Sodium chromium oxide, Na_2CrO_4	9m	48	Sodium praseodymium fluoride silicate, $(\text{Na}_2\text{Pr}_8)\text{F}_2(\text{SiO}_4)_6$	7m	68
Sodium chromium oxide hydrate, $\text{Na}_2\text{CrO}_4 \cdot 4\text{H}_2\text{O}$	9m	50	Sodium selenate, Na_2SeO_4	9m	55
Sodium chromium oxide hydrate, $\text{Na}_2\text{Cr}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$	7m	62	Sodium selenide, Na_2Se	10m	135
Sodium chromium oxide sulfate, $\text{Na}_4(\text{CrO}_4)(\text{SO}_4)$	11m	55	Sodium silicate, $\alpha\text{(III)}$, $\text{Na}_2\text{Si}_2\text{O}_5$	8m	141
Sodium cobalt nitrite, $\text{Na}_3\text{Co}(\text{NO}_2)_6$	15m	70	Sodium silicate, $\beta\text{-Na}_2\text{Si}_2\text{O}_5$	10m	136
Sodium cobalt(II) sulfate hydrate, $\text{Na}_2\text{Co}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$	6m	61	Sodium silicon fluoride (malladrite), Na_2SiF_6	16m	68
Sodium cyanate, NaCNO	2m	33	Sodium strontium phosphate, NaSrPO_4	19m	77
Sodium cyanide, NaCN (cubic)	1	78	Sodium sulfate, Na_2SO_4	11m	57
Sodium cyanide, NaCN (orthorhombic) at 6°C	1	79	Sodium sulfate (thenardite), Na_2SO_4	2	59
Sodium fluoride (villiaumite), NaF	1	63	Sodium sulfate hydrate, $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$	17m	74
Sodium hydrogen carbonate hydrate, trona, $\text{Na}_3\text{H}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$	15m	71	Sodium sulfide, Na_2S	10m	140
Sodium hydrogen fluoride, NaHF_2	5	63	Sodium sulfite, Na_2SO_3	3	60
Sodium hydrogen phosphate, $\text{Na}_3\text{H}(\text{PO}_3)_4$	10m	130	Sodium telluride, Na_2Te	10m	141
Sodium hydrogen silicate hydrate, $\text{Na}_2\text{H}_2\text{SiO}_4 \cdot 4\text{H}_2\text{O}$	7m	163	Sodium tin fluoride, NaSn_2F_5	7m	166
Sodium hydrogen sulfate hydrate, $\text{NaHSO}_4 \cdot \text{H}_2\text{O}$	9m	52	Sodium titanium oxide, $\text{Na}_2\text{Ti}_3\text{O}_7$	16m	69
Sodium hydroxide, NaOH at 300°C	4m	69	Sodium titanium phosphate, $\text{NaTi}_2(\text{PO}_4)_3$	19m	79
Sodium iodate, NaIO_3	7	47	Sodium tungsten oxide, Na_2WO_4	1m	47
Sodium iodate, NaIO_4	7	48	Sodium tungsten(VI) oxide hydrate, $\text{Na}_2\text{WO}_4 \cdot 2\text{H}_2\text{O}$	2m	33
Sodium iodate hydrate, $\text{NaIO}_3 \cdot \text{H}_2\text{O}$	17m	73	Sodium vanadium oxide, $\alpha\text{-NaVO}_3$	18m	67
Sodium iodide, NaI	4	31	Sodium vanadium oxide, $\beta\text{-NaVO}_3$	18m	68
Sodium iron fluoride, Na_3FeF_6	9m	54			

	Vol. or Sec.	Page	Vol. or Sec.	Page
Sodium zinc fluoride, NaZnF_3	6m	74	Tantalum, Ta	1 29
Sodium zinc sulfate hydrate, $\text{Na}_2\text{Zn}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$	6m	72	Tantalum silicide, TaSi_2	8 59
Sodium zirconium fluoride, $\text{Na}_7\text{Zr}_6\text{F}_{31}$	8m	144	Tellurium, Te	1 26
Sodium zirconium phosphate, $\text{NaZr}_2(\text{PO}_4)_3$	19m	81	Tellurium(IV) oxide (paratellurite), TeO_2 (tetragonal)	7 56
Strontium aluminum hydroxide, $\text{Sr}_3\text{Al}_2(\text{OH})_{12}$	10m	50	Tellurium(IV) oxide, paratellurite, TeO_2 (tetragonal)	10 55
Strontium aluminum oxide, $\text{Sr}_3\text{Al}_2\text{O}_6$	10m	52	Tellurium(IV) oxide, tellurite, TeO_2 (orthorhombic)	9 57
Strontium arsenate, $\text{Sr}_3(\text{AsO}_4)_2$	2m	36	Terbium arsenate, TbAsO_4	3m 54
Strontium azide, $\text{Sr}(\text{N}_3)_2$	8m	146	Terbium arsenide, TbAs	5m 75
Strontium borate, SrB_2O_4	3m	53	Terbium nitride, TbN	4m 70
Strontium borate, SrB_4O_7	4m	36	Terbium phosphide, TbP	5m 76
Strontium bromate hydrate, $\text{Sr}(\text{BrO}_3)_2 \cdot \text{H}_2\text{O}$	17m	76	Terbium selenide, TbSe	5m 76
Strontium bromide fluoride, SrBrF	10m	54	Terbium sulfide, TbS	5m 77
Strontium bromide hydrate, $\text{SrBr}_2 \cdot 6\text{H}_2\text{O}$	4	60	Terbium telluride, TbTe	5m 77
Strontium carbonate (strontianite), SrCO_3	3	56	Terbium vanadium oxide, TbVO_4	5m 56
Strontium chloride, SrCl_2	4	40	Thallium, $\alpha\text{-Tl}$	16m 73
Strontium chloride fluoride, SrClF	10m	55	Thallium aluminum sulfate hydrate, $\text{TlAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6 53
Strontium chloride hydrate, $\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$	11m	58	Thallium(I) arsenate, Tl_3AsO_4	2m 37
Strontium chloride hydrate, $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$	4	58	Thallium azide, TlN_3	8m 82
Strontium chloride hydroxide phosphate, $\text{Sr}_5\text{Cl}_{1.65}(\text{OH})_{.35}(\text{PO}_4)_3$	11m	60	Thallium(I) bromate, TlBrO_3	8 60
Strontium chromium oxide, SrCr_2O_7	17m	77	Thallium bromide, TlBr	7 57
Strontium chromium oxide, Sr_2CrO_4	16m	71	Thallium cadmium sulfate, $\text{Tl}_2\text{Cd}_2(\text{SO}_4)_3$	8m 83
Strontium chromium oxide hydrate, $\text{SrCr}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$	17m	79	Thallium(I) chlorate, TlClO_4	2m 38
Strontium fluoride, SrF_2	5	67	Thallium(I) chlorate, TlClO_3	8 61
Strontium hydroxide, $\text{Sr}(\text{OH})_2$	13m	41	Thallium(I) chloride, TlCl	4 51
Strontium hydroxide hydrate, $\text{Sr}(\text{OH})_2 \cdot \text{H}_2\text{O}$	13m	42	Thallium chromium oxide, Tl_2CrO_4 ..	3m 54
Strontium hydroxide hydrate, $\text{Sr}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$	13m	43	Thallium chromium sulfate hydrate, $\text{TlCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6 55
Strontium indium hydroxide, $\text{Sr}_3\text{In}_2(\text{OH})_{12}$	6m	76	Thallium cobalt sulfate, $\text{Tl}_2\text{Co}_2(\text{SO}_4)_3$	8m 85
Strontium iodide hydrate, $\text{SrI}_2 \cdot 6\text{H}_2\text{O}$	8	58	Thallium cobalt sulfate hydrate, $\text{Tl}_2\text{Co}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	7m 70
Strontium iron oxide, $\text{SrFe}_{12}\text{O}_{19}$	18m	69	Thallium copper sulfate hydrate, $\text{Tl}_2\text{Cu}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	7m 72
Strontium manganese oxide, SrMnO_3 (cubic)	10m	56	Thallium fluoride, TlF	16m 74
Strontium manganese oxide, SrMnO_3 (hexagonal)	10m	58	Thallium gallium sulfate hydrate, $\text{TlGa}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6 57
Strontium molybdenum oxide, SrMoO_4	7	50	Thallium(I) iodate, TlIO_3	8 62
Strontium nitrate, $\text{Sr}(\text{NO}_3)_2$	12m	31	Thallium(I) iodide, TlI (orthorhombic)	4 53
Strontium oxide, SrO	5	68	Thallium iron sulfate hydrate, $\text{Tl}_2\text{Fe}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	8m 87
Strontium oxide, SrO_2	6	52	Thallium lead sulfate, $\text{Tl}_2\text{Pb}(\text{SO}_4)_2$	15m 74
Strontium oxide hydrate, $\text{SrO}_2 \cdot 8\text{H}_2\text{O}$	11m	61	Thallium magnesium chromium oxide, $\text{Tl}_2\text{Mg}_2(\text{CrO}_4)_3$	8m 89
Strontium phosphate, $\alpha\text{-Sr}_2\text{P}_2\text{O}_7$	11m	62	Thallium magnesium sulfate hydrate, $\text{Tl}_2\text{Mg}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	7m 74
Strontium phosphate, $\alpha\text{-Sr}_3(\text{PO}_4)_2$	11m	64	Thallium manganese sulfate, $\text{Tl}_2\text{Mn}_2(\text{SO}_4)_3$	7m 76
Strontium scandium oxide hydrate, $\text{Sr}_3\text{Sc}_2\text{O}_6 \cdot 6\text{H}_2\text{O}$	6m	78	Thallium nickel sulfate hydrate, $\text{Tl}_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	7m 78
Strontium silicate, Sr_3SiO_5	13m	44	Thallium(I) nitrate, TlNO_3	6 58
Strontium sulfate (celestite), SrSO_4	2	61	Thallium oxide (avicennite), Tl_2O_3	16m 77
Strontium sulfide, SrS	7	52	Thallium(III) oxide, Tl_2O_3	2 28
Strontium telluride, SrTe	4m	69	Thallium(I) phosphate, Tl_3PO_4	7 58
Strontium tin oxide, SrSnO_3	8m	80	Thallium(III) phosphate, TlPO_4	7 59
Strontium titanium oxide, SrTiO_3	3	44	Thallium platinum chloride, Tl_2PtCl_6	5 70
Strontium tungsten oxide, SrW_4	7	53	Thallium silicon fluoride, Tl_2SiF_6	6 56
Strontium tungsten oxide, Sr_2W_5	12m	32	Thallium strontium sulfate, $\text{Tl}_2\text{Sr}(\text{SO}_4)_2$	15m 75
Strontium vanadium oxide, $\text{Sr}_3(\text{VO}_4)_2$	15m	73	Thallium(I) sulfate, Tl_2SO_4	6 59
Strontium zirconium oxide, SrZrO_3	9	51	Thallium(I) thiocyanate, TlCNS	8 63
Sulfamic acid, $\text{H}_2\text{NSO}_3\text{H}$	7	54	Thallium tin chloride, Tl_2SnCl_6	6 54
Sulfur, S (orthorhombic)	9	54		

