NBS MONOGRAPH 25—SECTION 4

Standard X-ray Diffraction Powder Patterns

U.S. DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

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Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, Marlene C. Morris, and Eloise H. Evans

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Contents

Standard x-ray powder patterns:

***Calculated powder patterns:**

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*Not previously listed in Powder Diffraction File.
**Mineral name in parentheses indicates a synthetics sample.

Errata

Monograph 25, Section 4

Circular 539
Vol. 3, p. 33; The space group should be D_{3d}^{3}-P$\bar{3}$m1.
Vol. 4, p. 26; The space group should be D_{3d}^{3}-P$\bar{3}$m1.
Vol. 6, p. 3; The space group should be T_{h}^{6}-Pa3.
p. 35; The space group should be D_{2d}^{12}-I$\bar{4}$2d.
Monograph 25
Sec. 1, p. 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.
Sec. 3, p. 7; The *d*-spacing 1.568 should be 1.537.
p. 5; *hkl* 341 should be 203.
p. 16; The *d*-spacing 2.113 should be 2.013.
p. 49; In the text for *NBS sample*, the first sentence should be corrected to read: ". . . by heating sodium trimetaphosphate sesquihydrate above the melting . . ."
p. 51; The NBS value for β for SnF_2 should be 109° 6.5′±0.3′.

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The thirteen previous volumes in this series are available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C., 20402, as follows:

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 4—Data for 103 Substances

Howard E. Swanson, Marlene Cook Morris,[1] and Eloise H. Evans [1]

Standard x-ray diffraction powder data are presented for 103 substances. Thirty-two of these patterns represent experimental data and 71 are calculated. Ten experimental patterns replace eleven cards already in the X-ray Powder Diffraction File published by the American Society for Testing and Materials; twenty-two experimental patterns and seventy-one calculated patterns are for substances not previously included in the File. The experimental x-ray powder diffraction patterns were made with a Geiger counter x-ray diffractometer, using samples of high purity. All *d*-values were assigned Miller indices determined by comparison with theoretical interplanar spacings and from space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were obtained from single crystal structure data. The reported peak height intensities for calculated patterns were converted from integrated intensities.

Accurate cell determination measurements for the internal standards were obtained by using a flat-plate back reflection focusing camera.

Key Words: standard, x-ray, diffraction, powder, patterns, crystal, structure, measurements, lattice, constants

INTRODUCTION

The X-ray Powder Diffraction File [1] [2] 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 [3] for the revision and evaluation of published x-ray data for the X-ray Powder Diffraction File presents data in this report for 103 compounds. This compilation is the fourteenth of a series of "Standard X-ray Diffraction Powder Patterns." [4] The designation "Circular 539" used for the first ten volumes has been discontinued in favor of the series, "Monograph 25." This compilation is the fourth section of the series Monograph 25. Included are patterns recommended to replace data on 11 cards now present in the File. The other patterns are for 93 compounds not included in the File. In this group of compounds, 22 patterns are experimental and 71 are calculated.

Experimental Powder Patterns

Powder data cards. Under this heading are given the Powder Diffraction File Card numbers and the literature reference for each card. Cards listed through the 1964 index to the Powder Diffraction File are included in the table.

Additional published patterns. Literature references for patterns that have not been published as Powder Diffraction 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. 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 analyses. 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 definition 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.

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 constants for the last five lines because of the greater accuracy of calculation in the large-angle region of the pattern. The unit cell values for noncubic substances were determined by means of a least-squares calculation made on the IBM 7094, using those *d*-values for which only one set of Miller indices could be assigned. The number of significant figures reported for the *d*-values in the NBS patterns varies slightly with the symmetry and crystallinity of each sample. A portion of the indexing and cell

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[1] Research Associate at the National Bureau of Standards sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods.

[2] Figures in brackets indicate the literature references at the end of each section of this paper.

[3] This project is sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods. This committee is composed of members from the American Society for Testing and Materials, the American Crystallographic Association, and the British Institute of Physics. Financial support is also provided by the National Bureau of Standards.

[4] Other volumes were published as follows: Circular 539 Vol. 1 and Vol. 2, June 1953; Vol. 3, June 1954; Vol. 4, March 1955; Vol. 5, October 1955; Vol. 6, September 1956; Vol. 7, September 1957; Vol. 8, April 1959; Vol. 9, February 1960; Vol. 10, September 1960; Monograph 25, Section 1, March 1962; Section 2, May 1963; and Section 3, July 1964.

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 [2]. 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 and data given in angstrom units prior to 1947 were converted to angstrom units using the factor 1.00202 as recommended by an international conference of crystallographers [3].

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 [4].

Orthorhombic cell dimensions are presented according to the Dana convention $b>a>c$ [5].

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 [6], and the Avogadro number (6.02252×10^{23}).

Intensity measurements. 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 μ [7]. In order to avoid the orientation effects which occur when samples are packed or pressed, a sample holder was made that had an extended rectangular cavity opened on its top face and at the 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.

Interplanar spacings. Specimens for the interplanar spacing 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 2θ, the pattern peak was measured in the center, at a place averaging about 75 percent of the peak height. For higher values of 2θ, where the α_1 and α_2 peaks were separated, the α_1 peak was measured in the same way. The internal standard correction appropriate to each region was then applied to the measurement of 2θ. The internal standard lattice constants used were 3.1648 Å for tungsten and 4.0861 Å for silver at 25 °C, as determined by Jette and Foote [8]. All of the NBS patterns, unless otherwise noted, are made at 25 °C using either filtered copper or cobalt radiation ($K\alpha_1$), having the wavelengths 1.5405 Å, and 1.7889 Å, respectively.

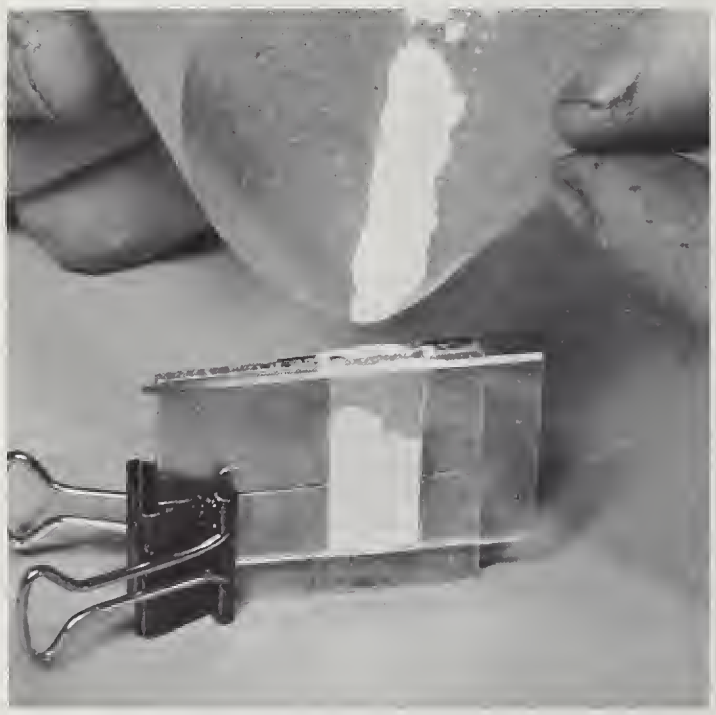

FIGURE 1

FIGURE 2

Calculated Powder Patterns

Some substances are not readily available for experimental powder measurements. Therefore, patterns were calculated from single crystal structure data, using a FORTRAN program developed by Smith [9].

Scattering factors were obtained from The International Tables [10].

Intensity calculations were based upon copper wavelength, 1.5405 Å. The integrated intensities were converted to peak height values by means of a graph [11]. Data with peak height intensities less than 0.1 were omitted. Peak height intensities from 0.1 to 0.9 were recorded as <1. Those intensities with *d*-values close enough to be unresolved were summed.

No temperature corrections were included.

Literature references are compiled at the end of the section of calculated patterns.

The authors are indebted to H. F. McMurdie for measurement of indices of refraction and for his continuous interest and supervision in this work, to J. H. deGroot for the preparation of many of the samples used, and to S. J. Carmel for his assistance on the work using the back reflection camera.

References

[1] Index to the X-ray Powder Diffraction File, (1964) American Society for Testing and Materials, 1916 Race Street, Philadelphia, Pa. 19103.

[2] H. T. Evans, D. E. Appleman, and D. S. Handwerker. The least-squares refinement of crystal unit cells with powder diffraction data by an automatic computer indexing method, (abs.) Am. Crystal. Assoc. Annual Meeting, Cambridge, Mass. Program 42–43, March (1963).

[3] The conversion factor for kX units to angstrom units, J. Sci. Instr. **24,** 27 (1947).

[4] International Tables for X-ray Crystallography, **I** (1952).

[5] Dana's System of Mineralogy, **I,** 6 (John Wiley & Sons, New York, 7th ed., 1944).

[6] International Union of Pure and Applied Chemistry, Chem. Eng. News, **Nov. 20,** 43 (1961).

[7] L. Alexander, H. P. Klug, and E. Kummer, Statistical factors affecting the intensity of X-rays diffracted by crystalline powders, J. Appl. Phys. **19,** No. 8, 742–753 (1948).

[8] E. R. Jette and F. Foote, Precision determination of lattice constants, J. Chem. Phys. **3,** 605–616 (1935).

[9] D. K. Smith, A FORTRAN program for calculating X-ray powder diffraction patterns, UCRL–7196 (1963) University of California, Lawrence Radiation Laboratory, Livermore, Calif.

[10] International Tables for X-ray Crystallography, **III** 202 (1962).

[11] H. E. Swanson, M. C. Morris, R. P. Stinchfield, and E. H. Evans, Standard X-ray Diffraction Powder Patterns, Natl. Bur. Std. Monograph 25, **Sec. 1,** 3 (1962).

Cell Determination for Internal Standards

In the search for new sources of supply for silver and tungsten which we have used to reference 2θ measurements, we became interested in obtaining lattice values of the various samples of high purity silver and tungsten. The cell values for these internal standards, adopted by this laboratory in 1950, will be changed after this issue from 3.1648 to 3.16504 Å for tungsten, and from 4.0861 to 4.08625 Å for silver. The greater change in tungsten is due to higher purity (four 9's) of the newer tungsten sample. The purity of the old tungsten sample is approximately three 9's.

