THE NATIONAL BUREAU OF STANDARDS

The National Bureau of Standards is a principal focal point in the Federal Government for assuring maximum application of the physical and engineering sciences to the advancement of technology in industry and commerce. Its responsibilities include development and maintenance of the national standards of measurement, and the provisions of means for making measurements consistent with those standards; determination of physical constants and properties of materials; development of methods for testing materials, mechanisms, and structures, and making such tests as may be necessary, particularly for government agencies; cooperation in the establishment of standard practices for incorporation in codes and specifications; advisory service to government agencies on scientific and technical problems; invention and development of devices to serve special needs of the government; assistance to industry, business, and consumers in the development and acceptance of commercial standards and simplified trade practice recommendations; administration of programs in cooperation with United States business groups and standards organizations for the development of international standards of practice; and maintenance of a clearinghouse for the collection and dissemination of scientific, technical, and engineering information. The scope of the Bureau's activities is suggested in the following listing of its four Institutes and their organizational units.


*NBS Group, Joint Institute for Laboratory Astrophysics at the University of Colorado.

**Located at Boulder, Colorado.
Standard X-ray Diffraction
Powder Patterns

Howard E. Swanson, Marlene Cook Morris,
Eloise H. Evans, and Linda Ulmer

National Bureau of Standards Monograph 25 — Section 3
Issued July 31, 1964
Introduction

Standard x-ray powder patterns:
- Copper Sulfate, (chalcocyanite), CuSO₄ (orthorhombic)
- Cesium Fluoride, CsF (cubic)
- Dysprosium Arsenate, DyAsO₄ (tetragonal)
- Indium Arsenide, InAs (cubic)
- Lanthanum Arsenate, LaAsO₄ (monoclinic)
- Lanthanum Niobium Titanium Oxide, LaNb₂O₇ (monoclinic)
- Lithium Phosphate, low form, (lithiophosphate), Li₃PO₄ (orthorhombic)
- Lithium Phosphate, high form, Li₃PO₄ (orthorhombic)
- Magnesium Ammonium Phosphate Hexahydrate, (struvite), MgNH₄PO₄·6H₂O (orthorhombic)
- Potassium Chlorate, KClO₃ (monoclinic)
- Potassium Lithium Sulfate, KLiSO₄ (hexagonal)
- Potassium Perchlorate, K₂CrO₄ (tetragonal)
- Potassium Persulfate, K₂S₂O₇ (trigonal)
- Potassium Persulfate, K₂S₂O₇ (orthorhombic)
- Potassium Persulfate, K₂S₂O₇ (tetragonal)
- Silver Antimony Telluride, AgSb₂Te₄ (cubic)
- Sodium Magnesium Aluminum Boron, Hydroxy Silicate, dravite, NaMg₂Al₂B₃Si₆O₁₇(OH)₄ (trigonal)

Vol. 9, Page 6, (NH₄)₂PtBr₆ table: Cu radiation applies to entire table.
Vol. 8, Page 42, Column 1: The density should be 4.697.
Vol. 5, Page 10, Column 1, bottom line, the index of refraction should read 1.710.
Vol. 3, Page 54, On the line below
Vol. 2, Page 46, Lattice constants paragraph, column 1, line 3: Puma should read Pnma. This change was made in the Vol. 2 reprint.
Vol. 1, Page 50, In the pattern of Swanson and Tatge, the d-values 0.8576, 0.8557, 0.8467, 0.8412, and 0.8383 should have the following hkl values, 422, 511, 513, 333, and 206.
Vol. 3, Page 54, On the line below hkl 121 insert hkl 012; on the line below hkl 200 insert hkl 031; hkl 040 should read 211; delete hkl values 230 and 410 and all those following 421.
Vol. 5, Page 10, Column 1, bottom line, the index of refraction should read 1.710.
Vol. 11, In pattern of Swanson, Gilfrich, and Ugrinic, for hkl 721 d should read 2.078.
Page 43, Reference No. 3: The fourth author's name should be F. E. Sennett.
Vol. 8, Page 42, Column 1: The density should be 4.697.
Vol. 9, Page 6, (NH₄)₂PtBr₆ table: Cu radiation applies to entire table.
Errata—Continued

Page 19, hkl 102 should be 012.
Page 47, The density of K$_2$ZrF$_7$ should be 3.123.

Monograph 25
Sec. 1, Page 10, Lattice constants table: headings $a$ $b$ $c$ should read $b$ $c$ $a$.
Page 12, The title should read: Erbium Gallium Oxide 3:5. . . .
Sec. 2, Page 1, Column 2 line 11: potassium nitroso chlororhenate should be potassium nitroso chlororuthenate.
Page 2, In the left hand column, the sentence beginning in the seventh line from the bottom should read: Factors for converting integrated intensities to peak height intensities are on the left side of the chart.
Page 8, CdWO$_4$ space group should be C$_{4}$—P2/c (No. 13).
Page 11, Spectrographic analysis should read: 0.01 to 0.1 percent sodium and . . . .
Page 34, The intensity of the line at $d = 4.21$ should be 61. Insert the reading: $hkl=102$, $d=3.94$, $I=2$.
Page 35, Reference No. 7 should read: Helen M. Ondik, to be published in Acta Cryst.

Addenda

Monograph 25
Sec. 2, Page 22, Insert this data:

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</table>

Sec. 2, Page 35, Add this data: The sample is optically negative and the indices of refraction are $N_\alpha=1.440$, $N_\beta=1.458$, $N_\gamma=1.474$, and $2V\approx90^\circ$.

Standard X-ray Diffraction Powder Patterns

The eleven previous volumes in this series are available from the Superintendent of Documents, U.S. Government Printing Office, Washington 25, D.C., as follows:

NBS Circular 539, Volume 1, Standard X-ray Diffraction Powder Patterns (Data for 54 inorganic substances) 45 cents
NBS Circular 539, Volume 2, Standard X-ray Diffraction Powder Patterns (Data for 30 inorganic substances) 45 cents
NBS Circular 539, Volume 3, Standard X-ray Diffraction Powder Patterns (Data for 34 inorganic substances) 45 cents
NBS Circular 539, Volume 4, Standard X-ray Diffraction Powder Patterns (Data for 42 inorganic substances) 45 cents
NBS Circular 539, Volume 5, Standard X-ray Diffraction Powder Patterns (Data for 45 inorganic substances) 45 cents
NBS Circular 539, Volume 6, Standard X-ray Diffraction Powder Patterns (Data for 44 inorganic substances) 40 cents
NBS Circular 539, Volume 7, Standard X-ray Diffraction Powder Patterns (Data for 53 substances) 40 cents
NBS Circular 539, Volume 8, Standard X-ray Diffraction Powder Patterns (Data for 61 substances) 45 cents
NBS Circular 539, Volume 9, Standard X-ray Diffraction Powder Patterns (Data for 43 substances) 40 cents
NBS Circular 539, Volume 10, Standard X-ray Diffraction Powder Patterns (Data for 40 substances) 40 cents
NBS Monograph 25, Section 1, Standard X-ray Diffraction Powder Patterns (Data for 46 substances) 40 cents
NBS Monograph 25, Section 2, Standard X-ray Diffraction Powder Patterns (Data for 37 substances) 35 cents

Those wishing to be notified of future issues should send mailing address to the Government Printing Office.
STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 3—Data for 51 Substances

Howard E. Swanson, Marlene Cook Morris, Eloise H. Evans, and Linda Ulmer

INTRODUCTION

The X-ray Powder Data File[1] is a compilation of diffraction patterns from many sources and is used for the identification of unknown crystalline materials by matching spacing and intensity measurements. The National Bureau of Standards in its program for the revision and evaluation of published x-ray data for the X-ray Powder Data File presents data in this report for 51 compounds. This compilation is the thirteenth of a series of "Standard X-ray Diffraction Patterns." The designation "Circular 539" used for the first 10 volumes has been discontinued in favor of the new series, "Monograph 25." This compilation is the third section of the new series Monograph 25. Included are patterns recommended to replace data on 26 cards now present in the File. The other patterns are for 30 compounds not included in the File. These compounds are: ampholyte; antimony telluride; arsenic oxide, claudetite; barium bromide monohydrate; bismuth orthophosphate (trigonal); bismuth orthovanadate (tetragonal); bismuth orthovanadate (monoclinic); cadmium perchlorate hexahydrate; cerium niobium titanium oxide; cesium chromate; cesium fluoride; cesium iodide; cesium oxide; cesium phosphate; cesium sulfide; cesium telluride; chromium arsenate; chromium oxide; chromic oxide; chromium perchlorate; cobalt arsenate; cobalt chromate; cobalt fluoride; cobalt perchlorate hexahydrate; cobalt perchlorate hexahydrate; dysprosium arsenate; erbium arsenate; europium arsenate; gallium arsenide; holmium arsenate; lanthanum arsenate; lanthanum niobium titanium oxide; potassium lithium sulfate; potassium perchlorate; potassium zinc decavanadate 16-hydrate; rubidium chromate; silver antimony telluride; sodium magnesium aluminum boron hydroxy phosphate; strontium chloride; strontium fluoride; strontium oxide; thallium arsenate; thallium chromate; thallium oxide; thulium arsenate. The experimental procedure and general plan of this Monograph section 3 have not changed greatly from previous publications. However, the basic technique is discussed, in this section, with minor changes.