	Vol. or Sec.	Page		Vol. or Sec.	Page
Thallium(I) tungsten oxide, Tl_2WO_4	1m	48	Yttrium vanadium oxide, YVO_4	5m	59
Thallium zinc sulfate hydrate, $Tl_2Zn(SO_4)_2 \cdot 6H_2O$	7m	80	Zinc, Zn	1	16
Thorium arsenide, ThAs	4m	70	Zinc aluminum oxide (gahnite), $ZnAl_2O_4$	2	38
Thorium carbide, ThC	18m	71	Zinc ammine bromide, $Zn(NH_3)_2Br_2$	11m	68
Thorium nitrate hydrate, $Th(NO_3)_4 \cdot 5H_2O$	18m	72	Zinc ammine chloride, $Zn(NH_3)_2Cl_2$	10m	59
Thorium oxide (thorianite), ThO_2 ..	1	57	Zinc antimony oxide, $ZnSb_2O_4$	4m	39
Thulium arsenate, $TmAsO_4$	3m	56	Zinc Arsenate Hydrate (koettigite), $Zn_3(AsO_4)_2 \cdot 8H_2O$	19m	85
Thulium arsenide, TmAs	4m	71	Zinc borate, $Zn_4B_6O_{13}$	13m	48
Thulium nitride, TmN	4m	71	Zinc carbonate, smithsonite, $ZnCO_3$	8	69
Thulium oxide, Tm_2O_3	9	58	Zinc chlorate hydrate, $Zn(ClO_4)_2 \cdot 6H_2O$	16m	79
Thulium telluride, TmTe	4m	72	Zinc chromium oxide, $ZnCr_2O_4$	9m	59
Thulium vanadium oxide, $TmVO_4$	5m	57	Zinc cobalt oxide, $ZnCo_2O_4$	10m	60
Tin, α -Sn (cubic)	2	12	Zinc cyanide, $Zn(CN)_2$	5	73
Tin, β -Sn (tetragonal)	1	24	Zinc fluoride, ZnF_2	6	60
Tin arsenide, SnAs	4m	37	Zinc fluoride hydrate, $ZnF_2 \cdot 4H_2O$	11m	69
Tin arsenide, $Sn_3 \cdot gAs_3$	15m	76	Zinc germanium oxide, Zn_2GeO_4	10	56
Tin chloride hydrate, $SnCl_2 \cdot 2H_2O$..	17m	84	Zinc hydroxide silicate hydrate, hemimorphite, $Zn_4(OH)_2Si_2O_7 \cdot H_2O$..	2	62
Tin(II) fluoride, SnF_2	3m	51	Zinc iodide, ZnI_2	9	60
Tin hydrogen phosphate, $SnHPO_4$	13m	46	Zinc iron oxide (franklinite), $ZnFe_2O_4$	9m	60
Tin(IV) iodide, SnI_4	5	71	Zinc manganese oxide (hetaerolite), $ZnMn_2O_4$	10m	61
Tin(II) oxide (romarchrite), SnO	4	28	Zinc molybdenum oxide, $Zn_2Mo_3O_8$	7m	173
Tin(IV) oxide (cassiterite), SnO_2	1	54	Zinc nitrate hydrate, α - $Zn(NO_3)_2 \cdot 6H_2O$	12m	36
Tin sulfide (berndtite), β - SnS_2	9m	57	Zinc oxide (zincite), ZnO	2	25
Tin(II) telluride, $SnTe$	7	61	Zinc phosphate, α - $Zn_3(PO_4)_2$	16m	80
Titanium, Ti	3	4	Zinc phosphate, β - $Zn_3(PO_4)_2$	16m	81
Titanium carbide, TiC	18m	73	Zinc phosphate, γ - $Zn_3(PO_4)_2$	16m	83
Titanium(III) oxide, $TiO_{1.515}$	9	59	Zinc phosphate hydrate (hopeite), $Zn_3(PO_4)_2 \cdot 4H_2O$	16m	85
Titanium oxide (anatase), TiO_2	7m	82	Zinc selenide, $ZnSe$	3	23
Titanium oxide, brookite, TiO_2 (orthorhombic)	3m	57	Zinc silicate (willemite), Zn_2SiO_4	7	62
Titanium oxide (rutile), TiO_2	7m	83	Zinc silicon fluoride hydrate, $ZnSiF_6 \cdot 6H_2O$	8	70
Titanium silicide, Ti_5Si_3	8	64	Zinc sulfate (zinkosite), $ZnSO_4$	7	64
Titanium sulfide, TiS_2	4m	72	Zinc sulfate hydrate (gunningite), $ZnSO_4 \cdot H_2O$	19m	86
Titanium sulfide, Ti_2S	8m	149	Zinc sulfate hydrate (goslarite), $ZnSO_4 \cdot 7H_2O$	8	71
Tungsten, W	1	28	Zinc sulfide (wurtzite), α - ZnS (hexagonal)	2	14
Tungsten, W (reference standard) ..	8m	2	Zinc sulfide (sphælerite), β - ZnS (cubic)	2	16
Tungsten oxide, WO_2	18m	74	Zinc telluride, $ZnTe$	3m	58
Tungsten sulfide (tungstenite), WS_2	8	65	Zinc tin oxide, Zn_2SnO_4	10m	62
Uranium nitride, UN	18m	75	Zinc titanium oxide, $ZnTiO_3$	13m	49
Uranium oxide, UO	5m	78	Zinc titanium oxide, Zn_2TiO_4	12m	37
Uranium oxide (uraninite), UO_2	2	33	Zinc tungsten oxide (sanmartinite), $ZnWO_4$	2m	40
Uranium selenide, USe	5m	78	Zirconium, α - Zr	2	11
Uranium telluride, UTe	4m	73	Zirconium fluoride, ZrF_4	18m	79
Vanadium, V	9m	58	Zirconium hydride, ZrH_2	5m	60
Vanadium(V) oxide (shcherbinaite), V_2O_5	8	66	Zirconium iodate, $Zr(IO_3)_4$	1m	51
Vanadium sulfide, α - V_3S	14m	118	Zirconium nitride, ZrN	5m	80
Vanadium sulfide, β - V_3S	14m	120	Zirconium oxide, ZrO	5m	81
Ytterbium arsenate, $YbAsO_4$	4m	38	Zirconium oxide chloride hydrate, $ZrOCl_2 \cdot 8H_2O$	18m	81
Ytterbium arsenide, $YbAs$	4m	73	Zirconium phosphide, ZrP	4m	75
Ytterbium nitride, YbN	4m	74	Zirconium silicate, zircon, $ZrSiO_4$	4	68
Ytterbium oxide, Yb_2O_3	6m	80	Zirconium silicide, $ZrSi_2$	17m	86
Ytterbium selenide, $YbSe$	5m	79	Zirconium sulfate hydrate (zircosulfate), $Zr(SO_4)_2 \cdot 4H_2O$	7	66
Ytterbium telluride, $YbTe$	5m	79			
Ytterbium(III) vanadium oxide, $YbVO_4$	5m	58			
Yttrium, Y	18m	77			
Yttrium arsenate, $YAsO_4$	2m	39			
Yttrium arsenide, YAs	4m	74			
Yttrium chloride oxide, $YCLO$	1m	51			
Yttrium chromium oxide, $YCrO_3$	19m	83			
Yttrium oxide, Y_2O_3	3	28			
Yttrium phosphate (xenotime), YPO_4	8	67			
Yttrium sulfide, YS	5m	80			
Yttrium telluride, YTE	4m	75			
Yttrium titanium oxide, Y_2TiO_5	11m	113			