A flat plate back reflection camera was specially constructed for these measurements. With this type of camera only one diffraction ring is in sharp focus with each setting. This tends to limit its use to cubic materials. For each sample, a radiation was selected which produced a back reflection ring between 165° and 178° (2θ). A micro focus tube was chosen partly because of the ease with which targets may be changed and partly because the small external tube dimension allowed the glass photographic plate to be close enough to the 0.1 mm X-ray target to satisfy focusing. The sample powders were mounted on a 5 cm diam rotating holder that was spherically shaped for the 50 cm focus. Samples of tungsten were run on a shorter focus of 25 cm with a shaped holder to fit a 25 cm sphere. The 10 in. × 2 in. photographic plates had a hole cut in the center prior to the emulsion coating.

An insulated box enclosed the camera and made possible the circulation of air or helium at 25.00 ± 0.02° C. A steady cooling effect was obtained by using a fin containing 18° C water in a circulated air stream. The temperature was controlled by a proportioning device that allowed varying amounts of current to heat a 7W light bulb also in the air flow. Temperature was read from two Beckmann thermometers calibrated at 25° C. The diffraction ring recorded on the photographic plate was scanned with a densitometer driven manually by a comparator. Densitometer readings were plotted for the $K\alpha_1$ portion of the peak and the center was chosen at the point where the center line intersected the top of the peak.

Measurements of the distance from sample to the photographic plate emulsion were made by an inside micrometer and end measuring rods. Calculation of *d*-values without sine tables was possible using the formula $d = \dfrac{\lambda}{2\sqrt{\dfrac{h+b}{2h}}}$

given: $a = \frac{1}{2}$ diam of diffraction ring
b = the distance from sample to the center of the plate
and $h = \sqrt{a^2 + b^2}$.

Samples of high purity tungsten and silver were obtained from several suppliers, but only three tungsten and four silver samples gave sufficiently sharp diffraction peaks for measurement of cell values. Since the variation of cell values for these samples was within the reproducibility of the equipment, it appears that most samples of tungsten or silver of four or five 9's purity and producing sharp diffraction peaks would be suitable for x-ray spacing reference standards.

Cadmium oxide was also considered and measured as a spacing standard, but the cell size was obtained from only one high purity sample.

Lattice constants

Sample source	λ[a]		Corrected for index of refraction [1]
		Å	Å
Tungsten:			
Spex [1]	Co	3. 16501	3. 16522
Spex	Ni	3. 16508	3. 16526
Parrish [2]	Ni	3. 16506	[b]3. 16524
Fairmount [3]	Co	3. 16501	3. 16522
Fairmount	Ni	3. 16503	3. 16521
Present NBS Standard	Co	3. 16493	3. 16514
Silver:			
Cominco [4]	Ni	4. 08625	4. 08639
Johnson & Matthey [5]	Ni	4. 08625	4. 08639
Engelhard [6]	Ni	4. 08623	4. 08637
Present NBS Standard	Ni	4. 08626	4. 08640
Cadmium oxide:			
Fairmount	Co	4. 69559	4. 69573
Fairmount	Ni	4. 69558	4. 69570

[a] CoKα_1=1.78890 Å, NiKα_1=1.65783 Å [2].

[b] a=3.16522 Å, mean value obtained in I.U. Cr. project using same tungsten sample [3].

[1] Spex Industries, Inc., 3880 Park Avenue, Metuchen, N.J.

[2] Dr. William Parrish. Philips Laboratories, Briarcliff Manor, N.Y.

[3]. Fairmount Chemical Co., Inc, 136 Liberty Street, New York, N.Y., 10006.

[4] Cominco Products, Inc., Electronic Materials Division, 933 West Third Avenue, Spokane 4, Washington.

[5] Johnson, Matthey & Co., Ltd., c/o Jarrell-Ash Co., Newtonville 60, Mass.

[6] Engelhard Industries, Inc., 113 Astor Street, Newark 14, N.J.

New lattice measurements will be used with the recently obtained standard reference samples beginning with the next Section of this Monograph. These changes will increase d-values by a factor of 1.00004 compared to the d-values obtained with the older standard samples.

The following 2θ angles for high purity tungsten, silver, and cadmium oxide are computed using copper radiation K_{α_1}=1.5405 Å and the cell dimensions without index of refraction corrections.

Calculated 2θ Angles

hkl	W a=3.16504 Å	Ag a=4.08625 Å	CdO a=4.69558 Å
110	40. 262°		
111		38. 112°	33. 012°
200	58. 252	44. 295	38. 304
211	73. 187		
220	87. 000	64. 440	55. 286
310	100. 630		
311		77. 390	65. 920
222	114. 922	81. 530	69. 256
321	131. 171		
400	153. 533	97. 874	82. 014
331		110. 498	91. 290
420		114. 914	94. 378
422		134. 897	106. 954
511		156. 735	116. 939
440			136. 230
531			152. 076
600			159. 618

References

[1] H. Lipson and A. J. C. Wilson, The derivation of lattice spacings from Debye-Scherrer photographs, J. Sci. Instr. **18**, 144 (1944).

[2] The conversion factor for kX units to angstrom units, J. Sci. Instr. **24**, 27 (1947).

[3] W. Parrish, Results of the I. U. Cr. precision lattice parameter project, Acta Cryst. **13**, 838 (1960).

Barium Boron Oxide, high form, BaB_2O_4 (trigonal)

Powder data cards. No. 6–0220 and No. 6–0224, Levin and McMurdie [1] 1949. The data on card No. 6–0220 was taken at 700 °C. Card No. 6–0224 is for a lower temperature form of BaB_2O_4.

Additional published patterns. None.

NBS sample. The sample of barium boron oxide was prepared at NBS by C. E. Weir from barium carbonate and boric acid. It was heated at 1,000 °C, then alternately ground and reheated several times. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium, silicon, and strontium; and 0.001 to 0.01 percent each of aluminum, sodium, and nickel.

The sample is colorless and optically negative. The indices of refraction are $N_e=1.530$ and $N_o=1.658$.

The d-values of the three strongest lines are 3.619, 3.324, and 5.98 Å.

Structural data. Block, Perloff, and Weir [2] in 1964 reported that there appear to be two polymorphic forms of barium boron oxide, the high form being trigonal having the space group C_{3v}^6—R3c (No. 161) or D_{3d}^6—R$\bar{3}$c (No. 167) with 18 (BaB_2O_4) per unit hexagonal cell.

Barium Boron Oxide, BaB$_2$O$_4$ (trigonal)

hkl (hex)	Internal Standard W, a=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
006	6.54	17
012	5.98	53
018	3.862	17
110	3.619	100
1·0·10	3.324	83
116	3.164	6
0·1·11, 202	3.094	26
024	2.986	3
205	2.912	2
119	2.783	4
208	2.639	16
0·2·10	2.448	33
1·1·12	2.425	31
211	2.365	2
2·0·11	2.352	23
214	2.302	8
1·0·16	2.282	5
217	2.180	3
0·0·18	2.177	6
128	2.131	18
1·1·15	2.120	<2
300, 2·0·14	2.088	30
2·1·10	2.0268	27
306	1.9897	2
1·2·11	1.9721	2
0·2·16	1.9301	2
0·1·20	1.8699	18
0·0·21, 1·1·18	1.8653	16
220, 1·2·14	1.8087	12
224	1.7784	<2
3·0·12	1.7599	8
312	1.7314	12
1·0·22	1.7133	4
2·0·20	1.6614	7
318	1.6377	4
1·3·10	1.5883	12
042	1.5613	<2
0·2·22	1.5487	4
1·2·20	1.5098	6
1·3·13	1.5060	9
1·1·24	1.4882	<2
3·1·14	1.4763	<2
4·0·10	1.4541	6
232	1.4332	2
2·1·22	1.4238	5
2·2·18	1.3910	3
238	1.3790	<2
410	1.3670	14
3·2·10	1.3493	8
0·0·30	1.3060	<2
3·1·20	1.3004	8
0·2·28	1.2775	<2
1·4·12	1.2610	<2
1·3·22	1.2442	6
1·1·30	1.2284	4
0·4·20	1.2239	4
2·1·28	1.2051	4
0·1·32	1.2020	2
0·5·10	1.1937	<2
422	1.1817	<2
4·0·22	1.1760	2
2·3·20, 274	1.1586	6
428	1.1511	<2
2·4·10	1.1334	<2
0·3·30	1.1074	2
158	1.0964	<2
1·3·28	1.0900	<2
1·2·32	1.0876	4
0·2·34	1.0814	4
2·2·30	1.0588	2
5·0·20	1.0558	2
600, 1·0·37, 1·5·14	1.0440	2
4·0·28	1.0436	2
4·2·20	1.0134	4
3·2·28	1.0026	4

Lattice constants

		a	*c*
		Å	Å
1964	Block, Perloff, and Weir [2]	7.23	39.17
1965	National Bureau of Standards, sample at 25 °C	7.2351	39.192

The density of the high form of barium boron oxide calculated from the NBS lattice constants is 3.751 g/cm^3 at 25 °C.

Reference

[1] E. M. Levin and H. F. McMurdie, The system BaO·Ba$_2$O$_3$, J. Res. NBS **42**, 131–7 (1949) RP 1956.

[2] S. Block, A. Perloff, and C. E. Weir, The crystallography of some M^{+2} borates, Acta Cryst. **17**, 314 (1964).

Barium Boron Oxide, BaB_4O_7 (monoclinic)

Powder data card. No. 6–0334, Levin and McMurdie [1].

Additional published pattern. None.

NBS sample. The sample of barium boron oxide was prepared at NBS from boric acid and barium carbonate, in a solid state reaction below the melting point of 910 °C. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon, and 0.01 to 0.1 percent each of aluminum, calcium, cobalt, and strontium.

The sample was colorless and optically positive with medium 2V. The indices of refraction are $N_\alpha=1.594\pm0.004$, $N_\beta=1.610\pm0.004$, and $N_\gamma=1.666\pm0.004$.

The *d*-values of the three strongest lines are 3.130, 3.805, and 4.908 Å.