Powder data cards. Under this heading are given the Powder Data File card numbers, the three strongest lines, and the literature references for each card. Cards listed through the 1962 index to the Powder Data File are included in the table.

Additional published patterns. Literature references for patterns that have not been published as Powder Data cards are listed.

NBS sample. Many of the samples used to make NBS patterns were special preparations of high purity obtained from a variety of sources or prepared in small quantities in our laboratory by J. deGroot. Unless otherwise noted, the spectrographic analyses were done at NBS after preparation of the sample was completed. The limit of detection for the alkali elements was 0.05 percent for the spectrographic analysis. A microscopic inspection for phase purity was made on the nonopaque materials during the refractive index determination. Another check of phase purity was...
usually provided by the x-ray pattern itself, when it was indexed by comparison with theoretical \(d\)-values. Treating the sample by appropriate annealing, recrystallization, or heating in hydrothermal bombs improved the quality of most of the patterns. The refractive index measurements were made by grain-immersion methods in white light, using oils standardized in sodium light, and covering the range 1.40 to 2.00.

**X-ray techniques.** At least three patterns for intensity measurements were prepared to check reproducibility. Samples that gave satisfactory intensity patterns usually had an average particle size smaller than 10 \(\mu\). [2]. In order to avoid the orientation effects when samples are packed or pressed, a sample holder was made that had an extended rectangular cavity open at its top face and end. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall. (See fig. 1.) The powdered sample was then drifted into the remaining end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample surface could be exposed to the x-ray beam (as shown in fig. 2). To powders that did not flow readily or were prone to orient excessively, approximately 50-volume percent of finely-ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the intensity of the strongest line. Additional patterns were obtained for \(d\)-value measurements. Specimens for these patterns were prepared by packing into a shallow holder a sample containing approximately 5-wt percent tungsten powder that served as an internal standard. When tungsten lines were found to interfere, 25 percent silver was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used for the regions between the peaks of the standard. For low values of \(2\theta\), the pattern peak was measured in the center, at a place averaging about 75 percent of the peak height. For higher values of \(2\theta\), where the \(c_1\) and \(c_2\) peaks were separated, the \(c_1\) peak was measured in the same way. The internal standard correction appropriate to each region was then applied to the measurement of \(2\theta\). The internal standard lattice constants used were 3.1648 \(\AA\) for tungsten and 4.0861 \(\AA\) for silver at 25 °C as determined by Jette and Foote [3]. All of the NBS patterns, unless otherwise noted, are made at 25 °C, using either filtered copper or cobalt radiation (\(K\alpha\)), having the wavelengths 1.5405 \(\AA\), and 1.7889 \(\AA\), respectively.

**Structural data.** For cubic materials a value for the lattice constant was calculated for each \(d\)-value. However, the constant reported is that obtained by averaging the last five lines because of the greater accuracy of measurement in the large-angle region of the pattern. The unit cell values for each noneubic substance were determined by means of a least-squares calculation made on the IBM 7090, using those \(d\)-values for which only one set of Miller indices could be assigned. The number of significant figures reported for \(d\)-values in the NBS pattern is limited by the quality of each sample as indicated by residuals obtained from least squares refinement. A portion of the indexing and cell refinement calculation was performed on a Burroughs B 220 computer at the United States Geological Survey using a program developed by H. T. Evans, Jr.
D. E. Appleman, and D. Handwerker. Lattice constant errors are given only for data refined on that program and are based on least squares refinement of the variance-covariance matrix derived from the unweighted $\Delta \theta$ residuals.

Published unit cell data in kX units were converted to angstrom units using the factor 1.00202 as recommended by an international conference of crystallographers [4].

The space groups are listed with both the Schoenflies and short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography [5].

Orthorhombic cell dimensions are presented according to the Dana convention [6] $b > a > c$.

The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter and are computed with atomic weights based on carbon 12 [7], and the Avogadro number $(6.02252 \times 10^{23})$.

References


Aluminum 3:2 Silicate (mullite)* $3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$ (orthorhombic)

Powder data cards

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<td>2. 54</td>
</tr>
<tr>
<td></td>
<td>3. 42</td>
<td>2. 54</td>
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</table>


NBS sample. The sample of aluminum 3:2 silicate was prepared at NBS by C. Robbins. Gamma Al$_2$O$_3$ and SiO$_2$-nH$_2$O were mechanically mixed in stoichiometric proportions of 3Al$_2$O$_3$ to 2SiO$_2$-nH$_2$O. This mixture was pressed into pellets and fired at 1400 °C and 1500 °C with little reaction, then remixed and fired in an open system at 1700 °C for 24 hr. Reaction was nearly complete. It was crushed, reground in an agate mortar and refired at 1725 °C for 24 hr. Chemical analysis of the finished product showed 61.6 mole percent Al$_2$O$_3$ and 38.4 mole percent SiO$_2$ instead of the beginning percentages of 60 and 40 in the 3:2 mixture. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent iron, and 0.001 to 0.01 percent each of calcium, chromium, magnesium, manganese, nickel, titanium, and zirconium.

*Some disagreement exists in the literature as to which ratio or ratios of alumina to silicas should be considered for mullite (3:2, 2:1, or both?). This sample was prepared as 3:2 at the request of P. Schroth of the Armco Steel Corp. to be used as an identification, diffraction standard for mullite in refractory brick.

The sample was colorless and optically positive with the indices of refraction $N_a = 1.637$, $N_g = 1.641$, and $N_r = 1.652$.

The $d$-values of the three strongest lines are: 3.390, 3.428 and 2.206 Å.

Structural data. Sadanaga, Tokonami, and Takeuchi [10] in 1962 determined that mullite has the space group $D_{3h}$-Pbam (No. 55). Wyckoff, Grieg, and Bowen [5] in 1926 determined that mullite has $3/4(3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2)$ per unit cell. Several lattice constants have been converted from kX to angstrom units for comparison with the NBS values.

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*These values are for $2\text{Al}_2\text{O}_3 \cdot \text{SiO}_2$.

The density calculated from the NBS lattice constants is 3.170 g/cm$^3$ at 25 °C.
Aluminum 3:2 Silicate (mullite) \(3\text{Al}_2\text{O}_3\cdot2\text{SiO}_2\) (orthorhombic)—Continued

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References

Ammonium Fluoberyllate, (NH₄)₂BeF₄ (orthorhombic)

Powder data cards

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Additional published patterns. None.

NBS sample. The sample of ammonium fluoberyllate was obtained from K and K Laboratories, Jamaica, Long Island, N.Y. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, calcium, and silicon.

The sample was colorless, and optically negative with \( N_a = 1.397, N_0 = 1.401 \), and \( N_\lambda = 1.403 \).

The \( d \)-values of the three strongest lines are: 4.275, 2.478, and 4.312 Å.

Structural data. Hultgren [1] in 1934 determined that ammonium fluoberyllate belongs to the space group \( \text{D}_{2h}^5 - \text{Pnam} \) (No. 62) with \( 4[(\text{NH}_4)_2\text{BeF}_4] \) per unit cell. The lattice constants of Mukherjee [2] have been converted from kX to ångstrom units for comparison with the NBS values.

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The density of ammonium fluoberyllate calculated from NBS lattice constants is 1.698 g/cm³ at 25 °C.

References

Ammonium Fluoborate, NH$_4$BF$_4$ (orthorhombic)

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Additional published patterns. None.

NBS sample. The sample of ammonium fluoborate was obtained from K and K Laboratories, Jamaica, Long Island, N.Y. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of calcium and phosphorus and 0.001 to 0.01 percent each of iron, titanium, and strontium.

The sample was colorless and had extremely low birefringence and indices of refraction.

The $d$-values of the three strongest lines are: 4.482, 3.542, and 3.186 Å.

Structural data. Hoard and Blair [1] in 1935 determined that ammonium fluoborate has the space group D$_{2h}^8$-Pbnm (No. 62) and 4(NH$_4$BF$_4$) per unit cell. The cell constants of Hoard and Blair have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

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Ammonium Fluoborate, $\text{NH}_4\text{BF}_4$ (orthorhombic)—Continued

The density of ammonium fluoborate calculated from the NBS lattice constants is 1.858 g/cm$^3$ at 26 $^\circ$C.

References


Antimony Selenide, $\text{Sb}_2\text{Se}_3$ (orthorhombic)

Powder data cards. None.


NBS sample. The sample of antimony selenide was obtained from Semitronics, Inc., Winchester, Mass. It was heated in an evacuated tube at 450 $^\circ$C overnight to obtain a sharper pattern. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent tellurium and 0.001 to 0.01 percent each of aluminum and silicon.

The sample was a dark gray opaque powder. The $d$-values of the three strongest lines are: 2.868, 3.162, and 3.253 $\AA$.