CUMULATIVE ORGANIC FORMULA INDEX

		Vol. or Sec.	Page
CHI ₃	Iodoform	18m	34
CH ₄ N ₂ O	Urea	7	61
CH ₄ N ₂ S	Thiourea	17m	83
CH ₅ NO ₂	Ammonium formate	11m	9
CH ₅ N ₃ ·HCl	Guanidinium chloride	17m	35
CH ₅ N ₃ S	Thiosemicarbazide	17m	81
C ₂ Ag ₂ O ₄	Silver oxalate	9m	47
C ₂ FeO ₄ ·2H ₂ O	Iron oxalate hydrate (humboldtine)	10m	24
C ₂ HNaO ₄ ·H ₂ O	Sodium hydrogen oxalate hydrate	17m	72
C ₂ H ₂ CaO ₄	Calcium formate	8	16
C ₂ H ₂ O ₄ ·2H ₂ O	Oxalic acid hydrate	16m	55
C ₂ H ₂ O ₄ Pb	Lead formate	8	30
C ₂ H ₂ O ₄ Sr	Strontium formate	8	55
C ₂ H ₂ O ₄ Sr·2H ₂ O	Strontium formate hydrate (orthorhombic)	8	56
C ₂ H ₃ KO ₄	Potassium formate-formic acid complex	9m	93
C ₂ H ₃ NaO ₂ ·3H ₂ O	Sodium acetate hydrate	15m	66
C ₂ H ₄ N ₂ O ₂	Glyoxime	8m	102
C ₂ H ₅ NO ₂	α-Glycine	17m	34
C ₂ H ₇ NO ₂	Ammonium acetate	8m	95
C ₂ H ₈ N ₂ ·2HCl	Ethylenediamine Hydrochloride	19m	43
C ₂ H ₈ N ₂ O ₄ ·H ₂ O	Ammonium oxalate hydrate (oxammite)	7	5
C ₂ K ₂ O ₄ ·H ₂ O	Potassium oxalate hydrate	9m	39
C ₂ Li ₂ O ₄	Lithium oxalate	10m	34
C ₂ Na ₂ O ₄	Sodium oxalate	6m	70
C ₂ O ₄ Rb ₂ ·H ₂ O ₂	Rubidium oxalate perhydrate	9m	102
C ₃ H ₇ NO ₂	L-Alanine	8m	93
C ₃ H ₇ NO ₂ S	L-Cysteine	11m	86
C ₃ H ₉ N·HCl	Trimethylammonium chloride	9m	113
C ₄ H ₃ KO ₈ ·2H ₂ O	Potassium hydrogen oxalate hydrate	17m	60
C ₄ H ₄ CaO ₅ ·2H ₂ O	Calcium malate hydrate	10m	76
C ₄ H ₄ KNaO ₆ ·4H ₂ O	Potassium sodium tartrate hydrate	15m	55
C ₄ H ₄ MnO ₆	Manganese Tartrate	19m	57
C ₄ H ₄ NO ₈ Y·H ₂ O	Ammonium yttrium oxalate hydrate	8m	97
C ₄ H ₄ Na ₂ O ₆ ·2H ₂ O	Sodium D-tartrate hydrate	11m	110
C ₄ H ₆ CoO ₄ ·4H ₂ O	Cobalt acetate hydrate	12m	19
C ₄ H ₆ Hg ₂ O ₄	Mercury acetate	17m	51
C ₄ H ₆ NiO ₄ ·4H ₂ O	Nickel acetate hydrate	13m	31
C ₄ H ₆ O ₄ Zn·2H ₂ O	Zinc acetate hydrate	18m	78
C ₄ H ₆ O ₆	D-Tartaric acid	7m	168
C ₄ H ₆ O ₆ U·2H ₂ O	Uranyl acetate hydrate	18m	76
C ₄ H ₇ N ₃ O	Creatinine	15m	31
C ₄ H ₈ N ₈ O ₈	α-HMX	11m	100
C ₄ H ₈ N ₈ O ₈	β-HMX	11m	102
C ₄ H ₈ N ₈ O ₈	Octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine, alpha-	11m	100
C ₄ H ₈ N ₈ O ₈	Octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine, beta- bis-(o-Dodecacarbonane)	11m	102
C ₄ H ₂₂ B ₂₀	Uric acid, phase 1 (calc. pattern)	6m	7
C ₅ H ₄ N ₄ O ₃	Uric acid, phase 1	8m	154
C ₅ H ₄ N ₄ O ₃	Copper glutamate hydrate	16m	78
C ₅ H ₇ CuNO ₄ ·2H ₂ O	Zinc glutamate hydrate	7m	110
C ₅ H ₇ NO ₄ Zn·2H ₂ O	Sodium glutamate hydrate	7m	170
C ₅ H ₈ NNaO ₄ ·H ₂ O	β-L-Glutamic acid	17m	70
C ₅ H ₉ NO ₄	Pentaerythritol	17m	32
C ₅ H ₁₂ O ₄	Picric acid	17m	55
C ₆ H ₃ N ₃ O ₇	Nicotinic acid	16m	56
C ₆ H ₅ NO ₂	γ-Hydroquinone	16m	54
C ₆ H ₆ O ₂	Zinc diimidazole chloride	8m	107
C ₆ H ₈ Cl ₂ N ₄ Zn	Phenylhydrazine hydrochloride	7m	123
C ₆ H ₈ N ₂ ·HCl	L-Ascorbic acid	17m	56
C ₆ H ₈ O ₆	Hexamethylenetetramine	8m	99
C ₆ H ₁₂ N ₄	Dextrose	17m	37
C ₆ H ₁₂ O ₆		11m	28