Structural data. Block, Perloff, and Weir [2] in 1964 determined that barium boron oxide has the space group C_{2h}^{5}—$P2_1/c$ (No. 14) and 8(BaB_4O_7) per unit cell.

hkl	Internal Standard W, $a=3.1648$ Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
100	10. 22	8
$\bar{1}02$, $\bar{1}11$	6. 120	49
200	5. 113	24
012	4. 995	39
$\bar{1}12$	4. 908	72
102	4. 831	42
$\bar{2}11$	4. 410	14
210	4. 335	64
112	4. 160	45
020	4. 096	40
$\bar{2}12$	4. 010	5
021	3. 897	54
211	3. 847	24
$\bar{1}13$, 120	3. 805	94
$\bar{1}21$, 013	3. 742	24
121	3. 548	65
$\bar{3}02$	3. 388	63
212	3, 246	65
$\bar{2}21$	3. 229	35
220	3. 196	49
$\bar{3}12$	3, 130	100
$\bar{2}04$, $\bar{2}22$	3. 060	55
$\bar{1}14$	3. 029	6
221	2. 983	12
$\bar{1}23$	2. 967	12
014	2. 939	32
311	2. 894	11
$\bar{3}13$, $\bar{2}14$	2. 870	12
104	2. 810	65
302	2. 712	10
123	2. 691	27
$\bar{3}21$	2. 674	29
130	2. 638	7
320. $\bar{1}31$	2. 620	17
$\bar{3}22$	2. 614	
$\bar{1}24$, 131	2. 549	20
032	2. 507	48
024, $\bar{1}32$	2. 495	58
$\bar{2}24$	2. 452	32
410	2. 439	27
230	2. 410	22
223	2. 365	12
$\bar{2}32$	2. 348	49
214, 231, +	2. 316	40
$\bar{4}04$	2. 299	38
313, 322	2. 266	14
$\bar{3}15$, $\bar{3}24$	2. 247	16
$\bar{4}21$	2. 219	25
402	2. 177	18
133, 420	2. 168	25
$\bar{2}25$	2. 158	19
$\bar{4}23$, $\bar{3}32$	2. 128	44
412	2. 104	27
$\bar{1}34$	2. 094	17
$\bar{2}16$	2. 077	19
421, 304	2. 060	13
$\bar{5}11$, $\bar{3}33$	2. 039	37
016	2. 033	
140	2. 008	21
314	1. 997	40
$\bar{3}16$	1. 980	21
134	1. 958	5
042	1. 946	7
422	1. 922	8
413	1. 914	14
$\bar{1}35$, 511	1. 887	7
$\bar{5}21$, $\bar{2}42$	1. 873	7
225	1. 837	7
315, 512	1. 768	10
044	1. 718	15
$\bar{2}36$	1. 688	9
325	1. 657	16
$\bar{3}27$, 334	1. 644	4
530, 226	1. 636	6
$\bar{3}44$, $\bar{2}08$	1. 629	15
$\bar{6}22$, $\bar{4}41$	1. 620	14
$\bar{2}45$	1. 593	13

Lattice constants

		a	b	c	β
		Å	Å	Å	
1964	Block, Perloff, and Weir [2]	10. 56	8. 20	13. 01	104. 95°
1965	National Bureau of Standards, sample at 25 °C	10. 586	8. 194	13. 045	105. 150°

The density of barium boron oxide calculated from the NBS lattice constants is 3.558 g/cm³ at 25 °C.

References

[1] E. M. Levin and H. F. McMurdie, The system $BaO \cdot B_2O_3$, J. Res. NBS **42,** 131–7 (1949) RP1956.

[2] S. Block, A. Perloff, and C. E. Weir, The crystallography of some M^{+2} borates, Acta Cryst. **17,** 314 (1964).

Barium Fluosilicate, $BaSiF_6$ (trigonal)

Powder data card. No. 1–0534, Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of barium fluosilicate was prepared at NBS from barium chloride and hydrofluosilic acid. The precipitate was dried at 60 °C. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent sodium; 0.01 to 0.1 percent each of aluminum, calcium, potassium, magnesium, and strontium; and 0.001 to 0.01 percent each of iron, nickel, lead, titanium, and zirconium.

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

The *d*-values of the three strongest lines are 3.593, 1.953, and 3.055 Å.

hkl (hex)	Internal Standard W, a=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	I
	Å	
101	4. 650	30
110	3. 593	100
012	3. 055	60
021	2. 845	11
003	2. 336	42
202	2. 327	27
211	2. 230	58
300	2. 075	9
113	1. 958	29
122	1. 953	62
220	1. 796	13
104	1. 686	5
131	1. 676	4
303	1. 550	6
312	1. 548	9
024	1. 5269	7
401	1. 5187	7
223	1. 4242	8
042	1. 4219	10
214	1. 4050	14
321	1. 3992	1
015	1. 3679	3
410	1. 3582	9
232	1. 3223	6
205	1. 2785	1
134	1. 2296	5
051	1. 2258	4
125	1. 2043	4
330	1. 1974	5
413	1. 1738	6
502	1. 1729	5
006	1. 1684	4
404	1. 1632	5
241	1. 1597	4
422	1. 1148	4
116	1. 1110	4
324	1. 1067	3
511	1. 1039	2
315	1. 0883	1
333	1. 0655	5
152	1. 0648	4
045	1. 0416	1
600	1. 0373	1
306	1. 0180	2
054	1. 0148	3
431	1. 0122	3
235	1. 0004	2
520	0. 9965	3
342	. 9821	3
226	. 9796	3
244	. 9765	2

Structural data. Hoard and Vincent [2] in 1940 determined that barium fluosilicate has the space group D_{3d}^5—$R\bar{3}m$ (No. 166), with 3($BaSiF_6$) per unit hexagonal cell.

References

[1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by x-ray diffraction, Anal. Chem. **10**, 457–512 (1938).

[2] J. L. Hoard and W. B. Vincent, Structures of complex fluorides. Barium fluosilicate and barium fluogermanate, J. Am. Chem. Soc. **62**, 3126–3129 (1940).

Lattice constants

		a	*c*
		Å	*Å*
1940	Hoard and Vincent [2]	7.19	7.01
1965	National Bureau of Standards, sample at 25 °C	7.1854 ±0.0003	7.0102 ±0.0004

The density of barium fluosilicate calculated from NBS lattice constants is 4.440 g/cm³ at 25 °C.

Cerium Arsenate, $CeAsO_4$ (monoclinic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of cerium arsenate was precipitated at NBS from a water solution of arsenic pentoxide and cerium trichloride. It was heated to 930 °C for 1 hr to sharpen the pattern. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium and antimony; and 0.001 to 0.01 percent

hkl	Internal Standard Ag, *a*=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
$\bar{1}01$	5.420	5
110	4.908	14
011	4.820	12
$\bar{1}11$	4.324	11
101	4.183	4
111	3.610	10
020	3.581	16
200	3.368	58
002	3.260	8
120	3.161	100
210, $\bar{2}11$	3.046	24
$\bar{1}12$	2.978	34
012	2.966	77
$\bar{2}02$	2.710	25
$\bar{2}12$	2.533	22
112	2.507	16
220, $\bar{2}21$	2.451	6
$\bar{1}22$	2.417	7
$\bar{3}01$	2.310	4
130	2.247	6
031, $\bar{1}03$	2.240	19
$\bar{3}11$	2.198	8
221	2.167	8
$\bar{2}22$	2.161	5
122, 310	2.142	5
131	2.072	4
$\bar{3}12$	2.029	5
212	2.008	31
301	1.972	4
230, $\bar{2}31$	1.945	11
103, $\bar{1}32$	1.930	31
311, 320	1.902	15
023	1.857	4
$\bar{3}22$	1.822	20
$\bar{3}03$	1.807	1
$\bar{2}23$	1.799	2
231	1.794	4
040	1.7892	8
132	1.7817	25
140	1.7293	12
400	1.6825	8
$\bar{4}04$	1.6791	12
$\bar{2}04$, 410	1.6385	16
$\bar{4}12$, 330	1.6345	14
004	1.6294	8
312	1.6184	4
$\bar{2}14$	1.5973	7
014	1.5883	4
$\bar{3}32$	1.5830	8
240, $\bar{2}41$	1.5796	6
$\bar{1}42$	1.5700	3
$\bar{1}24$, 420	1.5235	7
$\bar{4}22$	1.5197	4
322	1.5067	3
$\bar{2}42$	1.4931	5
$\bar{3}14$	1.4809	3
421	1.4127	1
$\bar{4}23$	1.4086	1
$\bar{4}31$	1.4058	1
340	1.3989	4
$\bar{3}24$, 303	1.3941	5
124	1.3824	9
$\bar{1}34$	1.3661	7
332	1.3634	9
151, 233	1.3542	<1
204	1.3392	6
412	1.3369	6
$\bar{4}14$	1.3315	7
510	1.3230	4
250	1.3176	4
052	1.3109	7
323	1.2986	1
$\bar{5}13$	1.2809	5
$\bar{3}34$	1.2784	8
$\bar{2}52$	1.2658	3

Lattice constants

		a	b	c	β
		Å	Å	Å	
1965	National Bureau of Standards, sample at 25 °C	6.9596 ±0.0005	7.1576 ±0.0005	6.7378 ±0.0005	104°42.7′ ±0.3′

each of aluminum, iron, magnesium, and silicon. Rare-earth impurities were less than 0.1 percent of total rare-earth content.

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

The *d*-values of the three strongest lines are 3.161, 2.966, and 3.688 Å.

Structural data. Schwarz [1] in 1963 reported that cerium arsenate is isostructural with huttonite, with the space group C^5_{2h}—$P2_1/n$ (No. 14) and 4($CeAsO_4$) per unit cell.

The density of cerium arsenate calculated from the NBS lattice constants is 5.709 g/cm³ at 25 °C.

Reference

[1] H. Schwarz, Über die Chromate (V) der Seltenen Erden, I. Lanthanchromat (V), $LaCrO_4$, Z. Anorg Allgem. Chem. **322,** 1–14 (1963).