Structural data. Dönges [1] in 1950 determined that antimony selenide has the antimony sulfide structure, the space group $D_{2h}^5$-Pbnm (No. 62), and 4($\text{Sb}_2\text{Se}_3$) per unit cell.

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Antimony Selenide, Sb$_2$Se$_3$ (orthorhombic)—Continued

The density of antimony selenide calculated from NBS lattice constants is 5.843 g/cm$^3$ at 25 °C.

**Reference**

Antimony Telluride, Sb$_2$Te$_3$ (trigonal)

**Powder data cards.** None.
**Additional published patterns.** None.

**NBS sample.** The sample of antimony telluride was obtained from Semitronics, Inc., Winchester, Mass. It was heated at 450 °C overnight in an evacuated tube to sharpen the pattern. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum and silicon.

The sample was dark gray opaque powder. The $d$-values of the three strongest lines are: 3.157, 2.349, and 2.130 Å.

**Structural data.** Dönges [1] in 1951 showed that antimony telluride is isomorphous with bismuth telluride, having the space group D$_{3d}^1$ - R$3m$ (No. 166), and 3(Sb$_2$Te$_3$) per unit hexagonal cell, or 1(Sb$_2$Te$_3$) per unit rhombohedral cell. The unit cell measurements reported by Semiletov [2] have been converted from kX to angstrom units for comparison with NBS values.

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The density of antimony telluride calculated from NBS lattice constants is 6.513 g/cm$^3$ at 25 °C.

**References**

Arsenic Trioxide, claudetite, $\text{As}_2\text{O}_3$ (monoclinic)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of claudetite was obtained from the National Museum, No. 1737 from the San Domingo mines, Portugal. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of aluminum, yttrium, and zinc; 0.01 to 0.1 percent each of barium, calcium, cobalt, chromium, iron, magnesium, titanium, and tungsten.

The sample was colorless. Due to the high indices of refraction a complete optical analysis was not obtained, but partial results seemed to confirm the data given in Dana [4].

The $d$-values of the three strongest lines are: 3.245, 3.454, and 2.771 Å.

**Structural data.** Buerger [1] in 1942 determined that claudetite has the space group $C_{2h}^-\text{P}2_1/n$ (No. 14) and 4($\text{As}_2\text{O}_3$) per unit cell.

The density of claudetite calculated from the NBS lattice constants is 4.186 g/cm$^3$ at 25 °C.

**References**


**Lattice constants**

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<td>&lt;3</td>
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**Lattice constants**

<table>
<thead>
<tr>
<th>Year</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1951</td>
<td>Becker, Plieth and Stranski [2]</td>
</tr>
<tr>
<td>1951</td>
<td>Frueh [3]</td>
</tr>
<tr>
<td>1963</td>
<td>National Bureau of Standards at 25 °C</td>
</tr>
</tbody>
</table>

- $a = 5.25 \pm 0.002 \text{ Å}$
- $b = 12.90 \pm 0.001 \text{ Å}$
- $c = 4.53 \pm 0.005 \text{ Å}$
- $\beta = 93^\circ 53'$
- $a = 5.25 \pm 0.002 \text{ Å}$
- $b = 12.87 \pm 0.001 \text{ Å}$
- $c = 4.54 \pm 0.005 \text{ Å}$
- $\beta = 93^\circ 49'$
- $a = 5.339 \pm 0.002 \text{ Å}$
- $b = 12.984 \pm 0.001 \text{ Å}$
- $c = 4.505 \pm 0.005 \text{ Å}$
- $\beta = 94^\circ 16', 1'$
- $a = 5.339 \pm 0.002 \text{ Å}$
- $b = 12.984 \pm 0.001 \text{ Å}$
- $c = 4.505 \pm 0.005 \text{ Å}$
- $\beta = 94^\circ 16', 1'$

9
Barium Bromide Monohydrate, BaBr₂·H₂O (orthorhombic)

Powder data cards. None.
Additional published patterns. None.
NBS sample. The sample of barium bromide monohydrate was prepared from barium bromide dihydrate obtained from City Chemical Co., New York, N.Y. The hydrate was heated overnight at 85 to 90 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of sodium and strontium; and 0.001 to 0.01 percent each of calcium, magnesium, silicon, and titanium.

The color of the sample was white. The refractive index could not be determined because the sample was too fine.

The $d$-values of the three strongest lines are: 3.170, 2.512, and 2.999 Å.

Structural data. Vainstein and Pinsker [1] in 1950 determined that barium bromide monohydrate has the barium chloride monohydrate structure, the space group $D_{2h}^5-Pbnm$ (No. 62), and 4 (BaBr₂·H₂O) per unit cell.

<table>
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<tr>
<th>$hkl$</th>
<th>Internal Standard, Tungsten, $a_0 = 3.1648$ Å</th>
<th>Cu, 1.5405 Å at 25 °C</th>
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</tbody>
</table>

The density of barium bromide monohydrate calculated from the NBS lattice constants is 4.135 g/cm³ at 25 °C.

Reference

Barium Stannate, BaSnO₃ (cubic)

The density of barium stannate calculated from the NBS lattice constant is 7.238 g/cm³ at 25 °C.

### Powder data cards

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**Additional published patterns.** None.

**NBS sample.** The sample of barium stannate was prepared at NBS from stoichiometric amounts of barium carbonate and stannic oxide, pressed into a pellet and heated at 1400 °C for 1 hr. Spectrographic analysis showed the following major impurities: 0.1 percent calcium and 0.01 to 0.1 percent each of aluminum, magnesium, silicon, and strontium.

The sample was very light gray. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 2.911, 2.376, and 2.058 Å.

**Structural data.** Megaw [1] in 1946 determined that barium stannate has the perovskite structure, the space group OJ-PmSm (No. 221), and 1 (BaSnO₃) per unit cell.

<table>
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<th>hkl</th>
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<tbody>
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<td></td>
<td>Cu, 1.5405 Å at 25 °C</td>
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<td>222</td>
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<td>.980504 15 4.1164</td>
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Average value of last five lines: 4.1163

**References**


Bismuth Orthophosphate, BiPO₄ (monoclinic)

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<tr>
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**NBS sample.** The sample of monoclinic bismuth orthophosphate was obtained from Bios Laboratories, Inc., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of silver, aluminum, copper, iron, magnesium, lead, and silicon.

The color of the sample was white. The indices of refraction could not be obtained because the sample was too fine.

The d-values of the three strongest lines are: 3.066, 2.862, and 4.156 Å.

**Structural data.** Zemann [2] in 1950 determined that monoclinic bismuth orthophosphate has the monazite structure, the space group C₂ᵥ-P2₁/n (No. 14), with 4(BiPO₄) per unit cell. According to Mooney-Slater [3] 1962, three forms of bismuth phosphate exist: a hexagonal low phase formed from precipitation at room temperature, a high monoclinic phase formed about 700 °C and the monoclinic monazite phase formed above 350 °C.
Bismuth Orthophosphate, BiPO₄ (monoclinic)—Continued

**Lattice constants**

<table>
<thead>
<tr>
<th>Year</th>
<th>Author(s)</th>
<th>a (Å)</th>
<th>b (Å)</th>
<th>c (Å)</th>
<th>β (°)</th>
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<th>$I$</th>
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</thead>
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<td>312</td>
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</tbody>
</table>

The density of monoclinic bismuth orthophosphate calculated from NBS lattice constants is 6.863 g/cm³ at 25 °C.

**References**

Bismuth Orthophosphate, BiPO₄ (trigonal)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of trigonal bismuth orthophosphate was precipitated at NBS from a mixture of bismuth nitrate and phosphoric acid. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent sodium and 0.001 to 0.01 percent silicon.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 4.421, 3.025, and 2.854 Å.

**Structural data.** Mooney-Slater [1] in 1962 determined the structure of the trigonal bismuth orthophosphate; it has the space group D₃h-P3₁2₁ (No. 152) and 3 (BiPO₄) per unit cell. This form is transformed to a monoclinic monazite structure at 350 °C and to another higher temperature monoclinic form above 700 °C.

### Lattice constants

<table>
<thead>
<tr>
<th></th>
<th>a</th>
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<tr>
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<td>± 0.0007Å</td>
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The density of trigonal bismuth orthophosphate calculated from NBS lattice constants is 5.538 g/cm³ at 25 °C.

**Reference**

Bismuth Orthovanadate (low form), BiVO₄ (tetragonal)

**Powder data cards.** None. (Card No. 12–293 gives data for a mineral pucherite, BiVO₄, which is orthorhombic and does not compare with either of the synthetic forms of BiVO₄.)

**Additional published patterns.** None.

**NBS sample.** The sample of low form bismuth orthovanadate was obtained from City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum and silicon. The sample was also precipitated at NBS from solutions of Na₃VO₄ and Bi(NO₃)₃. If the precipitate is heated below 400 °C, the tetragonal form is unchanged. Between 400 and 500 °C the changed to the stable monoclinic form occurs.

The color of the sample was orange-yellow. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.649, 2.738, and 1.879 Å.

**Structural data.** The structure of low form bismuth orthovanadate has not been reported in the literature. However, because of the similarity of patterns it is thought to be isostructural with zircon, having the space group D_{4h}⁻I₄/m (No. 141) and 4(BiVO₄) per unit cell.