	Vol. or Sec.	Page
C ₆ H ₁₂ O ₆		28
C ₆ H ₁₅ HO ₁₂ S ₃ ·9H ₂ O	11m	18
C ₆ H ₁₅ NdO ₁₂ S ₃ ·9H ₂ O	1m	41
C ₇ H ₅ BrO ₂	9	22
C ₇ H ₅ ClO ₂	16m	30
C ₇ H ₅ FO ₂	16m	36
C ₇ H ₅ IO ₂	19m	47
C ₇ H ₉ NO ₂ S	9m	78
C ₇ H ₁₂ O ₄	7m	153
C ₈ H ₄ Hg ₂ O ₄	10m	113
C ₈ H ₅ KO ₄	4m	30
C ₈ H ₅ O ₄ Tl	16m	75
C ₈ H ₇ N ₃ O ₇	8m	152
C ₈ H ₈ O ₃	16m	11
C ₈ H ₉ NO	14m	38
C ₈ H ₉ NO	16m	7
C ₈ H ₁₁ N ₂ NaO ₃	16m	157
C ₈ H ₁₂ N ₂ O ₃	15m	126
C ₈ H ₁₂ N ₂ O ₃	15m	128
C ₈ H ₁₂ N ₂ O ₃	15m	130
C ₉ H ₁₄ N ₂ O ₃	15m	177
C ₁₀ H ₁₂ N ₂ O ₃	14m	41
C ₁₀ H ₁₂ N ₂ O ₈	19m	45
C ₁₀ H ₁₅ NO·HC1	16m	124
C ₁₁ H ₁₆ N ₂ O ₃	16m	162
C ₁₁ H ₁₈ N ₂ O ₃	15m	114
C ₁₁ H ₁₈ N ₂ O ₃	15m	117
C ₁₂ H ₁₀ N ₂	7m	86
C ₁₂ H ₁₂ N ₂ ·2HC1	18m	14
C ₁₂ H ₁₂ N ₂ O ₃	16m	144
C ₁₂ H ₁₂ N ₂ O ₃ ·8H ₂ O	19m	88
C ₁₂ H ₁₆ Cl ₂ CuN ₈	8m	31
C ₁₂ H ₁₆ Cl ₂ N ₈ Ni	8m	44
C ₁₂ H ₁₆ CuN ₁₀ O ₆	13m	24
C ₁₂ H ₁₆ N ₂	14m	109
C ₁₂ H ₁₆ N ₂ O	15m	133
C ₁₂ H ₁₆ N ₂ O	16m	152
C ₁₂ H ₂₂ O ₁₁	11m	66
C ₁₂ H ₂₆ N ₂ O ₄	7m	121
C ₁₃ H ₂₀ N ₂ O ₂ ·HC1	16m	149
C ₁₃ H ₂₁ N ₂ O ₄ P	16m	154
C ₁₄ H ₁₁ FO	8m	91
C ₁₄ H ₁₉ N ₃ S·HC1	14m	112
C ₁₅ H ₁₂ N ₂ O	18m	24
C ₁₅ H ₁₂ O ₂	7m	115
C ₁₆ H ₁₃ ClN ₂ O	14m	106
C ₁₆ H ₁₃ N	6m	29
C ₁₇ H ₁₉ ClN ₂ S	14m	60
C ₁₇ H ₁₉ NO ₃ ·HC1·3H ₂ O	16m	133
C ₁₇ H ₂₁ NO ₄ ·HC1	16m	114
C ₁₇ H ₂₅ N·HC1	16m	141
C ₁₈ H ₂₁ NO ₃ ·HBr·2H ₂ O	16m	117
C ₁₈ H ₂₄ CdN ₁₄ O ₆	8m	23
C ₁₈ H ₂₄ N ₁₄ NiO ₆	7m	27
C ₁₈ H ₂₈ N ₂ O ₄ S	15m	119
C ₁₉ H ₂₁ NO ₄ ·HC1·2H ₂ O	16m	136
C ₁₉ H ₂₂ N ₂ O	17m	26
C ₁₉ H ₂₄ N ₂ ·HC1	16m	129
C ₂₀ H ₂₅ NO ₃ ·HC1	16m	92
C ₂₀ H ₃₄		
	16m	122
C ₂₁ H ₂₃ ClFNO ₂	16m	127
C ₂₁ H ₃₀ O ₂	16m	111
C ₂₂ H ₂₅ ClN ₂ OS·2H ₂ O	17m	28
C ₂₂ H ₃₀ O ₄	16m	160

	Vol. or Sec.	Page
C ₂₄ H ₃₂ N ₂ O ₂ Pd		
C ₂₅ H ₁₅ N ₆		
C ₃₃ H ₄₀ N ₂ O ₉		
Palladium bis-(N-isopropyl-3-ethylsalicylaldiminate)	7m	144
N-Methylphenazinium-7,7,8,8-tetracyanoquinodimethanide	7m	146
Reserpine	8m	123