Cesium Fluoantimonate, $CsSbF_6$ (trigonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium fluoantimonate was prepared at NBS by treating a mixture of antimony and cesium nitrates with hydrofluoric acid. The sample was dried at 100 °C. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent rubidium; 0.01 to 0.1 percent each of aluminum and nickel; and 0.001 to 0.01 percent each of silver, calcium, copper, iron, potassium, sodium, silicon, and thallium.

The sample is colorless. It is optically positive with the indices $N_o=1.400$ and $N_e=1.406$.

The *d*-values of the three strongest lines are 3.948, 3.534, and 2.192 Å.

Structural data. Schrewelius [1] in 1943 determined that cesium fluoantimonate has the space group D^5_{3d}—$R\bar{3}m$ (No. 166) and 3($CsSbF_6$) per unit hexagonal cell. The rhombohedral cell reported by Schrewelius has been converted to the equivalent hexagonal cell for comparison with the NBS values.

hkl (hex.)	Internal Standard Ag, *a*=4.0861 Å; temp. 25 °C Cu 1.5405 Å	
	d	*I*
	Å	
101	5.273	5
110	3.948	100
012	3.534	69
021	3.161	1
003	2.751	2
202	2.634	17
211	2.467	5
300	2.282	14
122	2.192	35
220, 104	1.976	15
024	1.767	6
312	1.724	8
214	1.613	9
042	1.580	5
410	1.494	8
232	1.468	5
134	1.396	3
006	1.375	<1
330, 404	1.318	3
502, 116	1.2991	4
324	1.2497	2
422	1.2338	2
152, 306	1.1781	2
600, 054	1.1402	1
520, 244	1.0956	1
612, 416	1.0119	1
440, 434, 208	0.9874	1
532, 336	.9512	1
164	.9310	<1
710, 318	.9068	1

Lattice constants

		a	c
		Å	Å
1943	Schrewelius [1]	7.98	8.05
1965	National Bureau of Standards, sample at 25 °C	7.9026 ±0.0006	8.252 ±0.001

The density of cesium fluoantimonate calculated from the NBS lattice constants is 4.115 g/cm³ at 25 °C.

Reference

[1] N. Schrewelius, X-ray analyses of thallium fluoantimonate $TlSbF_6$ and some isomorphous alkali compounds, Arkiv Kemi, **16B** No. 7, 1–6 (1943).

Cobalt, Co (cubic)

Powder data cards. None.

Additional published patterns. Hull [1] 1921, Sekito [2] 1927, and Hofer and Peebles [3] 1947.

NBS sample. The sample of cubic cobalt was prepared at NBS by heating cobalt oxalate in a stream of hydrogen at 800 °C for about 10 min. Spectographic analysis showed the following major impurities: 0.1 to 1.0 percent each of nickel and antimony; and 0.01 to 0.1 percent each of aluminum and iron.

The sample was a dark grey opaque powder. The *d*-values of the three strongest lines are 2.0467, 1.7723, and 1.0688 Å.

Structural data. Hull [1] in 1921 determined that the cubic form of cobalt has the copper structure, the space group O_h^5—Fm3m (No. 225) and 4(Co) per unit cell. There also exists a hexagonal close-packed form of cobalt and the forms commonly occur together.

hkl	Internal Standard W, a=3.1648 Å; temp. 25 °C Co λ 1.7889 Å		
	d	*I*	*a*
	Å		Å
111	2.0467	100	3.5449
200	1.7723	41	3.5446
220	1.2532	23	3.5446
311	1.0688	29	3.5448
222	1.0233	11	3.5448
Average value of last five lines			3.5447

The lattice constant reported by Hull has been recalculated with a Mo wavelength of 0.711 Å. The lattice constant reported by Sekito could not be converted because the wavelength used for iron radiation was not given.

Lattice constants

		Å
1921	Hull [1]	3.546
1927	Sekito [2]	3.558
1947	Hofer and Pebbles [3]	3.546
1950	Taylor and Floyd [4]	3.5442
1965	NationalBureau of Standards, sample at 25 °C	3.5447

The density of cubic cobalt calculated from the NBS lattice constant is 8.788 g/cm³ at 25 °C.

References

[1] A. W. Hull, X-ray crystal analysis of thirteen common metals, Phys. Rev. **17,** 571–587 (1921).

[2] S. Sekito, On the lattice constants of metallic cobalt, Sci. Repts. Tohoku Imp. Univ. **16,** 545–53 (1927).

[3] L. J. E. Hofer and W. C. Pebbles, X-ray diffraction studies of the action of carbon monoxide on cobalt-thoria-kieselguhr catalyst. I., J. Am. Chem. Soc. **69,** 2497–2500 (1947).

[4] A. Taylor and R. W. Floyd, Precision measurements of lattice parameters of non-cubic crystals, Acta Cryst. **3,** 285–289 (1950).

Cobalt Diarsenide, $CoAs_2$ (monoclinic), revised

Powder data card. The following pattern is the same pattern shown on No. 11–115 prepared in 1960 by NBS*; however, it has been reindexed using recent data from the literature.

Additional published pattern. Quesnel and Heyding [1] 1962.

NBS sample. Minor corrections and additions were made to the original patterns.

Structural data. Quesnel and Heyding [1] in 1962 reported that cobalt diarsenide was isostructural with rhodium diphosphide, with the space group C_{2h}^5—$P2_1/c$ (No. 14) and 4($CoAs_2$) per unit cell. However, the unit cell measurements reported by Quesnel and Heyding are not in close agreement with the indexing reported by them.

Lattice constants

		a	*b*	*c*	*β*
		Å	Å	Å	
1962	Quesnel and Heyding [1]	5.853	5.805	5.885	114°11′
1965	National Bureau of Standards, sample at 25 °C	5.916	5.872	5.960	116°27′

The density of cobalt diarsenide calculated from the NBS lattice constants is 7.480 g/cm³ at 25 °C.

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*NBS Circular 539, **10,** 26 (1961).

hkl	Internal Standard W, a=3.1648 Å; temp. 25 °C Co λ 1.7889 Å	
	d	I
	Å	
$\bar{1}11$	3. 826	8
020	2. 936	11
111	2. 758	18
002	2. 666	47
200	2. 648	44
$\bar{1}21$	2. 536	100
012	2. 429	60
210	2. 413	52
$\bar{2}12$	2. 319	26
$\bar{2}21$	2. 083	4
102	2. 045	6
022	1. 974	6
220	1. 966	4
$\bar{2}22$	1. 913	10
$\bar{1}13$	1. 870	28
$\bar{3}11$	1. 856	28
$\bar{2}13$	1. 829	16
$\bar{1}31$	1. 825	23
013	1. 702	<3
131	1. 658	35
$\bar{1}23$	1. 6370	13
$\bar{3}21$	1. 6274	18
$\bar{3}13$	1. 6176	18
032	1. 5777	9
230	1. 5744	13
202	1. 5637	16
$\bar{2}32$	1. 5463	5
023	1. 5217	3
$\bar{2}04$	1. 4869	<3
$\bar{4}02$	1. 4767	3
040	1. 4680	<3
$\bar{3}23$	1. 4600	<3
$\bar{1}41$	1. 4098	<3
$\bar{3}32, \bar{3}14$	1. 3694	3
004, 123	1. 3336	12
321	1. 3285	12
400	1. 3239	7
$\bar{4}22$	1. 3189	7
014	1. 3010	3
$\bar{2}42$	1. 2689	13

Reference

[1] J. C. Quesnel and R. D. Heyding, Transition metal arsenides V. A note on the rhodium arsenic system and the monoclinic diarsenides of the cobalt family, Can. J. Chem. **40**, 814–818 (1962).

Cobalt Silicate, Co_2SiO_4 (orthorhombic)

Powder data cards. None.

Additional published pattern. Gallitelli and Cola [1] 1954.

NBS sample. The sample of cobalt silicate was obtained from Alfa Inorganics Inc., Beverly, Mass. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent aluminum, and 0.01 to 0.1 percent each of calcium, copper, iron, sodium, nickel, lead, titanium, and zircon.

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

The d-values of the three strongest lines are 2.469, 2.790, and 3.516 Å.

Structural data. Gallitelli and Cola [1] in 1954 determined that cobalt silicate has the olivine structure, the space group D_{2h}^{16}—Pmnb (No. 62) and 4(Co_2SiO_4) per unit cell. Ringwood [2] in 1963 determined that the olivine form of cobalt silicate converts to a spinel form at 60 kilobars of pressure and over, at 700 °C.

The density of cobalt silicate calculated from the NBS lattice constants is 4.708 g/cm³ at 25 °C.

Lattice constants

		a	b	c
		Å	Å	Å
1954	Gallitelli and Cola [1]	5. 99	10. 27	4. 77
1963	Ringwood [2]	5. 996	10. 340	4. 779
1965	National Bureau of Standards, sample at 25 °C	6. 0074	10. 310	4. 7823

Cobalt Silicate, $CoSiO_4$ (orthorhombic)—Continued

hkl	Internal Standard W, a=3.1648 Å; temp. 25 °C Co λ 1.7889 Å	
	d	*I*
	Å	
020	5.151	11
011	4.336	13
120	3.910	15
101	3.739	6
111	3.516	78
121	3.026	7
200	3.004	<5
031	2.790	90
220	2.594	35
040	2.578	24
131	2.530	74
211	2.469	100
002	2.392	17
140	2.369	14
012	2.330	10
221	2.282	24
041	2.270	16
112	2.172	7
022	2.168	6
231	2.045	9
051	1.895	6
311	1.818	12
151	1.807	6
222	1.759	72
042	1.754	
321	1.739	<5
142	1.683	11
160	1.652	10
331	1.627	14
251	1.602	12
340	1.581	6
013	1.576	6
113, 023	1.523	5
312	1.518	5
242	1.515	5
152	1.511	5
400, 341	1.502	19
260	1.492	25
033	1.446	<5
071	1.407	13
062, 213	1.3954	7
351	1.3761	<5
223	1.3580	7
143	1.3226	14
360	1.3037	<5
402	1.2718	<5
303	1.2474	<5
004	1.1956	5
333	1.1723	<5
253	1.1630	10
511	1.1578	<5
442	1.1403	7
214, 531	1.1039	<5
224	1.0856	10
291	1.0446	8
433	1.0421	8
471	1.0270	8
611	0.9758	8

References

[1] P. Gallitelli and M. Cola, Synthesis and crystallographic and structural properties of cobalt orthosilicate (olivine type), Atti Accad. Nazl. Lincei Rend. Classe Sci. Fis. Mat. Nat. **17**, 172–7 (1954).