<table>
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<td>d</td>
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The density of low form bismuth orthovanadate calculated from NBS lattice constants is 6.252 g/cm³ at 26 °C.

Bismuth Orthovanadate (high form), BiVO₄ (monoclinic)

**Powder data cards.** None. (Card No. 12–293 gives data for a mineral pucherite, BiVO₄, which is orthorhombic and does not correspond to either form of BiVO₄ which we prepared.)

**Additional published patterns.** None.

**NBS sample.** The sample of high form bismuth orthovanadate was prepared by R. S. Roth at NBS by heating stoichiometric mixtures of bismuth oxide and vanadium oxide at 895 °C for 16 hr. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum and silicon. The monoclinic form was also prepared from the low form which was made by precipitation from solutions of Na₃VO₄ and Bi(NO₃)₃. The low form sample is tetragonal up to approximately 400 °C. The nonreversible change to the monoclinic form takes place between 400 and 500 °C.

The color of the sample was orange-yellow. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.095, 3.082, and 3.120 Å.

**Structural data.** Roth and Waring [1] in 1963 reported that high form BiVO₄ is thought to be isostructural with fergusonite because of the similarity of patterns. Ferguson [2] in 1955 reported that the fergusonite structure is monoclinic. The probable space group is C_{2h}⁻I2/a (No. 15) with 4(BiVO₄) per unit cell.
Bismuth Orthovanadate (high form), BiVO₄ (monoclinic)—Continued

### Lattice constants

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
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<th>β</th>
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</thead>
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The density of high form bismuth orthovanadate calculated from NBS lattice constants is 6.951 g/cm³ at 26 °C.

### References


Bismuth Telluride (tellurobismuthite), Bi₂Te₃ (trigonal)

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**NBS sample.** The sample of bismuth telluride was obtained as a single crystal from Semitronics Inc., Winchester, Mass. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of magnesium and silicon.

**Structure data.** Lange [4] in 1939 determined that bismuth telluride has the tetradymite structure with the space group D⁻₃d-R3m (No. 166) and 3(Bi₂Te₃) per unit hexagonal cell.

**Lattice constants**

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The density of bismuth telluride calculated from the NBS lattice constants is 7.857 g/cm³ at 25 °C.

- The sample was a gray opaque powder.
- The d-values of the three strongest lines are: 3.222, 2.376, and 2.192 Å.

**Lattice data.**

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Bismuth Telluride (tellurobismuthite), Bi₂Te₃ (trigonal)—Continued

References

Bismuth Trioxide (bismite), alpha Bi₂O₃ (pseudo-orthorhombic)

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NBS sample. The sample of bismuth trioxide was obtained from Johnson, Matthey, and Co., Ltd. Their spectrographic analysis showed the following major impurities: less than 0.001 percent each of silicon, aluminum, lead, silver, and sodium.

The color of the sample was light yellow. The refractive indices were too high to be determined by the usual liquid-grain immersion method.

The d-values of the three strongest lines are:
3.253, 2.693, and 2.708 Å.

Structural data. Sillén [1] in 1941 determined that alpha bismuth oxide is monoclinic or pseudo-orthorhombic having the monoclinic space group Cem–P2₁/c (No. 14), with 4(Bi₂O₃) per unit monoclinic cell, or 8(Bi₂O₃) per unit pseudo-orthorhombic cell. According to Sillén [1], the monoclinic indices hkl are transformed into the pseudo-orthorhombic indices h'k'l' by the following relations

\[ h' = h, \quad k' = k, \quad \pm l' = 2l - h \]

The lattice constants reported by Sillén have been converted from kX to angstrom units for comparison with the NBS values.

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Bismuth Trioxide (bismite), alpha Bi₂O₃ (pseudo-orthorhombic)—Continued

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| Lattice constants |
|-------------------|-----------------|-----------------|
|                  | \(a\) | \(b\) | \(c\) |
| 1941 Sillén [1]   | 8.16  | 13.81 | 5.84  |

The density of alpha bismuth trioxide calculated from NBS lattice constants is 9.371 g/cm³ at 25 °C.

References

Cadmium Perchlorate Hexahydrate, Cd(ClO₄)₂·6H₂O (trigonal)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of cadmium perchlorate hexahydrate was obtained from the City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.0001 to 0.001 percent each of lead and silicon.

The sample was colorless and optically negative with indices of refraction N₀ = 1.490 and Nₑ = 1.479.

The d-values of the three strongest lines are: 3.995, 4.223, and 2.902 Å.

**Structural data.** West [1] in 1935 reported that cadmium perchlorate hexahydrate is trigonal, the space group C₃ᵥ-P3₁m (No. 156) with 1[Cd(ClO₄)₂·6H₂O] per unit cell. West reported that the structure is very similar to the hexagonal magnesium perchlorate structure. Moss, Russell, and Sharp [2] confirmed West's determinations. The value of "a" reported by West has been divided by 2 as he suggested. The unit cell values reported by West have been converted from kX to angstrom units for comparison with the NBS values.

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The density of cadmium perchlorate hexahydrate calculated from the NBS lattice constants is 2.361 g/cm³ at 25 °C.

**References**


Cadmium Sulfate, CdSO₄ (orthorhombic)

The sample was white. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.329, 3.277, and 2.961 Å.

Structural data. Kokkoros and Rentzeperis [1] in 1961 determined cadmium sulfate is orthorhombic with the most probable space group D₂h-Pmmn (No. 59) with 2(CdSO₄) per unit cell.

The density of cadmium sulfate calculated from NBS lattice constants is 4.759 g/cm³ at 25 °C.

Additional published patterns. None.

NBS sample. The sample of cadmium sulfate was prepared at NBS from cadmium carbonate treated with an excess of sulfuric acid and heated to dryness. Spectrographic analysis showed the major impurities to be 0.001 to 0.01 percent each of aluminum and silicon.

The sample was white. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.329, 3.277, and 2.961 Å.

Structural data. Kokkoros and Rentzeperis [1] in 1961 determined cadmium sulfate is orthorhombic with the most probable space group D₂h-Pmmn (No. 59) with 2(CdSO₄) per unit cell.

Internal Standard, Tungsten, a=3.1648 Å
Cu, 1.5405 Å at 25 °C

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<th>Cu, 1.5405 Å at 25 °C</th>
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Reference
Cadmium Telluride, CdTe (cubic)

Powder data cards

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Additional published patterns. None.
NBS sample. The sample of cadmium telluride was obtained from Semi-Elements Inc., Saxonburg, Pa. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon and 0.0001 to 0.001 percent each of barium, iron, and lead.

The sample was a black opaque powder.
The d-values of the three strongest lines are: 3.741, 2.290, and 1.954 Å.

Structural data. Zachariasen [2] in 1926 determined that cadmium telluride has the zinc sulfide structure, the space group Td-F43m (No. 216), and 4(CdTe) per unit cell. The lattice constants of Zachariasen and Goldschmidt have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constant

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<th>1963</th>
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The density of cadmium telluride calculated from the NBS lattice constant is 5.856 g/cm³ at 25 °C.

References

[1] D. A. Vaughan, Battelle Memorial Institute, Columbus, Ohio.
Calcium Fluoride Phosphate (fluorapatite), Ca₅F(PO₄)₃ (hexagonal)

Powder data cards

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NBS sample. The sample of calcium fluoride phosphate was prepared at NBS by J. H. deGroot. A mixture of calcium fluoride and tricalcium orthophosphate was heated in a covered platinum dish to 1250 °C. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of magnesium and sodium; and 0.01 to 0.1 percent each of aluminum, barium, germanium, iron, silicon, and strontium.

<table>
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The sample was colorless and optically negative with the indices of refraction $N_0 = 1.633$ and $N_e = 1.628$.

The $d$-values of the three strongest lines are: 2.800, 2.702, and 2.772 Å.

Structural data. Hentschel [1] in 1923 determined that fluorapatite has the space group $C_{6h}-P6/m$ (No. 176) and $2[Ca_5F(PO_4)_3]$ per unit cell.

The density of synthetic fluorapatite calculated from the NBS lattice constants is 3.201 g/cm$^3$ at 25 °C.

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<th>$a$</th>
<th>$c$</th>
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<tr>
<td>1952 Altschuler, Cisney and Barlow [12]</td>
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<td>Sample from Durango, Mex.</td>
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<td>6.8821 at 25 °C</td>
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<tr>
<td>Sample from Llallagua, Bolivia.</td>
<td>9.3712</td>
<td>6.8824 at 26 °C</td>
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The error in these values was ±0.0003.

*These samples were obtained from the National Museum; the number of the Mexican sample is 104021, of the Bolivian sample 103869. These cell constants were derived from powder diffraction measurements made at the same time as those on the synthetic sample.

*This particular sample from Durango may not be typical because of its lanthanum content. Spectropraphic analysis showed 1 to 4 percent of lanthanum and 0.1 to 1.0 percent each of cerium and sodium as major impurities. The error on these lattice constants was ±0.0003.