CUMULATIVE ORGANIC NAME INDEX

		Vol. or Sec.	Page
Acetanilide	C ₈ H ₉ NO (calc. pattern)	14m	38
Acetanilide	C ₈ H ₉ NO	16m	7
4-Acetyl-2'-fluorodiphenyl	C ₁₄ H ₁₁ FO	8m	91
Alanine, L-	CH ₃ CHNH ₂ CO ₂ H	8m	93
Allobarbital	C ₁₀ H ₁₂ N ₂ O ₃	14m	41
Amobarbital, form I	C ₁₁ H ₁₈ N ₂ O ₃	15m	114
Amobarbital, form II	C ₁₁ H ₁₈ N ₂ O ₃	15m	117
Ammonium acetate	NH ₄ ·CH ₃ CO ₂	8m	95
Ammonium formate	NH ₄ HCO ₂	11m	9
Ammonium oxalate hydrate (oxammite)	(NH ₄) ₂ C ₂ O ₄ ·H ₂ O	7	5
Ammonium yttrium oxalate hydrate	NH ₄ Y(C ₂ O ₄) ₂ ·H ₂ O	8m	97
Ampphetamine sulfate, (+)-	C ₁₈ H ₂₈ N ₂ O ₄ S	15m	119
p-Anisic acid	C ₈ H ₈ O ₃	16m	11
Ascorbic acid, L-	C ₆ H ₈ O ₆	8m	99
Azobenzene	C ₆ H ₅ NNC ₆ H ₅	7m	86
Barbital, form I	C ₈ H ₁₂ N ₂ O ₃	15m	126
Barbital, form II	C ₈ H ₁₂ N ₂ O ₃	15m	128
Barbital, form IV	C ₈ H ₁₂ N ₂ O ₃	15m	130
Benactyzine hydrochloride	C ₂₀ H ₂₅ NO ₃ ·HCl	16m	92
Benzidine hydrochloride	C ₁₂ H ₁₂ N ₂ ·2HCl	18m	14
o-Bromobenzoic acid	C ₇ H ₅ BrO ₂	16m	22
Bufofenine	C ₁₂ H ₁₆ N ₂ O	15m	133
Cadmium hexaimidazole nitrate	Cd(C ₃ H ₄ N ₂) ₆ (NO ₃) ₂	8m	23
Calcium formate	Ca(HCO ₂) ₂	8	16
Calcium malate hydrate	Ca(O ₂ C) ₂ (CH ₂ CHOH)·2H ₂ O	10m	76
Cannabidiol	C ₂₁ H ₃₀ O ₂	16m	111
Carbamazepine, β-	C ₁₅ H ₁₂ N ₂ O	18m	24
m-Chlorobenzoic acid	C ₇ H ₅ ClO ₂	16m	30
Chlorpromazine	C ₁₇ H ₁₉ ClN ₂ S	14m	60
Cinchonine	C ₁₉ H ₂₂ N ₂ O	17m	26
Cloperthixol hydrate	C ₂₂ H ₂₅ ClN ₂ OS·2H ₂ O	17m	28
Cobalt acetate hydrate	Co(C ₂ H ₃ O ₂) ₂ ·4H ₂ O	12m	19
Cocaine hydrochloride, L-	C ₁₇ H ₂₁ NO ₄ ·HCl	16m	114
Codeine hydrobromide hydrate	C ₁₈ H ₂₁ NO ₃ ·HBr·2H ₂ O	16m	117
Copper glutamate hydrate	Cu(O ₂ C) ₂ (H ₂ NCHCH ₂ CH ₂)·2H ₂ O	7m	110
Copper tetraimidazole nitrate	Cu(C ₃ H ₄ N ₂) ₄ (NO ₃) ₂	13m	24
Copper tetracyrazole chloride	Cu(C ₃ H ₄ N ₂) ₄ Cl ₂	8m	31
Creatinine	C ₄ H ₇ N ₃ O	15m	31
Cysteine, L-	HSCH ₂ ·CH(NH ₂)·COOH	11m	86
Dextrose	C ₆ H ₁₂ O ₆	11m	28
Diazepam	C ₁₆ H ₁₃ ClN ₂ O	14m	106
Dibenzoylmethane	(C ₆ H ₅ CO) ₂ CH ₂	7m	115
Dihydrophyllocladene, α-, hartite (or bombiccite)	C ₂₀ H ₃₄	16m	122
(N,N)-Dimethyltryptamine	C ₁₂ H ₁₆ N ₂	14m	109
bis-(o-Dodecacarborane)	C ₄ B ₂₀ H ₂₂	6m	7
Ephedrine hydrochloride, (-)-	C ₁₀ H ₁₅ NO·HCl	16m	124
Ethylenediamine hydrochloride	C ₂ H ₈ N ₂ ·2HCl	19m	43
Ethylenediaminetetraacetic acid	C ₁₀ H ₁₂ N ₂ O ₈	19m	45
p-Fluorobenzoic acid	C ₇ H ₅ FO ₂	16m	36
Glucose, α-D-	C ₆ H ₁₂ O ₆	11m	28
Glutamic acid, β-L-	C ₅ H ₉ NO ₄	17m	32
Glycine, α-	C ₂ H ₅ NO ₂	17m	34
Glyoxime	H ₂ C ₂ (NOH) ₂	8m	102
Guanidinium chloride	CH ₅ N ₃ ·HCl	17m	35
Haloperidol	C ₂₁ H ₂₃ ClFNO ₂	16m	127
Hexamethylenediammonium adipate	(CH ₂) ₄ (CO ₂ H ₃ N) ₂ (CH ₂) ₆	7m	121
Hexamethylenetetramine	C ₆ H ₁₂ N ₄	17m	37
HMX, α-	C ₄ H ₈ N ₈ O ₈	11m	100
HMX, β-	C ₄ H ₈ N ₈ O ₈	11m	102
Holmium ethylsulfate hydrate	Ho[(C ₂ H ₅)SO ₄] ₃ ·9H ₂ O	1m	18
Hydroquinone, γ-	HO ₂ C ₆ H ₄ OH	8m	107