[2] A. E. Ringwood, Olivine-spinel transformation in cobalt orthosilicate, Nature **198**, 79–80 (1963).

Cobalt Titanate, $CoTiO_3$ (trigonal)

Powder data card. No. 1–1040, New Jersey Zinc Co.

Additional published pattern. Barth and Posnjak [1] 1934.

NBS sample. The sample of cobalt titanate, obtained from Alfa Inorganics Inc., Beverly, Mass., was pressed into a pellet and heated 4½ hr at 1,350 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, calcium, copper, iron, nickel, and silicon.

The color of the sample was dark green. The indices of refraction could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are 2.727, 2.5340, and 1.7114Å.

Structural data. Barth and Posnjak [1] in 1934 determined that cobalt titanate has the ilmenite structure, the space group C_{3i}^2—R$\bar{3}$ (No. 148) and 6($CoTiO_3$) per unit hexagonal cell.

The rhombohedral cell reported by Barth and Posnjak was converted to the equivalent hexagonal cell for comparison with the NBS values.

hkl (hex)	Internal Standard W, a=3.1648 Å; temp. 25 °C Co λ 1.7889 Å	
	d	*I*
	Å	
012	3. 717	37
104	2. 727	100
110	2. 5340	73
006	2. 3202	<5
113	2. 2240	26
202	2. 0934	<5
024	1. 8566	30
107	1. 8114	<5
116	1. 7114	39
018	1. 6178	9
122	1. 6140	
214	1. 4974	25
300	1. 4628	29
208	1. 3636	5
1·0·10	1. 3272	7
119	1. 3203	7
220	1. 2672	6
306	1. 2379	<5
128	1. 2007	<5
0·2·10	1. 1756	6
134	1. 1488	<5
226	1. 1124	8
042	1. 0840	<5
2·1·10	1. 0664	7
404	1. 0465	5
318	0. 9977	6
0·1·14	. 9699	8
324	. 9675	7
410	. 9578	5
0·0·15, 048	. 9283	5
1·3·10	. 9165	10

Lattice constants

		a	c
		Å	Å
1934	Barth and Posnjak [1]	5. 054	13. 989
1965	National Bureau of Standards, sample at 25 °C	5. 0683	13. 9225

The density of cobalt titanate calculated from the NBS lattice constants is 4.980 g/cm³ at 25 °C.

Reference

[1] T. F. W. Barth and E. Posnjak, Notes on some structures of the ilmenite type, Z. Krist. **A88,** 271 (1934).

Cobalt Tungstate, $CoWO_4$ (monoclinic)

Powder data cards. None.

Additional published pattern. Broch [1] 1929.

NBS sample. The sample of cobalt tungstate was obtained from Alfa Inorganics Inc., Beverly, Mass. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of nickel and silicon, and 0.001 to 0.01 percent each of calcium, copper, iron, magnesium, manganese, lead, and vanadium.

The sample was a blue opaque powder.

The *d*-values of the three strongest lines are 2.916, 3.733, and 3.608 Å.

Structural data. Broch [1] in 1929 determined that cobalt tungstate is isostructural with magnesium tungstate, with the space group C_{2h}^4—P2/a (No. 13) and 2($CoWO_4$) per unit cell. Since monoclinic doublets were not seen in the NBS pattern, it was indexed as orthorhombic.

Cobalt Tungstate, $CoWO_4$ (monoclinic)—Continued

Lattice constants

		a	b	c	β
		Å	Å	Å	
1929	Broch [1]	4.93	5.68	4.66	90.0°
1965	National Bureau of Standards, sample at 25 °C	4.9478	5.6827	4.6694	90.0°

The density of cobalt tungstate calculated from the NBS lattice constants is 7.760 g/cm³ at 25 °C.

hkl (ortho.)	Internal Standard W, $a=3.1648$ Å; temp. 25 °C Co λ 1.7889 Å	
	d	*I*
	Å	
010	5.683	8
001	4.673	28
110	3.733	31
011	3.608	29
111	2.916	100
020	2.842	10
200	2.473	20
120	2.464	22
021	2.428	6
002	2.335	10
210	2.269	<1
201	2.185	14
121	2.180	14
012	2.160	<1
211	2.041	8
112	1.979	8
030	1.894	1
220	1.866	7
022	1.803	5
031	1.755	13
221	1.733	4
202	1.698	24
122	1.695	24
131	1.654	1
212	1.626	2
310	1.583	3
003	1.556	<1
311	1.500	14
032	1.471	3
222	1.457	6
113	1.436	10
231	1.432	14
320	1.426	8
132	1.410	1
140, 023	1.365	7
123	1.3162	4
312, 141	1.3108	7
213	1.2833	3
232	1.2644	4
400	1.2370	<1
322	1.2172	4
033, 331	1.2024	4
401	1.1956	3
142	1.1788	6
411	1.1701	3
004	1.1673	3
420	1.1342	3
114	1.1140	3
313	1.1101	5
051	1.1043	3
402	1.0933	3
233	1.0815	5
151	1.0777	6
124	1.0552	6
341	1.0489	2
430	1.0356	<1
143	1.0265	<1
052	1.0215	2
422	1.0201	2
431	1.0112	5
251	1.0086	5
224	0.9897	3

Reference

[1] E. K. Broch, Untersuchungen über Kristallstrukturen des Wolframittypus und des Scheelittypus, Skrifter Norske Videnskaps-Akad. Oslo I: Mat.-Naturv. Kl. No. 8, (1929).

Dysprosium Vanadate, $DyVO_4$ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of dysprosium vanadate was prepared at NBS by adding hot sodium orthovanadate solution to a hot acidic solution of dysprosium chloride. After the sample was dried at 110 °C for 1 hr, it was heated for 20 min at 700 °C to improve the crystallinity. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent iron; 0.01 to 0.1 percent each of aluminum, calcium, and silicon; and 0.001 to 0.01 percent each of copper, manganese, and antimony. Rare-earth impurities were less than 0.1 percent of total rare-earth content.

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

The *d*-values of the three strongest lines are 3.571, 2.675, and 1.837 Å.

Structural data. Milligan, Watt, and Rachford [1] in 1949 determined that dysprosium vanadate has the zircon structure, the space group D_{4h}^{19}—$I4_1/amd$ (No. 141) and $4(DyVO_4)$ per unit cell.

Lattice constants

		a	*c*
		Å	Å
1949	Milligan, Watt, and Rachford [1]	7.09	6.27
1965	National Bureau of Standards, sample at 25 °C	7.1434 ±0.0004	6.313 ±0.001

The density of dysprosium vanadate calculated from the NBS lattice constants is 5.720 g/cm³ at 25 °C.

hkl	Internal Standard W, *a*=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
101	4.728	36
200	3.571	100
211	2.851	12
112	2.675	65
220	2.525	23
202	2.363	7
301	2.227	12
103	2.018	12
321	1.890	12
312	1.837	58
400	1.786	13
213	1.758	6
411	1.671	5
420	1.597	14
004	1.579	6
332	1.4856	12
204	1.4435	11
501	1.3937	7
413	1.3377	9
512	1.2805	9
440	1.2627	7
600	1.1904	8
404	1.1830	8
503	1.1821	7
532	1.1420	9
620	1.1296	5
424, 523	1.1225	7
305	1.1158	3
116	1.0297	5
640	0.9909	4
444, 543	.9858	4
552	.9622	6

Reference

[1] W. O. Milligan, L. M. Watt, and H. H. Rachford, X-ray diffraction studies on heavy metal orthovanadates, J. Phys. Chem. **53,** 227–234 (1949).

Europium(III) Vanadate, $EuVO_4$ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of europium(III) vanadate was prepared at NBS by adding a hot solution of sodium orthovanadate to a hot acidic solution of europium chloride. After the sample was dried at 110° C for 1 hr., it was heated for 10 min at 700° C to improve the crystallinity. Spectrographic analysis showed the following major nonrare-earth impurities: 0.1 to 1.0 percent silicon; 0.01 to 0.1 percent each of aluminum and magnesium; and 0.001 to 0.01 percent each of cadmium, iron, and antimony. Rare-earth impurities were less than 0.2 percent of total rare-earth content.

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

The *d*-values of the three strongest lines are 3.619, 2.703, and 1.858 Å.

Structural data. Milligan, Watt, and Rachford [1] in 1949 determined that europium(III) vanadate has the zircon structure, the space group D_{4h}^{19}—$I4_1/amd$ (No. 141) and $4(EuVO_4)$ per unit cell.

Lattice constants

		a	c
		Å	Å
1949	Milligan, Watt, and Rachford [1]	7.19	6.33
1965	National Bureau of Standards, sample at 25 °C	7.2365 ±0.0002	6.3675 ±0.0003

The density of europium(III) vanadate calculated from the NBS lattice constants is 5.316 g/cm^3 at 25 °C.

hkl	Internal Standard W, *a*=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
101	4.779	30
200	3.619	100
211	2.884	12
112	2.703	65
220	2.559	21
202	2.390	8
301	2.256	17
103	2.037	11
321	1.914	11
312	1.858	49
400	1.810	18
213	1.7752	5
411	1.6923	6
420	1.6179	11
303	1.5930	5
332	1.5034	14
204	1.4570	11
501	1.4112	4
224	1.3515	10
512	1.2963	10
440	1.2794	4
600	1.2062	4
404	1.1953	5
215	1.1854	4
611	1.1696	3
532	1.1565	6
620	1.1444	2
523, 424	1.1349	6
325	1.0753	4
116	1.0390	4
640	1.0034	4
552	0.9742	5
316	.9626	8
604	.9613	6
624	.9291	5
732	.9104	4
820	.8774	2
516, 653	.8496	7

Reference

[1] W. O. Milligan, L. M. Watt, and H. H Rachford, X-ray diffraction studies on heavy metal orthovanadates, J. Phys. Chem. **53,** 227–234 (1949).