*Spectrographic analysis showed major impurities to be 0.1 to 1.0 percent of manganese and 0.01 to 0.1 percent each of iron and strontium.

References

[4] D. McConnell, The substitution of SiO$_4$- and SO$_4$- groups for PO$_4$- groups in the apatite structure; olistedite, the end-member, Am. Mineralogist 22, 981 (1937).
Cerium Niobium Titanium Oxide (eschynite), CeNbTiO₆ (orthorhombic)

**Powder data cards.** None.


**NBS sample.** The sample of cerium niobium titanium oxide was prepared at NBS by R. S. Roth from stoichiometric mixtures of cerium oxide, niobium oxide, and titanium oxide. The sample was heated first at 1300 °C for 3 hrs. and then reheated at 1325 °C for three more hours. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, and silicon.

The sample was a dark brown opaque powder.

The $d$-values of the three strongest lines are: 2.975, 3.024, and 3.106 Å.

**Structural data.** Komkov [1] in 1959 determined that cerium niobium titanium oxide has the space group $D_{2h}^-Pmnb$ (No. 62) with 4(CeNbTiO₆) per unit cell. The lattice constants reported by Komkov have been converted from kX to angstrom units for comparison with NBS values.

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The density of cerium niobium titanium oxide calculated from NBS lattice constants is 5.617 g/cm³ at 26 °C.

**Reference**

Cesium Chromate, $\text{Cs}_2\text{CrO}_4$ (orthorhombic)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of cesium chromate was obtained from the Fairmount Chemical Co. Inc., Newark, N.J. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent rubidium; 0.01 to 0.1 percent each of potassium and sodium; and 0.001 to 0.01 percent each of aluminum, barium, calcium, and silicon.

The color of the sample was yellow and it is optically positive. The refractive indices are $n_\alpha=1.750$, $n_\beta=1.753$, and $n_\gamma=1.762$.

The $d$-values of the three strongest lines are: 3.342, 3.207, and 3.364 Å.

**Structural data.** Miller [1] in 1938 determined that cesium chromate has the potassium sulfate structure, the space group $D_{6h}$-Pnam (No. 62) with 4($\text{Cs}_2\text{CrO}_4$) per unit cell.

The lattice constants reported by Miller have been converted from kX to angstrom units for comparison with NBS values.

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The density of cesium chromate calculated from the NBS lattice constants is 4.266 g/cm³ at 25 °C.

**Reference**

Cesium Fluoride, CsF (cubic)

Powder data cards

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Additional published patterns. None.

NBS sample. The sample of cesium fluoride was obtained from Semi-Elements Inc., Saxonburg, Pa. X-ray patterns were prepared from samples maintained in dry air because of the deliquesence. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent potassium; and 0.001 to 0.01 percent each of aluminum, calcium, copper, iron, lithium, magnesium, nickel, silicon, and sodium. The amount of rubidium impurity was not determined. The sample was colorless.

The d-values of the three strongest lines are: 3.003, 3.469, and 2.125 Å.

Structural data. Posnjak and Wyckoff [2] in 1922 determined that cesium fluoride has the sodium chloride structure, the space group $O_h^*$ Fm3m (No. 225), and 4(CsF) per unit cell. The unit cell measurements reported by Davey, Posnjak, and Wyckoff, have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

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The density of cesium fluoride calculated from the NBS lattice constant is 4.638 g/cm$^3$ at 25 °C.

References

Cobalt Fluosilicate Hexahydrate, CoSiF₆·6H₂O (trigonal)

**Powder Data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of cobalt fluosilicate hexahydrate was obtained from the City Chemical Co., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, copper, magnesium, nickel, and sodium; and 0.001 to 0.01 percent each of calcium, iron, and manganese.

The color of the sample was pink. The indices of refraction were too low to be measured by the usual liquid grain immersion method.

The d-values of the three strongest lines are: 4.69, 4.18, and 2.595Å.

**Structural data.** Hassel and Richter-Salvesen [1] in 1927 determined that cobalt fluosilicate hexahydrate has the nickel chlorostannate structure, the space group C₅₅v-R₃m (No. 160), and 1[CoSiF₆·6H₂O] per unit rhombohedral cell, or 3[CoSiF₆·6H₂O] per unit hexagonal cell. The unit cell measurements of Hassel and Richter-Salvesen have been converted from kX to angstrom units for comparison with the NBS values.

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The density of cobalt fluosilicate hexahydrate calculated from the NBS lattice constants is 2.081 g/cm³ at 25 °C.

Reference

Cobalt Perchlorate Hexahydrate, Co(ClO₄)₂·6H₂O (hexagonal)

**Powder data cards.** None.


**NBS sample.** The sample of cobalt perchlorate hexahydrate was obtained from the City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent of nickel, and 0.001 to 0.01 percent each of copper, magnesium, and silicon.

The color of the sample was pink. It is optically negative with the indices of refraction N₆=1.492 and N₀=1.512.

The d-values of the three strongest lines are: 3.900, 4.139, and 2.840 Å.

**Structural data.** West [1] in 1935 determined that cobalt perchlorate hexahydrate has the magnesium perchlorate hexahydrate structure, the space group D_{6h}-P6/mmm (No. 191), and 4[Co(ClO₄)₂·6H₂O] per unit cell. The lattice constants of West have been converted from kX to angstrom units for comparison with the NBS values.

### Lattice constants

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The density of cobalt perchlorate hexahydrate calculated from the NBS lattice constants is 2.199±0.001 g/cm³ at 26 °C.

### Table

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**Reference**

Copper Sulfate (chalcoyanite), CuSO₄ (orthorhombic)

Powder data cards

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NBS sample. The sample of copper sulfate was obtained from the NBS laboratories in Boulder, Colo. The sample was ground and fumed off with sulfuric acid and placed immediately in a dry atmosphere. Special care was necessary to keep it anhydrous. The sample was mounted in a holder which maintained a dry atmosphere while the patterns were run. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, iron, magnesium, and nickel.
The sample was colorless. The indices of refraction could not be obtained because the sample was too fine.
The d-values of the three strongest lines are: 3.549, (2.616 and 2.611), and 4.187 Å.


Lattice constants

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References


Dysprosium Arsenate, DyAsO₄ (tetragonal)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of dysprosium arsenate was prepared at NBS from a water solution of dysprosium trichloride and arsenic pentoxide. The sample was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent antimony and 0.001 to 0.01 percent each of calcium, magnesium, lead, and silicon.

The sample is colorless. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.537, 2.669, and 1.8246 Å.

**Structural data.** Durif and Forrat [1] in 1957 determined that dysprosium arsenate has the zircon structure with the space group D₄h-I₄₁/amd (No. 141) and 4[DyAsO₄] per unit cell.

### Lattice constants

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The density of dysprosium arsenate calculated from the NBS lattice constants is 6.338 g/cm³ at 25 °C.

**Reference**

Erbium Arsenate, ErAsO₄ (tetragonal)

Powder data cards. None.
Additional published patterns. None.
NBS sample. The sample of erbium arsenate was prepared at NBS from a water solution of arsenic pentoxide and erbium trichloride. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of nickel and antimony and 0.001 to 0.01 percent each of aluminum, calcium, magnesium, lead, and silicon.

The sample was very pale pink. The indices of refraction could not be determined because the sample was too fine.

The $d$-values of the three strongest lines are: 3.510, 2.652, and 1.812 Å.

Structural data. Durif and Forrat [1] in 1957 determined that erbium arsenate has the zircon structure with the space group $D_{4h}^8-I_4_1/amd$ (No. 141) and 4(ErAsO₄) per unit cell.

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The density of erbium arsenate calculated from the NBS lattice constants is 6.574 g/cm³ at 25 °C.

Reference
**Europium Arsenate, EuAsO₄ (tetragonal)**

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of europium arsenate was prepared at NBS from a water solution of arsenic pentoxide and europium trichloride. It was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of antimony and silicon; 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, and titanium.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.578, 2.704, and 1.8467 Å

**Structural data.** No reference to the structure of europium arsenate was found but it is apparently isostructural with yttrium arsenate with the space group D₁₄h-I₄₁/amd (No. 141) and 4(EuAsO₄) per unit cell.

**Lattice Constants**

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The density of europium arsenate calculated from the NBS lattice constants is 5.902 g/cm³ at 25 °C.

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32
Gallium Arsenide, GaAs (cubic)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of gallium arsenide was obtained from Semitronics Inc., Winchester, Mass. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent iron, 0.01 to 0.1 percent chromium, nickel, and lead; and 0.001 to 0.01 percent each of cobalt, copper, indium, manganese, molybdenum, and silicon.

The sample was a dark gray opaque powder. The d-values of the three strongest lines are: 3.262, 1.998, and 1.704 Å.

**Structural data.** Goldschmidt [1] in 1927 determined that gallium arsenide has the zinc sulfide structure, the space group T₂-F₄₃m (No. 216), and 4(GaAs) per unit cell.

The density of gallium arsenide calculated from the NBS lattice constant is 5.321 g/cm³ at 25 °C.