	Vol. or Sec.	Page
Imipramine hydrochloride	$C_{19}H_{24}N_2 \cdot HC1$	16m
p-Iodobenzoic acid	$C_7H_5IO_2$	19m
Iodoform	CHI_3	18m
Iron oxalate hydrate (humboldtine)	$FeC_2O_4 \cdot 2H_2O$	10m
Lead formate	$Pb(HCO_2)_2$	8
Lithium oxalate	$Li_2C_2O_4$	10m
Manganese tartrate	$C_4H_4MnO_6$	19m
Mercury acetate	$C_4H_6Hg_2O_4$	17m
Mercury o-phthalate	$C_6H_4(CO_2Hg)_2$	10m
Methapyrilene hydrochloride	$C_{14}H_{19}N_3S \cdot HC1$	14m
Metharbital	$C_9H_{14}N_2O_3$	15m
Methyl sulfonanilide	$C_6H_5NSO_2CH_3$	9m
N-Methylphenazinium-7,7,8,8-tetra-cyanoquinodimethanide	$C_{25}H_{15}N_6$	7m
Morphine hydrochloride hydrate	$C_{17}H_{19}NO_3 \cdot HC1 \cdot 3H_2O$	16m
Naloxone hydrochloride hydrate	$C_{19}H_{21}NO_4 \cdot HC1 \cdot 2H_2O$	16m
2-Naphthylamine, N-phenyl-	$C_{10}H_7NHC_6H_5$	6m
Neodymium ethylsulfate hydrate	$Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$	9
Nickel acetate hydrate	$Ni(C_2H_3O_2)_2 \cdot 4H_2O$	13m
Nickel hexaimidazole nitrate	$Ni(C_3H_4N_2)_6(NO_3)_2$	7m
Nickel tetracyrazole chloride	$Ni(C_3H_4N_2)_4Cl_2$	8m
Nicotinic acid	$C_6H_5NO_2$	16m
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (α -HMX)	$C_4H_8N_8O_8$	11m
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (β -HMX)	$C_4H_8N_8O_8$	11m
Oxalic acid hydrate	$C_2H_2O_4 \cdot 2H_2O$	16m
Palladium bis-(N-isopropyl-3-ethylsalicylaldiminate)	$Pd(C_{12}H_{16}NO)_2$	7m
Pentaerythritol	$C_5H_{12}O_4$	17m
Phencyclidine hydrochloride	$C_{17}H_{25}N \cdot HC1$	16m
Phenobarbital, form III	$C_{12}H_{12}N_2O_3$	16m
Phenobarbital hydrate	$C_{12}H_{12}N_2O_3 \cdot H_2O$	19m
Phenylhydrazine hydrochloride	$C_6H_8N_2 \cdot HC1$	17m
Picric acid	$C_6H_3N_3O_7$	16m
Pimelic acid	$(CH_2)_5(CO_2H)_2$	7m
Potassium formate-formic acid complex	$KO_2CH \cdot HO_2CH$	9m
Potassium hydrogen o-phthalate	$C_6H_4(COOH)(COOK)$	4m
Potassium hydrogen oxalate hydrate	$C_4H_3KO_8 \cdot 2H_2O$	17m
Potassium oxalate hydrate	$K_2C_2O_4 \cdot H_2O$	9m
Potassium oxalate perhydrate	$K_2C_2O_4 \cdot H_2O_2$	9m
Potassium sodium tartrate hydrate	$C_4H_4KNaO_6 \cdot 4H_2O$	15m
Procaine hydrochloride	$C_{13}H_{20}N_2O_2 \cdot HC1$	16m
Psilocin	$C_{12}H_{16}N_2O$	16m
Psilocybin methanolate	$C_{13}H_{21}N_2O_4P$	16m
Reserpine	$C_{33}H_{40}N_2O_9$	8m
Rubidium oxalate perhydrate	$Rb_2C_2O_4 \cdot H_2O_2$	9m
Silver oxalate	$Ag_2C_2O_4$	9m
Sodium acetate hydrate	$C_2H_3NaO_2 \cdot 3H_2O$	15m
Sodium barbital	$C_8H_{11}N_2NaO_3$	16m
Sodium glutamate hydrate	$C_5H_8NNaO_4 \cdot H_2O$	17m
Sodium hydrogen oxalate hydrate	$C_2HNaO_4 \cdot H_2O$	17m
Sodium oxalate	$Na_2C_2O_4$	6m
Sodium D-tartrate hydrate	$(CHOH-CO_2Na)_2 \cdot 2H_2O$	11m
Strontium formate	$Sr(CHO_2)_2$	8
Strontium formate hydrate	$Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic)	8
Sucrose	$C_{12}H_{22}O_{11}$	11m
Tartaric acid, D-	$(CHOHCO_2H)_2$	7m
Δ^9 -Tetrahydrocannabinolic acid B	$C_{22}H_{30}O_4$	16m
Thallium hydrogen phthalate	$C_8H_5O_4Tl$	16m
Thiosemicarbazide	CH_5N_3S	17m
Thiourea	CH_4N_2S	17m
Trimethylammonium chloride	$C_3H_9N \cdot HC1$	9m
2,4,6-Trinitrophenetole	$C_8H_7N_3O_7$	8m
Uranyl acetate hydrate	$C_4H_6O_6U \cdot 2H_2O$	18m
Urea	$CO(NH_2)_2$	7
Uric acid, phase 1, (calc. pattern)	$C_5H_4N_4O_3$	8m
Uric acid (phase 1)	$C_5H_4N_4O_3$	16m
Vinbarbital, form I	$C_{11}H_{16}N_2O_3$	16m

		Vol. or Sec.	Page
Zinc acetate hydrate	C ₄ H ₆ O ₄ · 2H ₂ O	18m	78
Zinc diimidazole chloride	Zn(C ₃ H ₄ N ₂) ₂ Cl ₂	7m	123
Zinc glutamate hydrate,	Zn(O ₂ CCHNH ₂ CH ₂ CH ₂ CO ₂) · 2H ₂ O	7m	170