Gadolinium Arsenate, $GdAsO_4$ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of gadolinium arsenate was prepared at NBS from a water solution of gadolinium trichloride and arsenic pentoxide and heated for 30 min at 900 °C. Spectrographic analysis showed the following major nonrare-earth impurities: 0.01 to 0.1 percent each of aluminum and antimony, and 0.001 to 0.01 percent each of iron, magnesium, lead, silicon, and titanium. Rare-earth impurities were less than 0.1 percent of total rare-earth content.

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

The *d*-values of the three strongest lines are 3.566, 2.689, and 1.8395 Å.

Structural data. Durif and Forrat [1] in 1957 determined that gadolinium arsenate has the zircon structure with the space group D_{4h}^{19}—$I4_1/amd$ (No. 141) and $4(GdAsO_4)$ per unit cell.

Lattice constants

		a	c
		Å	Å
1957	Durif and Forrat [1]	7.14	6.34
1965	National Bureau of Standards, sample at 25° C	7.1326 ±0.0002	6.3578 ±0.0003

The density of gadolinium arsenate calculated from the NBS lattice constants is 6.082 g/cm³ at 25 °C.

hkl	Internal Standard W, a=3.1648 Å; temp. 25 °C Co λ 1.7889 Å	
	d	I
	Å	
101	4.747	10
200	3.566	100
112	2.689	64
220	2.522	20
202	2.374	4
301	2.228	6
103	2.032	6
321	1.888	5
312	1.8395	46
400	1.7832	13
420	1.5948	10
332	1.4859	11
204	1.4517	9
501	1.3915	<1
224	1.3444	8
512	1.2805	11
440	1.2608	2
600	1.1890	6
404	1.1866	
532	1.1419	7
424	1.1258	11
116	1.0367	5
640	0.9891	5
444	.9876	
712	.9614	10
316	.9591	10
624	.9196	7

Reference

[1] A. Durif and F. Forrat, Sur quelques arséniates des terres rares à structure zircon, Compt. Rend. **245,** 1636–38 (1957).

Holmium Vanadate, $HoVO_4$ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of holmium vanadate was precipitated at NBS by adding hot sodium orthovanadate solution to a hot acidic solution of holmium chloride. The sample was first dried at 110 °C for 1 hr. To improve the crystallinity, the sample was heated at 600 °C for 2 hr. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of iron and silicon, and 0.001 to 0.01 percent each of silver, aluminum, calcium, copper, magnesium, and antimony. Rare-earth impurities were less than 0.1 percent of total rare-earth content.

The color of the sample was dark brown. The indices of refraction could not be determined because the sample was too fine.

The *d*-valves of the three strongest lines are 3.564, 2.668, and 1.8311 Å.

Structural data. Milligan and Vernon [1] in 1952 determined that holmium vanadate has the zircon structure, the space group D_{4h}^{19}—$I4_1/amd$ (No. 141) and $4(HoVO_4)$ per unit cell.

Lattice constants

		a	*c*
		Å	Å
1952	Milligan and Vernon [1]	7.06	6.25
1965	National Bureau of Standards, sample at 25 °C	7.1214 ±0.0002	6.2926 ±0.0005

The density of holmium vanadate calculated from the NBS lattice constants is 5.825 g/cm^3 at 25 °C.

hkl	Internal Standard W, *a*=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
101	4.716	27
200	3.564	100
211	2.841	7
112	2.668	66
220	2.517	18
202	2.358	6
301	2.221	15
103	2.0111	9
321	1.8841	9
312	1.8311	51
400	1.7807	15
213	1.7511	3
411	1.6659	2
420	1.5926	10
004, 303	1.5722	5
332	1.4809	13
204, 323	1.4385	9
501	1.3888	3
413	1.3334	10
314	1.2899	1
512	1.2765	9
440	1.2590	2
600	1.1870	4
503	1.1783	5
215	1.1709	1
442	1.1694	2
611	1.1511	1
532	1.1385	6
620	1.1259	3
523	1.1188	11
325	1.0609	2
631	1.0470	<1
116	1.0261	4
613	1.0223	1
640	0.9874	2
444, 543	.9826	3
712	.9592	4
316	.9508	3
633, 604	.9473	3
703	.9153	4
732	.8964	4

Reference

[1] W. O. Milligan and L. W. Vernon, Crystal structure of heavy metal orthovanadates, J. Phys. Chem. **56**, 145–148 (1952).

Iridium Dioxide, IrO_2 (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of iridium dioxide was obtained from K&K Laboratories Inc., Jamaica, N.Y. It was heated in an evacuated sealed Vycor tube for 6 hrs at 900 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of sodium, lead, and platinum.

The sample was a black opaque powder.

The *d*-values of the three strongest lines are 3.178, 2.582, and 1.6960 Å.

Structural data. Goldschmidt [1] in 1926 determined that iridium dioxide has the rutile structure, the space group D_{4h}^{14}—$P4_2/mnm$ (No. 136), and $2(IrO_2)$ per unit cell.

Lattice constants

		a	*c*
		Å	*Å*
1926	Goldschmidt [1]	4.50	3.15
1965	National Bureau of Standards, sample at 25 °C	4.4983	3.1544

The density of iridium dioxide calculated from the NBS lattice constants is 11.665 g/cm³ at 25 °C.

Reference

[1] V. M. Goldschmidt, Crystal structure of the rutile type with remarks on the geochemistry of the bivalent and quadrivalent elements, Skrifter Norske Videnskaps-Akad. Oslo I: Mat. Naturv. K1. No. 1 (1926)

hkl	Internal Standard Ag, $a=4.0861$ Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
110	3.178	100
101	2.582	92
200	2.2488	26
210	2.0119	<1
211	1.6960	56
220	1.5903	12
002	1.5771	6
310	1.4227	12
112	1.4133	13
301	1.3542	14
202	1.2914	8
321	1.1604	10
400	1.1247	3
222	1.1199	6
330	1.0602	3
312	1.0563	9
411	1.0310	8
103	1.0240	4
420	1.0058	4
213	0.9318	8
402	.9157	3
510	.8822	4
332	.8799	4
501	.8652	11
303	.8609	5
422	.8480	7
521	.8075	9
323	.8040	8
440	.7953	3
004	.7886	2

Lead Boron Oxide, PbB_4O_7 (orthorhombic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of lead boron oxide was prepared at NBS from lead oxide and boric acid. It was heated at temperatures below the melting point (768 °C), ground, and then alternately reheated and reground several times. 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 determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are 2.673, 3.952, and 4.122 Å.

Structural data. Block, Perloff, and Weir [1] in 1964 determined that lead boron oxide has the space group C_{2v}^7—$Pnm2_1$ (No. 31) and $2(PbB_4O_7)$ per unit cell.

Lattice constants

		a	*b*	*c*
		Å	*Å*	*Å*
1964	Block, Perloff, and Weir [1]	4.457	10.840	4.244
1965	National Bureau of Standards, sample at 25 °C	4.4562 ±0.0002	10.8401 ±0.0005	4.2434 ±0.0002

Lead Boron Oxide, PbB_4O_7 (orthorhombic)—Continued

The density of lead boron oxide calculated from the NBS lattice constants is 5.872 g/cm^3 at 25 °C.

Reference

[1] S. Block, A. Perloff, and C. E. Weir, The crystallography of some M^{+2} borates, Acta Cryst. **17,** 314 (1964).

hkl	Internal Standard W, *a*=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
020	5.423	73
100	4.456	10
110	4.122	74
011	3.952	80
120	3.442	4
101	3.072	52
111	2.955	21
130	2.806	57
031	2.752	62
040	2.709	22
121	2.673	100
131	2.341	5
140	2.315	13
200	2.229	20
210	2.182	8
002	2.121	18
220	2.061	14
141	2.033	53
022	1.976	26
201	1.972	21
150	1.949	17
211	1.941	21
051	1.931	19
102	1.916	<1
230	1.896	11
112	1.887	34
221	1.854	12
060, 122	1.807	13
151	1.772	2
231	1.7317	14
240	1.7211	6
132	1.6929	15
042	1.6709	10
241	1.5950	5
142	1.5642	4
161	1.5575	16
202	1.5366	5
212	1.5215	6
300	1.4852	3
222	1.4782	9
170	1.4625	7
251	1.4592	11
071	1.4551	9
152	1.4357	12
320	1.4322	10
232	1.4135	4
013, 301	1.4024	10
311	1.3902	8
171	1.3826	2
062	1.3751	5
321	1.3568	5
080	1.3546	6
103	1.3481	5
242	1.3366	8
261	1.3328	6
033	1.3169	5
123	1.3081	11
340	1.3026	8
270	1.2715	2
252	1.2538	3
341	1.2453	3
181	1.2399	7
350	1.2254	1
271	1.2177	5
312	1.2090	3
143	1.2069	3
172	1.2043	6
203	1.1942	<1
322, 213	1.1871	7
053	1.1847	8
351	1.1772	3
262	1.1704	2
223	1.1663	4
190	1.1632	2
280	1.1581	4
332	1.1529	1
360	1.1473	<1
082	1.1421	3
233	1.1340	4
281	1.1172	2
342	1.1101	5
410, 361	1.1078	5
243	1.0927	2
272	1.0905	2
0·10·0	1.0841	<1
163	1.0807	4
401	1.0778	3
411, 370	1.0721	<1
430	1.0646	1
352, 004	1.0612	2
421	1.0570	5
253	1.0460	3
024	1.0412	2
371	1.0393	3
291	1.0277	4
1·10·1	1.0222	5
313, 192	1.0198	8
173, 282	1.0164	4
362	1.0093	2

Lithium Phosphate, low form (lithiophosphate), Li_3PO_4 (orthorhombic) revised

This compound was described in earlier work [1] from this laboratory. Recently the structure of the low form was determined by Keffer, Mighell, Mauer, Swanson, and Block [2]. The following pattern is intended to replace the earlier one in Monograph 25, Section 3.

Powder data card. No. 12–230, Fisher [3] 1958.

Additional published patterns. Matias and Bondareva [4] 1957 and National Bureau of Standards [1] 1964.

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. Two indices of refraction are $N_\alpha=1.550$ and $N_\gamma=1.538$. It is optically negative with a large 2V. N_β could not be determined because of the crystal shape.