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Average value of last five lines: 5.652

**Reference**

Holmium Arsenate, HoAsO₄ (tetragonal)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of holmium arsenate was prepared at NBS from a water solution of arsenic pentoxide and holmium trichloride. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent antimony and 0.001 to 0.01 percent each of aluminum, calcium, iron, lead, and silicon.

The color of the sample was very pale pinkish white. The indices of refraction could not be determined because the sample was too fine.

The \( d \)-values of the three strongest lines are: 3.528, 2.668, and 1.822 Å.

**Structural data.** The structure of holmium arsenate was not found in the literature; however, it is apparently isostructural with erbium arsenate having the space group \( D_{4h}^{14} \) amd (No. 141) and 4 (HoAsO₄) per unit cell.

## Lattice constants

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<th>( hkl )</th>
<th>( a )</th>
<th>( c )</th>
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<td>( \AA )</td>
<td>( \pm .0003 )</td>
<td>( \pm .0005 )</td>
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The density of holmium arsenate calculated from NBS lattice constants is 6.420 g/cm³ at 25 °C.
Indium Arsenide, InAs (cubic)

Powder data cards

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<tr>
<th>Card number</th>
<th>Index lines</th>
<th>Source</th>
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NBS sample. The sample of indium arsenide was obtained from Semitronics, Inc., Winchester Mass. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of silver, aluminum, bismuth, chromium, iron, gallium, and titanium; and 0.001 to 0.01 percent each of barium, calcium, cobalt, magnesium, nickel, antimony, and tin.

The sample was an opaque metallic powder. The d-values of the three strongest lines are: 3.498, 2.142, and 1.8263 Å.

Structural data. Iandelli [2] in 1941 determined that indium arsenide has the zinc sulfide structure, the space group Td-F43m (No. 216), and 4(InAs) per unit cell. The unit cell measurement reported by Iandelli has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

<table>
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Average value of last five lines: 6.058

The density of indium arsenide calculated from NBS lattice constant is 5.668 g/cm³ at 25 °C.

References


**Lanthanum Arsenate, LaAsO₄ (monoclinic)**

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of lanthanum arsenate was prepared at NBS from a water solution of arsenic pentoxide and lanthanum trichloride. It was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, iron, and silicon, and 0.001 to 0.01 percent each of calcium, magnesium, lead, and antimony.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The rf-values of the three strongest lines are: 3.185, 2.983, and 3.391 Å.

**Structural data.** No reference to the structure of lanthanum arsenate was found; however, it is apparently isostructural with lanthanum phosphate with the space group C₆₅₋₋₂₁/ₙ (No. 14) and 4(LaAsO₄) per unit cell.

<table>
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The density of lanthanum arsenate calculated from the NBS lattice constants is 5.572 g/cm³ at 25 °C.

<table>
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<th>I</th>
<th>d Å</th>
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<td>1.868</td>
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<td>1.320</td>
<td>8</td>
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</tbody>
</table>
**Lanthanum Niobium Titanium Oxide, LaNbTiO$_6$ (monoclinic)**

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of lanthanum niobium titanium oxide was prepared at NBS by R. S. Roth from stoichiometric mixtures of the oxides of lanthanum, niobium, and titanium. The sample was first heated at 1300 °C for 3 hr and then heated at 1350 °C for 3 hr. Spectrographic analysis of the original oxides showed no impurities greater than 0.05 percent.

The sample was colorless. The refractive indices could not be determined because the sample was too fine.

The $d$-values of the three strongest lines are: 3.444, 3.331, and 3.306 Å.

**Structural data.** P. M. de Wolff [1] in 1962 determined that lanthanum niobium titanium oxide has a C-centered monoclinic lattice.

<table>
<thead>
<tr>
<th>Lattice constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$ $b$ $c$ $\beta$</td>
</tr>
<tr>
<td>A A A °</td>
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<tr>
<td>11.20 8.85 5.27 115°18'</td>
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</table>

<table>
<thead>
<tr>
<th>$h$ $k$ $l$</th>
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</thead>
<tbody>
<tr>
<td>$d$ $I$</td>
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<tr>
<td>110 1.68 22</td>
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<tr>
<td>200 5.063 10</td>
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<tr>
<td>111 4.523 10</td>
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<td>220 3.331 100</td>
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<td>221 3.183 16</td>
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<td>130 2.833 11</td>
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<td>312 2.421 6</td>
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<td>311 2.249 4</td>
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<td>330 2.223 10</td>
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<td>132 1.941 8</td>
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<td>530 1.669 9</td>
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<td>113 1.651 6</td>
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<td>711 1.563 5</td>
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<td>333 1.507 9</td>
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<tr>
<td>152 1.459 4</td>
</tr>
<tr>
<td>531 1.427 4</td>
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</table>

**Reference**

**Lithium Phosphate, low form (lithiophosphate), Li₃PO₄ (orthorhombic)**

**Powder data cards**

<table>
<thead>
<tr>
<th>Card number</th>
<th>Index lines</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3.80</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.67</td>
<td></td>
</tr>
</tbody>
</table>

A high form is obtained from samples that have been heated above approximately 500 °C.


**NBS sample.** The sample of lithium phosphate was obtained from the City Chemical Co., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent calcium; 0.01 to 0.1 percent each of aluminum, sodium, and strontium; and 0.001 to 0.01 percent each of barium, iron, magnesium, and silicon.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.973, 3.797, and 2.640 Å.

**Structural data.** Zemann [3] in 1960 studied a crystal of Li₃PO₄ that had been grown in molten LiCl and determined that it has the space group D₄h-Pmn2₁ (No. 62) and 4(Li₃PO₄) per unit cell. We find that the lower form apparently has the same structure with only slight changes in the lattice constants, principally in the c-direction. The cell constants of Zambonini and Laves have been converted from kX to angstrom units for comparison with the NBS values.

**Lattice constants**

<table>
<thead>
<tr>
<th>Year</th>
<th>Authors</th>
<th>a (Å)</th>
<th>b (Å)</th>
<th>c (Å)</th>
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<tbody>
<tr>
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<td>± 0.0004</td>
<td>± 0.001</td>
<td>± 0.005</td>
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</table>

**References**

**Lithium Phosphate, high form, \( \text{Li}_3\text{PO}_4 \) (orthorhombic)**

**Powder data cards.** None. Powder data card No. 12-230 has a pattern by Fisher [1] which seems to be for the low form. The sample is changed to the high form when it has been heated above approximately 500 °C.

**Additional published patterns.** Tien and Hummel [2], 1961.

**NBS sample.** The sample of lithium phosphate was obtained from the City Chemical Co, New York, N.Y. It was heated at 800 °C for 15 min. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent calcium; 0.01 to 0.1 percent each of aluminum, sodium, and strontium; and 0.001 to 0.01 percent each of barium, iron, magnesium, and silicon.

The sample was colorless and optically positive, with the indices of refraction \( N_\alpha = 1.550, N_\beta = 1.556, \) and \( N_\gamma = 1.560. \)

The \( d \)-values of the three strongest lines are: 3.978, 3.834 and 2.640 Å.

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<th>Cu 1.5405 Å at 25 °C</th>
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<td>( I )</td>
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<tr>
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</table>
Lithium Phosphate, high form, Li₃PO₄ (orthorhombic)—Continued

Structural data. Zemann [3] in 1960 studied a crystal of Li₃PO₄ that had been grown in molten LiCl and determined that it has the space group D_{2h}^5-Pmnb (No. 62) and 4(Li₃PO₄) per unit cell. The cell constants of Zambonini and Laves have been converted from kX to angstrom units for comparison with the NBS values.

The density of lithium phosphate, high form, calculated from the NBS lattice constants is 2.439 g/cm³ at 25 °C.

<table>
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<th>c</th>
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<tbody>
<tr>
<td>1932</td>
<td>Zambonini and Laves [4].</td>
<td>6.08</td>
<td>10.28</td>
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References
Magnesium Ammonium Phosphate Hexahydrate (struvite), MgNH₄PO₄·6H₂O
(orthorhombic)

Powder data cards

<table>
<thead>
<tr>
<th>Card number</th>
<th>Index lines</th>
<th>Source</th>
</tr>
</thead>
</table>

Additional published patterns. None.

NBS sample. The sample of struvite was precipitated at NBS from a solution of magnesium sulfate by adding a solution of ammonium monohydrogen orthophosphate. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent sodium, and 0.001 to 0.01 percent each of calcium, iron, and silicon.

The sample was colorless and optically positive. The indices of refraction are Na—1,493, N^=1.496, and N? = 1.501.

The d-values of the three strongest lines are: 4.257, 5.601, and 2.919 Å.

Structural data. Bland and Basinski [2] in 1959 determined that struvite has the space group C2/vPm21n (No. 31) and 2(MgNH₄PO₄·6H₂O) per unit cell.

Lattice constants

<table>
<thead>
<tr>
<th>Year</th>
<th>Authors</th>
<th>a</th>
<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>± 0.001</td>
<td>± 0.002</td>
<td>± 0.0008</td>
</tr>
</tbody>
</table>

The density calculated from the NBS lattice constants is 1.706 g/cm³ at 25 °C.