CUMULATIVE MINERAL INDEX

Vol. or
Sec. Page

Vol. or
Sec. Page

Acanthite, Ag ₂ S	10	51	Clausthalite, PbSe	5	38
Aeschynite CeNbTiO ₆	3m	24	Clinobisvanite, BiVO ₄	3m	14
Alabandite, MnS	4	11	Copper, Cu	1	15
Anatase, TiO ₂	7m	82	Cordierite, Mg ₂ Al ₄ Si ₅ O ₁₈	1m	28
Andradite, Ca ₃ Fe ₂ Si ₃ O ₁₂	9	22	Corundum, Al ₂ O ₃	9	3
Anglesite, PbSO ₄	3	67	Cotunnite, PbCl ₂	12m	23
Anhydrite, CaSO ₄	4	65	Covellite, CuS	4	13
Annabergite, Ni ₃ (AsO ₄) ₂ ·8H ₂ O	19m	60	Cristobalite (α or low) SiO ₂	10	48
Antarcticite, CaCl ₂ ·6H ₂ O	12m	16	Cristobalite (α or low) SiO ₂	15m	180
Antimony; Sb	3	14	(tetragonal)	1	42
Aphthitalite, K ₃ Na(SO ₄) ₂	6m	52	Cristobalite (β or high) SiO ₂ (cubic)	9m	23
Aragonite, CaCO ₃	3	53	Cryolithionite, Li ₃ Na ₃ Al ₂ F ₁₂	5	5
Aragonite, CaCO ₃ (calculated pattern)	14m	44	Cryptohalite, (NH ₄) ₂ SiF ₆	2	23
Arcanite, K ₂ SO ₄	3	62	Cuprite, Cu ₂ O	11m	56
Arsenic, As	3	6	*Derbylite, SbFe ₄ Ti ₃ O ₁₃ (OH)	16m	89
Arsenolite, As ₂ O ₃	1	51	*Diamond, C	2	5
Aurostibite, AuSb ₂	7	18	*Diaspore, Al ₂ O ₃ ·H ₂ O	3	41
Avicennite, Tl ₂ O ₃	16m	77	Diopside, CaMg(SiO ₃) ₂	5m	17
*Azurite, Cu ₃ (OH) ₂ (CO ₃) ₂	10	30	*Dravite, NaMg ₃ Al ₆ B ₃ Si ₆ O ₂₇ (OH) ₄	3m	47
*Bahianite, Al _{5.66} Fe _{0.09} Sb _{2.95} O ₁₆	16m	87	Eitelite, Na ₂ Mg(CO ₃) ₂	11m	43
Baryte, BaSO ₄	10m	12	Elpasolite, K ₂ NaAlF ₆	9m	32
Bassanite, CaSO ₄ ·0.5H ₂ O	18m	22	*Enstatite, MgSiO ₃	6	30
Berlinite, AlPO ₄	10	3	Epsomite, MgSO ₄ ·7H ₂ O	7	39
Berndtite, SnS ₂	9m	57	Eriochalcite, CuCl ₂ ·2H ₂ O	18m	27
*Beryl, Be ₃ Al ₂ Si ₆ O ₁₈	9	13	Erythrite, Co ₃ (AsO ₄) ₂ ·8H ₂ O	19m	33
Bischofite, MgCl ₂ ·6H ₂ O	11m	37	Erythrosiderite, K ₂ FeCl ₅ ·H ₂ O	14m	22
Bismite, α -Bi ₂ O ₃	3m	17	Eskolaite, Cr ₂ O ₃	5	35
Bismoclite, BiOCl	4	54	Ettringite, Ca ₆ Al ₂ S ₃ O ₁₈ ·3H ₂ O	8	3
Bismuth, Bi	3	20	Fairchildite, K ₂ Ca(CO ₃) ₂	8m	48
Bismuthinite, Bi ₂ S ₃	5m	13	Farringtonite, Mg ₃ (PO ₄) ₂	19m	55
Bixbyite, α -Mn ₂ O ₃	11m	95	Fluorapatite, Ca ₅ F(PO ₄) ₃	3m	22
*Bloedite, Na ₂ Mg(SO ₄) ₂ ·4H ₂ O	6m	63	Fluorite, CaF ₂	1	69
Boehmite, Al ₂ O ₃ ·H ₂ O	3	38	Forsterite, Mg ₂ SiO ₄	1	83
*Bombiccite, C ₂₀ H ₃₄	16m	122	Franklinite, ZnFe ₂ O ₄	9m	60
Borax, Na ₂ B ₄ O ₅ (OH) ₄ ·8H ₂ O	16m	66	Fresnoite, Ba ₂ TiSi ₂ O ₈	9m	14
Bromargyrite, AgBr	4	46	Gahnite, ZnAl ₂ O ₄	2	38
Bromellite, BeO	1	36	Galaxite, MnAl ₂ O ₄	9	35
*Brookite, TiO ₂	3m	57	Galena, PbS	2	18
Brownmillerite, Ca ₄ Al ₂ Fe ₂ O ₁₀	16m	28	Gaspeite, NiCO ₃	1m	36
Brucite, Mg(OH) ₂	6	30	Geikielite, MgTiO ₃	5	43
Bunsenite, NiO	1	47	Gersdorffite, NiAsS	1m	35
Burkeite, Na ₆ CO ₃ (SO ₄) ₂	11m	52	Glauberite, Na ₂ Ca(SO ₄) ₂	6m	59
*Butlerite, Fe(OH)SO ₄ ·2H ₂ O	10m	95	Gold, Au	1	33
Cadmoselite, CdSe	7	12	Goslarite, ZnSO ₄ ·7H ₂ O	8	71
Calcite, CaCO ₃	2	51	Greenockite, CdS	4	15
Calomel, Hg ₂ Cl ₂	13m	30	*Groutite, MnO(OH)	11m	97
Carnallite, KMgCl ₃ ·6H ₂ O	8m	50	Gunningite, ZnSO ₄ ·H ₂ O	19m	86
Carrobiite, KF	1	64	Gypsum, CaSO ₄ ·2H ₂ O	17m	16
Cassiterite, SnO ₂	1	54	Halite, NaCl	2	41
Celestite, SrSO ₄	2	61	*Hartite, C ₂₀ H ₃₄	16m	122
Cerianite, CeO ₂	1	56	Hausmannite, Mn ₃ O ₄	10m	38
Cerussite, PbCO ₃	2	56	Hematite, α -Fe ₂ O ₃	18m	37
Cervantite, Sb ₂ O ₄	10	8	*Hemimorphite, Zn ₄ (OH) ₂ Si ₂ O ₇ ·H ₂ O	2	62
*Chabazite, Ca ₂ Al ₄ Si ₈ O ₂₄ ·12H ₂ O	19m	27	Hercynite, FeAl ₂ O ₄	19m	48
Chalcocyanite, CuSO ₄	3m	29	Hessite, Ag ₂ Te	19m	73
Chernovite, YAsO ₄	2m	39	Hetaerolite, ZnMn ₂ O ₄	10m	61
Chiolite, Na ₅ Al ₃ F ₁₄	16m	63	*Hexahydroborite, Ca[B(OH) ₄] ₂ ·2H ₂ O	16m	104
Chloraluminite, AlCl ₃ ·6H ₂ O	7	3	Hieratite, K ₂ SiF ₆	5	50
Chlorargyrite, AgCl	4	44	Hoernesite, Mg ₃ (AsO ₄) ₂ ·8H ₂ O	19m	53
Chloromagnesite, MgCl ₂	11m	94	Hopeite, Zn ₃ (PO ₄) ₂ ·4H ₂ O	16m	85
Chromatite, CaCrO ₄	7	13	Huebnerite, MnWO ₄	2m	24
Chromite, FeCr ₂ O ₄	19m	50	Humboldtine, FeC ₂ O ₄ ·2H ₂ O	10m	24
Chrysoberyl, BeAl ₂ O ₄	9	10	Humite, Mg ₇ F ₂ Si ₃ O ₁₂	1m	30
Cinnabar, HgS	4	17	Hydromolysite, FeCl ₃ ·6H ₂ O	17m	40
Claudetite, As ₂ O ₃	3m	9	Hydrophilite, CaCl ₂	11m	18
			Ilmenite, FeTiO ₃	15m	34