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

Structural data. Keffer, Swanson, Mighell, Mauer, and Block [2] in 1964 determined that low form lithium phosphate has the space group C_{2v}^7–$Pmn2_1$ (No. 31) and $2(Li_3PO_4)$ per unit cell.

hkl	Internal Standard Ag, *a*=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
010	5. 232	34
110	3. 973	100
101	3. 797	98
011	3. 554	56
111	3. 071	26
200	3. 059	
210	2. 640	64
020	2. 616	36
002	2. 423	47
211	2. 318	31
021	2. 303	
012	2. 199	<1
121	2. 155	4
112	2. 070	3
310, 202	1. 899	1
301	1. 879	2
221	1. 839	4
212	1. 785	14
311	1. 769	9
122	1. 7074	1
130	1. 6777	2
031	1. 6415	1
320	1. 6083	3
131	1. 5855	2
103	1. 5616	4
013	1. 5431	3
400	1. 5287	11
230	1. 5152	16
113	1. 4959	1
410	1. 4675	1
411	1. 4043	2
213	1. 3776	14
123	1. 3409	2
420	1. 3203	2
040	1. 3078	<1
402	1. 2931	4
232	1. 2848	8
331	1. 2788	4
303	1. 2656	2
412	1. 2550	1
223	1. 2533	1
240	1. 2027	<1
510	1. 1909	2
501	1. 1860	2
241	1. 1676	3
422	1. 1591	2
430	1. 1498	<1
323	1. 1394	<1
340	1. 1014	2

References

[1] H. E. Swanson, M. C. Morris, E. H. Evans, and L. Ulmer, Standard X-ray Diffraction Powder Patterns, NBS Mono. 25, **Sec. 3,** 38 (1964).

[2] C. Keffer, A. Mighell, F. Mauer, H. Swanson, and S. Block, The crystal structure of low temperature lithium phosphate (to be published in Inorg. Chem.).

[3] D. J. Fisher, Note on lithiophosphate, Am. Mineralogist **43,** 761–2 (1958).

[4] V. V. Matias and A. M. Bondareva, Lithiophosphate, a new mineral, Dokl. Akad. Nauk SSSR 112, 124–6 (1957); an English abstract exists in Am. Mineralogist **42,** 585 (1957).

[5] F. Zambonini and F. Laves, Über die Kristallstruktur des Li_3PO_4 und seine Beziehung Zum Strukturtyp des Olivin, Z. Krist. **83,** 26–28 (1932).

Lattice Constants

		a	b	c
		Å	Å	Å
1932	Zambonini and Laves [5]	6. 08	10. 28	4. 87
1965	National Bureau of Standards, sample at 25 °C	6. 1155 ±0. 0004	5. 2340 ±0. 0005	4. 8452 ±0. 0005

The density of lithium phosphate, low form, calculated from the NBS lattice constants is 2.479 g/cm^3 at 25 °C.

Lithium Sulfate Monohydrate, $Li_2SO_4 \cdot H_2O$ (monoclinic)

Powder data card. No. 1–0425, Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of lithium sulfate monohydrate was prepared at NBS from lithium metal and sulfuric acid, using enough heat to fume off the excess acid. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of silver, calcium, sodium, and tungsten; and 0.001 to 0.01 percent each of aluminum, barium, iron, potassium, magnesium, silicon, and strontium.

The sample was colorless and optically negative. The indices of refraction are $N_\alpha=1.460$, $N_\beta=1.477$, and $N_\gamma=1.487$; 2V is large.

The *d*-values of the three strongest lines are 5.084, 4.133, and 3.559 Å.

Structural data. Ziegler [2] in 1934 determined that lithium sulfate monohydrate has the space group C_2^2—$P2_1$ (No. 4) with $2(Li_2SO_4 \cdot H_2O)$ per unit cell.

Lattice Constants

		a	b	c	β
		Å	Å	Å	
1934	Ziegler [2]	5. 44	4. 84	8. 16	107°35′
1952	Bechmann [3]	5. 45	4. 87	8. 18	107°18′
1954	Larson and Helmholz [4]	5. 430	4. 836	8. 140	107°14′
1965	National Bureau of Standards, sample at 25 °C	5. 4518 ±0. 0005	4. 8707 ±0. 0004	8. 175 ±0. 001	107°19. 8′ ±0. 4′

The density of lithium sulfate monohydrate calculated from the NBS lattice constants is 1.939 g/cm^3 at 25° C.

References

[1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by x-ray diffraction, Anal. Chem. **10,** 457–512 (1938).

[2] G. E. Ziegler, The crystal structure of lithium sulphate monohydrate, $Li_2SO_4 \cdot H_2O$, Z. Krist. **89,** 456–459 (1934).

[3] R. Bechmann, Elastic and piezoelectric coefficients of lithium sulphate monohydrate, Proc. Phys. Soc. **65B,** 375–77 (1952).

[4] A. C. Larson and L. Helmholz, Redetermination of the crystal structure of lithium sulfate monohydrate, $Li_2SO_4 \cdot H_2O$, J. Chem. Phys. **22,** 2049–2050 (1954).

Lithium Sulfate Monohydrate, $Li_2SO_4 \cdot H_2O$ (monoclinic)—Continued

hkl	Internal Standard W, *a*=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
001	7. 82	11
100	5. 205	31
$\bar{1}01$	5. 084	100
011	4. 133	95
002	3. 904	35
101	3. 837	86
$\bar{1}02$	3. 696	34
110	3. 559	92
$\bar{1}11$	3. 520	3
012	3. 049	61
111	3. 014	8
$\bar{1}12$	2. 944	52
102	2. 752	19
$\bar{2}01$	2. 724	52
$\bar{1}03$	2. 666	16
200, 003	2. 603	6
$\bar{2}02$	2. 543	6
020	2. 435	34
112	2. 396	10
$\bar{2}11$	2. 377	6
$\bar{1}13$	2. 339	15
021	2. 324	4
210, 013	2. 295	19
201	2. 274	7
$\bar{2}12$	2. 254	8
120	2. 207	11
$\bar{1}21$, $\bar{2}03$	2. 197	
103	2. 091	2
211	2. 061	10
121	2. 056	8
104	2. 036	6
$\bar{1}22$	2. 032	
$\bar{2}13$	2. 001	5
004	1. 950	2
113	1. 921	12
202	1. 917	
$\bar{2}04$	1. 847	4
122	1. 825	3
$\bar{2}11$	1. 815	5
$\bar{3}01$, 014	1. 811	
$\bar{1}23$, $\bar{3}02$	1. 797	5
212	1. 784	2
220, 023	1. 778	
$\bar{2}22$	1. 759	<1
300	1. 7344	7
$\bar{2}14$	1, 7272	4
104	1. 6701	<1
221	1. 6617	<1
310	1. 6342	3
$\bar{2}23$	1. 6310	2
203	1. 6150	1
$\bar{3}13$	1. 6006	5
301	1. 5961	6
031	1. 5893	3
114	1. 5800	2
005	1. 5613	8
$\bar{1}15$, 130	1. 5496	8
$\bar{3}04$	1. 5451	8
213	1. 5331	<1
311	1. 5167	<1
032	1. 4992	4
$\bar{1}32$, 015	1. 4860	4
$\bar{3}14$	1. 4723	3
$\bar{3}21$	1. 4537	2
302	1. 4343	2
320	1. 4129	2
132	1. 3983	3
$\bar{2}31$	1. 3946	3
$\bar{1}33$	1. 3866	3
$\bar{3}05$	1. 3832	2
204, 312	1. 3765	8
$\bar{2}32$	1. 3686	1
$\bar{1}06$	1. 3609	2
$\bar{2}01$	1. 3505	1

Magnesium Aluminum Silicate (pyrope), $Mg_3Al_2(SiO_4)_3$ (cubic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of pyrope was obtained from Dr. F. R. Boyd [5] at the Geophysical Laboratory, Carnegie Institute, Washington, D.C. The sample was prepared from magnesium silicate and aluminum silicate glasses at 40 kilobars of pressure and at 1,400 °C for 1 hr. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of bismuth and iron; and 0.01 to 0.1 percent each of calcium, nickel, titanium and vanadium.

The sample was colorless. The index of refraction is 1.702.

The *d*-values of the three strongest lines are 2.562, 2.865, and 1.5312 Å.

Structural data. Menzer [1] in 1926 determined that pyrope was an end-member of the garnet group, having the space group O_h^{10}—Ia3d (No. 230) with $8[Mg_3Al_2(SiO_4)_3]$ per unit cell.

The density of pyrope calculated from the NBS lattice constant is 3.563 g/cm³ at 25 °C.

hkl	Internal Standard Ag, a=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å		
	d	*I*	*a*
	Å		Å
211	4. 677	8	11. 46
220	4. 053	4	11. 46
321	3. 063	8	11. 46
400	2. 865	61	11. 46
420	2. 562	100	11. 458
332	2. 443	40	11. 459
422	2. 339	22	11. 459
431	2. 247	27	11. 457
521	2. 092	13	11. 459
440	2. 0256	8	11. 458
611	1. 8588	16	11. 458
620	1. 8120	7	11. 460
541	1. 7678	1	11. 457
631	1. 6894	1	11. 458
444	1. 6540	12	11. 459
543	1. 6205	1	11. 459
640	1. 5890	32	11. 458
721	1. 5594	2	11. 459
642	1. 5312	52	11. 458
732	1. 4551	2	11. 457
800	1. 4320	9	11. 456
741	1. 4102	4	11. 456
820	1. 3897	3	11. 460
653	1. 3696	4	11. 459
822	1. 3506	1	11. 460
831	1. 3323	2	11. 461
752	1. 2976	3	11. 460
840	1. 2811	10	11. 458
842	1. 2503	9	11. 459
921	1. 2355	5	11. 458
664	1. 2216	6	11. 460
851	1. 2079	3	11. 459
844	1. 1693	<1	11. 457
941	1. 1575	5	11. 459
10·1·1	1. 1343	1	11. 456
10·2·0	1. 1235	2	11. 457
943	1. 1128	<1	11. 457

hkl	Internal Standard Ag, a=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å		
	d	*I*	*a*
	Å		Å
10·3·1	1. 0927	<1	11. 460
871	1. 0729	1	11. 455
10·4·0	1. 0638	7	11. 459
10·4·2	1. 0459	7	11. 457
11·1·0	1. 0374	1	11. 458
880	1. 0126	6	11. 456
11·3·2	0. 9897	1	11. 457
10·6·0	. 9826	1	11. 459
11·4·1	. 9751	<1	11. 455
10·6·2	. 9685	<1	11. 459
12·0·0	. 9548	2	11. 458
12·1·1	. 9482	1	11. 457
12·2·0	. 9418	1	11. 457
11·5·2	. 9355	1	11. 457
12·2·2	. 9293	10	11. 457
12·3·1	. 9230	<1	11. 454
12·4·0	. 9057	<1	11. 456
11·6·3	. 8892	1	11. 457
13·2·1	. 8685	<1	11. 456
12·4·4	. 8634	2	11. 456
12·5·3	. 8587	2	11. 456
12·6·0	. 8539	8	11. 456
12·6·2	. 8445	2	11. 455
11·4·1	. 8399	1	11. 455
888	. 8268	4	11. 457
13·4·3	. 8224	2	11. 455
14·1·1	. 8141	3	11. 455
14·2·0	. 8100	2	11. 455
12·7·3	. 8060	1	11. 455
14·3·1	. 7981	2	11. 455
12·8·0	. 7943	2	11. 456
13·5·4	. 7906	1	11. 457
14·4·0	. 7867	10	11. 454
Average value of last five lines			11. 455