References

## Powder Data cards

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<td>12-571</td>
<td>3.46 2.88 2.80</td>
<td>Institute of Physics, University College, Cardiff.</td>
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</table>

## Additional published patterns

**NBS sample.** The sample of potassium chlorate was obtained from the General Chemical Co., New York, N.Y., and recrystallized to sharpen the pattern. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, barium, iron, rubidium, silicon, sodium, and strontium.

The color of the sample was white. It is optically negative with the indices of refraction $N_a=1.408$, $N_g=1.516$, and $N_r=1.524$; $2V$ was very small.

The $d$-values of the three strongest lines are: 3.45, 3.34, and 2.86 Å.

**Structural data.** Zachariasen [2] and [3] in 1928 determined that potassium chlorate has the space group $C_{1h}P2_1/m$ (No. 11) and 2[KClO$_3$] per unit cell. The unit cell measurements of Ieviņš and Ozols and Zachariasen have been converted from kX to angstrom units for comparison with the NBS values.

The density of potassium chlorate calculated from the NBS lattice constants is 2.339 g/cm$^3$ at 26 °C.

## References


Potassium Chlorate, KCIO₃ (monoclinic)—Continued

Lattice constants

<table>
<thead>
<tr>
<th>Year</th>
<th>Source</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>β</th>
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<td>5.5905</td>
<td>7.1006</td>
<td>109°41.1’</td>
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</tbody>
</table>

Potassium Lithium Sulfate, KLiSO₄ (hexagonal)

Powder data cards. None.
Additional published patterns. None.
NBS sample. The sample of potassium lithium sulfate was prepared at NBS by dissolving stoichiometric amounts of solid potassium hydroxide and lithium hydroxide in a small amount of water. When the mixture was at room temperature a drop of 1 percent bromcresol-purple was added and the mixture neutralized with H₂SO₄. The solution was evaporated to dryness and the precipitate was then heated to about 750 °C to sharpen the pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, indium, and sodium; and 0.001 to 0.01 percent each of aluminum, rubidium, and silicon.

The sample is colorless and optically negative. The indices of refraction are N₀ = 1.471 and Nₑ = 1.469.

The d-values of the three strongest lines are: 3.960, 3.099, and 2.573 Å.

Structural data. Nowacki [1] in 1942 determined that potassium lithium sulfate has the space group C₄ᵥ-P6/3 (No. 173) and 2(KLiSO₄) per unit cell. The lattice constants of Nowacki have been converted from kX to angstrom units for comparison with the NBS values.

The density of potassium lithium sulfate calculated from NBS lattice constants is 2.385 g/cm³ at 26 °C.

Reference
Potassium Perchromate, $\text{K}_2\text{CrO}_4$ (tetragonal)

**Powder data cards.** None.


**NBS sample.** The sample of potassium perchromate was obtained from City Chemical Corp., New York, N.Y. Spectrographic analysis did not show any impurities greater than the range 0.0001 to 0.001 percent.

The color of the sample was deep red. The indices of refraction are $N_0 = 1.774$ and $N_e = 1.730$. It is optically negative.

The $d$-values of the three strongest lines are: 2.979, 2.372, and 1.856 Å.

**Structural data.** Wilson [1] in 1941 determined that potassium perchromate has the space group $D_{4h}^8$-142m (No. 121) and $2(K_2\text{CrO}_4)$ per unit cell. Potassium perchromate is used as a structure type. The unit cell measurements reported by Wilson have been converted from kX to angstrom units for comparison with NBS values.

<table>
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<tr>
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<td>$d$</td>
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The density of potassium perchromate calculated from NBS lattice constants is 2.869 g/cm$^3$ at 25 °C.

**Reference**

Potassium Zinc Decavanadate 16 Hydrate, $K_2Zn_2V_{10}O_{28} \cdot 16H_2O$ (triclinic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium zinc decavanadate 16 hydrate, was obtained from H. T. Evans, Jr., U.S. Geological Survey, Washington, D.C. It was prepared from a solution of potassium metavanadate and zinc acetate in water with the pH adjusted between 3 and 4 with acetic acid. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent sodium; 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, barium, calcium, chromium, iron, magnesium, molybdenum, lead, and rubidium.

The color of the sample was bright orange. The indices of refraction could not be determined because of imperfections in the crystals.

The $d$-values of the three strongest lines are: 8.18, 7.40, and 9.45 Å.

Structural data. Evans, Mrose, and Marvin [1], in 1955 determined that potassium zinc decavanadate 16 hydrate, has the space group $C_i-Pi$ (No. 2) and $1(K_2Zn_2V_{10}O_{28}\cdot 16H_2O)$ per unit cell.

The density of potassium zinc decavanadate calculated from the NBS lattice constants is 2.708 g/cm³ at 25 °C.

Reference

Potassium Zinc Decavanadate 16 Hydrate, K₂Zn₂V₁₀O₄₈·16H₂O (triclinic)—Continued

### Lattice constants

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Rubidium Chromate, Rb₂CrO₄ (orthorhombic)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of rubidium chromate was obtained from the Fairmount Chemical Co., Inc., Newark, N.J. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent potassium; 0.01 to 0.1 percent sodium; and 0.001 to 0.01 percent each of aluminum, barium, calcium, and silicon.

The color of the sample was yellow and it is optically positive. The refractive indices are N₀=1.715, N₁=1.725, and N₂=1.759.

The d-values of the three strongest lines are: 3.207, 3.191, and 3.083 Å.

**Structural data.** Smith and Colby [1] in 1940 determined that rubidium chromate has the potassium sulfate structure and the space group D₄h̅-Pnam (No. 62) with 4(Rb₂CrO₄) per unit cell.

The lattice constants reported by Smith and Colby have been converted from kX to angstrom units for comparison with NBS values.

<table>
<thead>
<tr>
<th>hkl</th>
<th>Internal Standard, Tungsten a=3.1648 Å</th>
<th>Cu, 1.5405 Å at 25°C</th>
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The density of rubidium chromate calculated from NBS lattice constants is 3.657 g/cm³ at 25°C.

**Reference**

Silver Antimony Telluride, AgSbTe₂ (cubic)

Powder data cards. None.

NBS sample. The sample of silver antimony telluride was obtained from Semitronics Inc., Winchester, Mass. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, bismuth, copper, iron, indium, and tin; and 0.001 to 0.01 percent each of gold, calcium, chromium, magnesium, nickel, and titanium.

The sample was an opaque metallic gray powder.

The d-values of the three strongest lines are: 3.042, 2.151, and 1.7554 Å.

Structural data. Geller and Wernick [1] in 1959 determined that silver antimony telluride has the sodium chloride structure, the space group P6₃–Fm3m (No. 225), and 2(AgSbTe₂) per unit cell.

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Average value of last five lines........... 6.080

Reference

Sodium Magnesium Aluminum Boron Hydroxy Silicate, dravite (var. of tourmaline), NaMg₃Al₆B₃Si₆O₂₂(OH)₄ (trigonal)

Powder Data cards. None.
Additional published patterns. None.

NBS sample. The sample of dravite is U.S. National Museum No. 103791 from Dobruva, Carinthia, Austria. This mineral sample was picked by C. R. Robbins, NBS, as a true end member representative of the magnesium rich variety of tourmaline. The chemical analysis by H. B. Wiik, Hilsingfors, Westend, Finland, showed the following: 36.99 percent SiO₂; 0.39 percent TiO₂; 32.00 percent Al₂O₃; 0.01 percent MnO; 11.58 percent MgO; 0.50 percent CaO; 0.01 percent Li₂O; 3.11 percent Na₂O; 0.08 percent K₂O; 3.08 percent H₂O⁺; 10.77 percent B₂O₃; 0.25 percent F; and 0.90 percent total Fe as FeO. The color of the sample was light brown and it is optically negative. The indices of refraction are Nₑ=1.634 and Nₚ=1.613.

The d-values of the three strongest lines are: 2.576, 3.985, and 2.961 Å.

Structural data. Buerger and Parrish [1] in 1937 determined the structure of the tourmalines; they have the space group C₃₅–R3m (No. 160) and 3[NaMg₃Al₆B₃Si₆O₂₂(OH)₄] per unit hexagonal cell.

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The density of dravite calculated from NBS lattice constants is 3.019 g/cm³ at 25 °C.

47
Sodium Magnesium Aluminum Boron Hydroxy Silicate, dravite (var. of tourmaline), NaMg₃Al₆B₃Si₆O₂₇(OH)₄ (trigonal)—Continued

<table>
<thead>
<tr>
<th>hkl (hex)</th>
<th>Internal Standard Tungsten, $a$=3.1648 Å Cu, 1.5405 Å at 25 °C</th>
<th>Internal Standard Tungsten, $a$=3.1648 Å Cu, 1.5405 Å at 25 °C</th>
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References
Sodium Trimetaphosphate, Na₅P₃O₉ (orthorhombic)

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The $d$-values of the three strongest lines are: 3.407, 3.850, and 3.037 Å.

**Structural data.** Ondik and Gryder [2] in 1960 determined that sodium trimetaphosphate has the space group $C_{2v}$-P2$_1$cn (No. 33) or $D_{4h}$-Pmcn (No. 62) with $4(Na_5P_3O_9)$ per unit cell.