* Natural mineral

	Vol. or Sec.	Page		Vol. or Sec.	Page
Indialite, $Mg_2Al_4Si_5O_{18}$	1m	29	Palladium, Pd	1	21
Iodargyrite, AgI	8	51	Palladseite, $Pd_{17}Se_{15}$	16m	139
Iron, α -Fe	4	3	Palmierite, $K_2Pb(SO_4)_2$	14m	30
Jacobsite, $MnFe_2O_4$	9	36	Paraguanajuatite, Bi_2Se_3	18m	16
*Julgoldite, $Ca_2Fe_3Si_3O_{10}(OH,0)_2(OH)_2$	10m	72	*Paratellurite, TeO_2	10	55
Kalistrontite, $K_2Sr(SO_4)_2$	14m	31	Paratellurite, TeO_2	7	56
Kieserite, $MgSO_4 \cdot H_2O$	16m	46	Periclase, MgO	1	37
Koettigite, $Zn_3(AsO_4)_2 \cdot 8H_2O$	19m	85	Perovskite, $CaTiO_3$	9m	17
Kremersite, $(NH_4,K)_2FeCl_5 \cdot H_2O$	14m	8	*Phenakite, Be_2SiO_4	8	11
Langbeinite, $K_2Mg_2(SO_4)_3$	6m	40	Picromerite, $K_2Mg(SO_4)_2 \cdot 6H_2O$	8m	54
Larnite, β - Ca_2SiO_4	19m	29	*Pirssonite, $Na_2Ca(CO_3)_2 \cdot 2H_2O$	9m	106
Lautarite, $Ca(IO_3)_2$	14m	12	Platinum, Pt	1	31
Lead, Pb	1	34	Portlandite, $Ca(OH)_2$	1	58
*Leucophanite, $NaCaBeFSi_2O_6$	8m	138	Potash alum, $KAl(SO_4)_2 \cdot 12H_2O$	6	36
Libethenite, $Cu_2(OH)PO_4$	17m	30	Powellite, $CaMoO_4$	6	22
*Liddicoatite, $Ca(Li,Al)_3Al_6B_3Si_6O_{27}$ $(O,OH)_3(OH,F)$	16m	42	Pyrargyrite, Ag_3SbS_3	5m	51
Lime, CaO	1	43	Pyrite, FeS_2	5	29
Lime, CaO (calculated pattern)	14m	49	*Pyroaurite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$	10m	104
*Linarite, $CuPb(OH)_2(SO_4)$	16m	34	Pyrolusite, β - MnO_2	10m	39
Litharge, PbO (red)	2	30	Pyrope, $Mg_3Al_2(SiO_4)_3$	4m	24
Lithiophosphate, Li_3PO_4	4m	21	Pyrophanite, $MnTiO_3$	15m	42
Loellingite, $FeAs_2$	10	34	*Quartz, SiO_2 (α or low)	3	24
Loeweite, $Na_{12}Mg_7(SO_4)_{13} \cdot 15H_2O$	14m	35	Quartz, low, α - SiO_2	18m	61
Lopezite, $K_2Cr_2O_7$	15m	47	Rammelsbergite, $NiAs_2$	10	42
*Loveringite, $Ca_{.72}RE_{.33}(Y,Th,U,$ $Pb).05Ti_{12.48}Fe_{3.38}Cr_{2.24}Mg_{.92}$ $Zr_{.58}Al_{.39}V_{.21}Mn_{.04}O_{.38}$	16m	106	Retgersite, $NiSO_4 \cdot 6H_2O$	7	36
Lueshite, $NaNbO_3$	18m	64	Rhodochrosite, $MnCO_3$	7	32
Macedonite, $PbTiO_3$	5	39	Rokuhnite, $FeCl_2 \cdot 2H_2O$	11m	32
Magnesiochromite, $MgCr_2O_4$	9	34	Romarchite, SnO	4	28
Magnesite, $MgCO_3$	7	28	*Roscherite, (monoclinic), $Be_2Ca(Fe_{.3}Mg_{.7})_2Al_{.67}(PO_4)_3(OH)_3 \cdot$ $2H_2O$	16m	96
Magnetite, Fe_3O_4	5m	31	*Roscherite, (triclinic), Be_4Ca_2 $(Mn_{3.91}Mg_{.04}Ca_{.05})(Al_{.13}Fe_{.42}Mn_{.12})$ $(PO_4)_6(OH)_4 \cdot 6H_2O$	16m	100
Malachite, $Cu_2(OH)_2CO_3$	10	31	Rutile, TiO_2	7m	83
Malladrite, Na_2SiF_6	16m	68	Safflorite, $CoFeAs_4$	10	28
Manganolangbeinite, $K_2Mn_2(SO_4)_3$	6m	43	Salammoniac, NH_4Cl	1	59
Manganosite, MnO	5	45	Sanbornite, β - $BaSi_2O_5$	13m	10
Marshite, CuI	4	38	Sanmartinite, $ZnWO_4$	2m	40
Mascagnite, $(NH_4)_2SO_4$	9	8	Scacchite, $MnCl_2$	8m	43
Massicot, PbO (yellow)	2	32	*Scheelite, $CaWO_4$	6	23
Matlockite, $PbFCl$	13m	25	Schultenite, $PbHAsO_4$	14m	18
Matteuccite, $NaHSO_4 \cdot H_2O$	9m	52	Selenium, Se	5	54
Mayenite, $Ca_{12}Al_{14}O_{33}$	9	20	Selenolite, SeO_2	7m	60
Melanterite, $FeSO_4 \cdot 7H_2O$	8m	38	Sellaite, MgF_2	4	33
*Meliphanite, $Na_{.63}Ca_{1.37}BeAl_{.13}Si_{1.87}O_{6.25}F_{.75}$	8m	135	Senarmontite, Sb_2O_3	3	31
Metaborite, HBO_2	4m	27	Shcherbinaite, V_2O_5	8	66
Metacinnabar, HgS	4	21	*Siderite, $FeCO_3$	15m	32
Miargyrite, $AgSbS_2$	5m	49	Silver, Ag	1	23
*Millerite, NiS	1m	37	Silver, Ag (reference standard)	8m	2
Minium, Pb_3O_4	8	32	*Sjögrenite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$	10m	103
Mitscherlichite, $K_2CuCl_4 \cdot 2H_2O$	9m	34	Skutterudite, $CoAs_3$	10	21
Molybdenite, MoS_2	5	47	*Smithsonite, $ZnCO_3$	8	69
Molybdite, MoO_3	3	30	Soda alum, $NaAl(SO_4)_2 \cdot 12H_2O$	15m	68
Monteponite, CdO	2	27	*Sodalite, $Na_8Si_6Al_6O_{24}Cl_2$	7m	158
Montroydite, HgO	9	39	Soda niter, $NaNO_3$	6	50
Mullite, $Al_6Si_2O_{13}$	3m	3	Sphaerocobaltite, $CoCO_3$	10	24
Nantokite, $CuCl$	4	35	Sphalerite, ZnS	2	16
*Newberryite, $MgHPO_4 \cdot 3H_2O$	7m	139	Spinel, $MgAl_2O_4$	9m	25
Nickel-hexahydrite, β - $NiSO_4 \cdot 6H_2O$	19m	65	Stibnite, Sb_2S_3	5	6
Niter, KNO_3	3	58	Stilleite, $ZnSe$	3	23
Nitrammite, NH_4NO_3	7	4	Stolzite, $PbWO_4$	5m	34
Nitrobarite, $Ba(NO_3)_2$	11m	14	Strontianite, $SrCO_3$	3	56
Norbergite, $Mg_3F_2SiO_4$	10	39	Struvite, $MgNH_4PO_4 \cdot 6H_2O$	3m	41
Oldhamite, CaS	7	15	Sulfur, S (orthorhombic)	9	54
Otavite, $CdCO_3$	7	11	Sylvite, KCl	1	65
Oxammite, $(NH_4)_2C_2O_4 \cdot H_2O$	7	5	Syngenite, $K_2Ca(SO_4)_2 \cdot H_2O$	14m	25
			Szmikite, $MnSO_4 \cdot H_2O$	16m	49

Tellurantimony, Sb ₂ Te ₃	3m	8
*Tellurite, TeO ₂	9	57
Tellurium, Te	1	26
Tellurobismuthite, Bi ₂ Te ₃	3m	16
Tenorite, CuO	1	49
Teschemacherite, NH ₄ HCO ₃	9	5
Thenardite, Na ₂ SO ₄	2	59
Thermonatrite, Na ₂ CO ₃ ·H ₂ O	8	54
*Thomsenolite, NaCaAlF ₆ ·H ₂ O	8m	132
Thorianite, ThO ₂	1	57
Thortveitite, Sc ₂ Si ₂ O ₇	7m	58
Tiemannite, HgSe	7	35
Tin, α-Sn (cubic)	2	12
~ Tin, β-Sn (tetragonal)	1	24
*Topaz, Al ₂ SiO ₄ (F,OH) ₂	1m	4
Trevorite, NiFe ₂ O ₄	10	44
Trippkeite, CuAs ₂ O ₄	16m	120
*Trona, Na ₃ H(CO ₃) ₂ ·2H ₂ O	15m	71
Tschermigite, NH ₄ Al(SO ₄) ₂ ·12H ₂ O	6	3
Tungstenite, WS ₂	8	65
Unnamed mineral, K _{1.16} Ba _{.72} Fe _{.36} Ti _{5.58} O ₁₃	16m	147
Uraninite, UO ₂	2	33
Uvarovite, Ca ₃ Cr ₂ (SiO ₄) ₃	10	17
*Valentinitite, Sb ₂ O ₃	10	6
Vanthoffite, Na ₆ Mg(SO ₄) ₄	15m	72
Villiaumite, NaF	1	63
Vivianite, Fe ₃ (PO ₄) ₂ ·8H ₂ O	16m	38
Wakefieldite, YVO ₄	5m	59
Willemite, Zn ₂ SiO ₄	7	62
Witherite, BaCO ₃	2	54
Wulfenite, PbMoO ₄	7	23
Wurtzite, ZnS	2	14
*Xanthoconite, Ag ₃ AsS ₃	8m	126
Xenotime, YPO ₄	8	67
Yavapaitite, KFe(SO ₄) ₂	16m	59
Zinc, Zn	1	16
Zincite, ZnO	2	25
Zinkosite, ZnSO ₄	7	64
*Zircon, ZrSiO ₄	4	68
Zircosulfate, Zr(SO ₄) ₂ ·4H ₂ O	7	66

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

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NOTE: The principal publication outlet for the foregoing data is the Journal of Physical and Chemical Reference Data (JPCRD) published quarterly for NBS by the American Chemical Society (ACS) and the American Institute of Physics (AIP). Subscriptions, reprints, and supplements available from ACS, 1155 Sixteenth St., NW, Washington, DC 20056.

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