Additional published patterns. Corbridge and Tromans [1].

**NBS sample.** The sample of sodium trimetaphosphate was crystallized by heating sodium trimetaphosphate above the melting point (about 650 °C) and then cooling slowly at the rate of 5 to 10 °C an hour. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, barium, calcium, iron, potassium, magnesium, silicon, and titanium. The sample is colorless.

<table>
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Internal Standard, Tungsten $a=3.1648$ Å, Cu, 1.5405 Å at 25 °C.
Sodium Trimetaphosphate, $\text{Na}_3\text{P}_3\text{O}_9$ (orthorhombic)—Continued

### Lattice constants

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The density of sodium trimetaphosphate calculated from the NBS lattice constants is 2.515 g/cm$^3$ at 25 °C.

### References


Sodium Trimetaphosphate Monohydrate, $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$ (orthorhombic)

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Card number 12-10 also is called $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$; however, it contains a very different pattern, perhaps another form.

### Additional published patterns

None.

### NBS sample

The sample of sodium trimetaphosphate monohydrate was prepared at NBS by heating sodium dihydrogen orthophosphate for 5 hr at 530 °C. Solid sodium trimetaphosphate was salted out with NaCl and then recrystallized several times. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, barium, calcium, iron, potassium, magnesium, silicon, and titanium.

The sample is colorless and it is probably optically negative. The indices of refraction are $n_\alpha = 1.493$, $n_\beta = 1.502$, and $n_\gamma = 1.504$.

The $d$-values of the three strongest lines are: 3.566, 2.825, and (2.605 and 2.601) Å.

### Structural data

Ondik and Gryder [2] in 1960 determined that sodium trimetaphosphate monohydrate has the space group $C_{2h}^2-P2_1cn$ (No. 33) or $D_{2h}^-Pmcn$ (No. 62) with $4(\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O})$ per unit cell.
Sodium Trimetaphosphate Monohydrate, Na₃P₃O₁₀·H₂O (orthorhombic)—Continued

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**Lattice constants**

| 1960 | Ondik and Gryder [2]. |
| 1963 | National Bureau of Standards at 25 °C. |
| a | $\hat{a}$ | $\hat{b}$ | $\hat{c}$ |
| 8.53 | ± 0.001 |
| 13.21 | ± 0.001 |
| 7.58 | ± 0.001 |

The density of sodium trimetaphosphate monohydrate calculated from NBS lattice constants is 2.539 g/cm³ at 25 °C.

**References**


Stannous Fluoride, SnF₂ (monoclinic)

**Powder data cards.** None


**NBS sample.** The sample of stannous fluoride was obtained from the Indiana University School of Dentistry, Indianapolis, Ind. Spectrographic analysis showed the following major impurities: 1.001 to 0.01 percent each of calcium and silicon.

The sample was colorless. The indices of refraction were not determined because the sample reacted with the index liquids.

**Lattice constants**

| 1962 | Bergerhoff [2]. |
| 1963 | National Bureau of Standards at 25 °C. |
| a | $\hat{a}$ | $\hat{b}$ | $\hat{c}$ | $\beta$ |
| 13.46 | 4.92 | 13.86 | 109°30' |
| 13.353 | 4.9089 | 13.787 | 019°5.5' |
| ± .001 | ± .0004 | ± .001 | ± .3' |

The $d$-values of the three strongest lines are: 3.552, 3.200 and 3.379 Å.

**Structural data.** Bergerhoff [2] in 1962 determined that stannous fluoride has the space group $C_{2h}-C2/c$ (No. 15) and 16 [SnF₂] per unit cell.

Difficulties in indexing the NBS pattern were overcome with the help of single crystal work done by Dr. Howard T. Evans Jr., of the U.S. Geological Survey.
Stannous Fluoride, SnF₂ (monoclinic)—Continued

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The density of stannous fluoride calculated from the NBS lattice constants is 4.875 g/cm³ at 25 °C.

References

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of strontium 1:1 borate was prepared at NBS by C. E. Weir. A suspension of hydrogen 3:1 borate (boric acid) and strontium carbonate was evaporated to dryness and heated at 1000 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of barium and silicon; 0.001 to 0.01 percent each of calcium and sodium.

The sample is colorless and optically negative with \( n_\lambda = 1.632, n_\lambda^1 = 1.650, \) and \( n_\lambda^2 = 1.660. \)

**Structural data.** Block, Perloff, and Weir [1] in 1963 determined that strontium 1:1 borate has the space group \( D_{\text{4h}}^5 - \text{Pnca} \) (No. 60) and 4(SrO-B\(_2\)O\(_3\)) per unit cell.

**Lattice constants**

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The density of strontium 1:1 borate calculated from the NBS lattice constants is 3.350 g/cm\(^3\) at 25 °C.

**Reference**

Terbium Arsenate, TbAsO₄ (tetragonal)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of terbium arsenate was prepared at NBS from a water solution of arsenic pentoxide and terbium trichloride. It was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon; 0.001 to 0.1 percent each of antimony, calcium, iron, magnesium, and lead.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.550, 2.685, and 1.834 Å.

**Structural data.** No reference to the structure of terbium arsenate was found, but it is apparently isostructural with yttrium arsenate with the space group D₄h-14/m (No. 141) and 4(TbAsO₄) per unit cell.

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The density of terbium arsenate calculated from the NBS lattice constants is 6.172 g/cm³ at 25 °C.

Thallium Chromate, Tl₂CrO₄ (orthorhombic)

**Powder data cards.** None.


**NBS sample.** The sample of thallium chromate was prepared at NBS from solutions of thallium nitrate and sodium chromate. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent lead; 0.01 to 0.1 percent each of aluminum and silicon; and 0.001 to 0.01 percent each of barium, calcium, and antimony.

The color of the sample was yellow. The refractive indices could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.145, 3.060, and 3.186 Å.

**Structural data.** Abbad and Rivoir [1] in 1947 determined that thallium chromate has the potassium sulfate structure, the space group D₄h-Pnam (No. 62), and 4(Tl₂CrO₄) per unit cell.

The lattice constants reported by Abbad and Rivoir have been converted from kX to angstrom units for comparison with the NBS values.

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The density of thallium chromate calculated from the NBS lattice constants is 6.946 g/cm³ at 25 °C.
### Thallium Chromate, $\text{Tl}_2\text{CrO}_4$ (orthorhombic)—Continued

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### Reference

Thulium Arsenate, TmAsO₄ (tetragonal)

**Powder data cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of thulium arsenate was prepared at NBS from a water solution of arsenic pentoxide and thulium trichloride. It was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of silicon and antimony; 0.001 to 0.01 percent each of aluminum, calcium, iron, lead, and magnesium.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The d-values of the three strongest lines are: 3.497, 2.644, and 1.8064 Å.

**Structural data.** No reference to the structure of thulium arsenate was found, but it is apparently isostructural with yttrium arsenate with the space group D₄h-D₄h/amd (No. 141) and 4(TmAsO₄) per unit cell.

**Lattice constants**

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The density of thulium arsenate calculated from the NBS lattice constants is 6.678 g/cm³ at 25 °C.
Titanium Dioxide, brookite, TiO₂ (orthorhombic)

Powder data cards

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<td>3-0380</td>
<td>3.47, 2.90, 1.88</td>
<td>British Museum.</td>
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Additional published patterns. Sturdivant and Pauling [1].

NBS sample. The sample of brookite was obtained from the U.S. National Museum. No. 97661 from Magnet Cove, Ark. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon; 0.01 to 0.1 percent each of aluminum, iron, and vanadium; 0.001 to 0.01 percent magnesium.

The color of the sample was black. The indices of refraction were not determined because they were higher than 2.00.

The d-values of the three strongest lines are: 3.512, 2.900, and 3.465 Å.

Structural data. Sturdivant and Pauling [1] in 1928 determined that brookite has the space group D²-Pcab (No. 61) and 8(TiO₂) per unit cell. Several lattice constants have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

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<th>b (Å)</th>
<th>c (Å)</th>
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The density of brookite calculated from the NBS lattice constants (a) is 4.120 g/cm³ at 25 °C.

References

Zinc Telluride, ZnTe (cubic)

Powder data cards

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Additional published patterns. None.

NBS sample. The sample of zinc telluride was obtained from Semi-Elements, Inc., Saxonburg, Pa. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent of silicon, and 0.001 to 0.01 percent each of aluminum, barium, iron, and magnesium.

The color of the sample was reddish-brown. The indices of refraction were too high to be determined by the usual grain-immersion method.

The d-values of the three strongest lines are: 3.523, 2.159, and 1.840 Å.

Structural data. Zachariasen [1] in 1925 determined that zinc telluride has the zinc sulfide structure, the space group Td-F43m (No. 216), and 4[ZnTe] per unit cell. The unit cell measurement reported by Zachariasen has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

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The density of zinc telluride calculated from the NBS lattice constant is 5.639 g/cm³ at 25 °C.

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* 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.

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*Natural minerals.

m—Monograph 26.