Magnesium Aluminum Silcate (pyrope), $Mg_3Al_2(SiO_4)_3$ (cubic)—Continued

Lattice constants

		Å
1926	Menzer (natural)[a] [1]	11. 53
1927	Stockwell[b] [2]	11. 453
1937	Fleischer[b] [3]	11. 463
1956	Skinner [5]	11. 459
1959	Boyd and England [6]	11. 456
1965	National Bureau of Standards, sample at 25 °C	11. 455

[a] Natural pyrope contains iron.
[b] Extrapolated from natural garnets.

References

[1] G. Menzer, Die Gitterkonstanten der Granate, Centr. Mineral. Geol. **A** and **B**, 343–344 (1926).

[2] C. H. Stockwell, An x-ray study of the garnet group, Am. Mineralogist **12**, 327–344 (1927).

[3] M. H. Fleischer, The relation between chemical composition and physical properties in the garnet group, Am. Mineralogist **22**, 751–759 (1937).

[4] B. J. Skinner, Physical properties of end-members of the garnet group, Am. Mineralogist **41**, 428–436 (1956).

[5] F. R. Boyd and J. L. England, Experimentation at high pressures and temperatures, Pyrope, Ann. Rept. Director Geophys. Lab. No. **1320**, 82–87 (1958–1959).

Magnesium Boron Oxide, $Mg_2B_2O_5$ (triclinic)

Powder data cards. No. 3–0841, Dow Chemical Co., Midland, Mich. This card is called magnesium metaborate, $MgO{\cdot}B_2O_3$; however, the data is comparable to ours. Two other cards, Nos. 10–327 and 11–427, by Takéuchi [1] 1952 give patterns for a monoclinic and the triclinic form.

Additional published patterns. None.

NBS sample. The sample of magnesium boron oxide was prepared at NBS by C. E. Weir from a slurry of magnesium carbonate and boric acid in water. The sample was alternately fired and ground several times reaching a maximum temperature of 1,150 °C. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of barium, beryllium, calcium, iron, silicon, and strontium.

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

The *d*-values of the three strongest lines are 2.579, 2.536, and 2.009 Å.

Structural data. Block, Burley, Perloff and Mason [2] in 1959 determined that magnesium boron oxide is isomorphous with cobalt boron oxide having the space group C_i^1—$P\bar{1}$ (No. 2) with $2(Mg_2B_2O_5)$ per unit cell.

The density of magnesium boron oxide calculated from NBS lattice constants is 2.910 g/cm³ at 25 °C.

Lattice constants

		a	b	c	α	β	γ
		Å	Å	Å			
1952	Takéuchi [1]	5. 93	9. 03	3. 12	90°54′	90°0′	103°54′
1959	Block, Burley, Perloff & Mason [2]	6. 187	9. 219	3. 119	90°24′	92°08′	104°19′
1965	National Bureau of Standards, sample at 25 °C	6. 155 ±0. 001	9. 220 ±0. 002	3. 122 ±0. 001	90°28′ ±1′	92°09′ ±1′	104°25′ ±1′

Magnesium Boron Oxide, $Mg_2B_2O_5$ (triclinic)—Continued

hkl	Internal Standard W, a=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
010	8. 94	6
100	5. 96	10
110, 020	4. 473	44
$\bar{1}20$	4. 099	14
120	3. 211	9
001	3. 121	9
$\bar{2}10$	3. 065	4
200, 030, $\bar{1}30$	2. 979	26
011	2. 928	3
$\bar{2}20$	2. 824	46
101	2. 717	3
$1\bar{1}1$	2. 700	22
210	2. 635	14
$0\bar{2}1$	2. 579	100
021	2. 536	54
111	2. 513	8
130, $\bar{2}30$	2. 431	7
$\bar{1}40$	2. 287	6
040	2. 232	6
$0\bar{3}1$	2. 173	2
$\bar{1}31$	2. 155	2
031	2. 134	20
201	2. 111	4
$2\bar{2}1$	2. 066	2
$\bar{3}10$, $\bar{2}40$	2. 050	7
$\bar{3}20$	2. 009	47
211	1. 973	<1
$\bar{1}\bar{3}1$	1. 948	30
131	1. 888	25
$\bar{2}\bar{2}1$	1. 850	11
$\bar{1}50$, $\bar{1}41$	1. 842	16
221	1. 783	8
$\bar{2}41$	1. 721	8
$\bar{3}21$	1. 717	
$\bar{3}01$	1. 707	11
$2\bar{4}1$	1. 704	
$3\bar{1}1$	1. 683	1
$\bar{1}\bar{4}1$, 320	1. 667	1
$\bar{2}\bar{3}1$	1. 640	3
141	1. 624	1
$\bar{3}\bar{1}1$	1. 616	6
240, 150	1. 604	10
$1\bar{5}1$	1. 589	4
002, 311	1. 558	24
051, $\bar{1}60$	1. 537	4
$\bar{4}10$, $\bar{4}20$	1. 532	10
$\bar{2}51$	1. 519	10
$\bar{1}12$, $\bar{3}41$	1. 514	12
$2\bar{5}1$	1. 512	
$\bar{4}30$, 060	1. 489	10
$3\bar{4}1$	1. 486	

References

[1] Y. Takéuchi, The crystal structure of magnesium pyroborate, Acta Cryst. **5**, 574–581 (1952).

[2] S. Block, G. Burley, A. Perloff, and R. Mason, Refinement of the crystal structure of triclinic magnesium pyroborate, J. Res. NBS **62**, No. 3, (1959) RP2936.

Metaboric Acid, HBO_2 (cubic)

Powder data cards. None. Nos. 1–0409 and 9–15 are for other modifications of metaboric acid.

Additional published patterns. None.

NBS sample. The sample of cubic metaboric acid was prepared at NBS by Kilday and Prosen [1] 1964 by holding orthoboric acid in a vacuum with orthorhombic metaboric acid followed by heating at 180 °C. Spectrographic analysis of the starting materials showed no impurity greater than 0.001 percent.

The sample was colorless. The refractive index is 1.616.

The *d*-values of the three strongest lines are 4.442, 1.939, and 3.627 Å.

Structural data. Zachariasen [2] in 1963 determined that cubic metaboric acid has the space group T_d^4—$P\bar{4}3n$ (No. 218) with 24(HBO_2) per unit cell. Three other forms of metaboric acid have been reported in the literature: a monoclinic, an orthorhombic, and a tetragonal.

hkl	Internal Standard W, *a*=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å		
	d	*I*	*a*
	Å		Å
110	6.280	47	8.881
200	4.442	100	8.884
210	3.973	43	8.884
211	3.627	50	8.884
220	3.140	26	8.881
310	2.809	42	8.883
222	2.565	26	8.885
320	2.464	4	8.884
321	2.374	32	8.883
400	2.221	20	8.884
410	2.155	8	8.885
411	2.094	36	8.884
420	1.986	6	8.882
421	1.939	93	8.886
332	1.894	17	8.884
422	1.8134	5	8.884
500	1.7768	2	8.884
510	1.7424	5	8.882
520	1.6496	3	8.883
521	1.6215	5	8.881
440	1.5708	2	8.886
530	1.5232	13	8.882
531	1.5016	6	8.884
600	1.4805	2	8.883
611	1.4411	6	8.884
620	1.4044	6	8.882
621	1.3877	4	8.886
541	1.3714	2	8.888
622	1.3395	11	8.885
630	1.3245	14	8.885
631	1.3103	5	8.887
444	1.2824	4	8.885
700	1.2693	1	8.885
710	1.2567	4	8.886
720	1.2205	1	8.885
721	1.2090	7	8.884
731	1.1567	5	8.885
650	1.1374	1	8.883
732	1.1283	3	8.884
800	1.1106	3	8.885
810	1.1022	4	8.886
811	1.0937	4	8.885
820	1.0774	4	8.884
821	1.0695	7	8.884
653	1.0620	4	8.885
822	1.0472	4	8.885
830	1.0397	5	8.883
831	1.0326	4	8.883
751	1.0260	4	8.885
662	1.0190	3	8.883
832	1.0124	1	8.884
752	1.0058	1	8.883
840	0.9934	1	8.885
900	.9875	1	8.888
910	.9811	2	8.884
911	.9753	3	8.885
920	.9639	1	8.887
921	.9581	5	8.885
922	.9418	2	8.885
930	.9366	1	8.885
931	.9313	2	8.884
852	.9212	2	8.884
932	.9164	2	8.885
844	.9064	1	8.886
941	.8976	1	8.886
10·1·0	.8842	2	8.886
10·1·1	.8799	1	8.887
10·2·0	.8712	2	8.884
10·2·1	.8670	2	8.884
950	.8630	2	8.885
951	.8590	3	8.886
10·2·2	.8549	2	8.884
10·3·0	.8510	1	8.885
Average value of last five lines			8.885

Lattice constants

		Å
1963	Zachariasen [2]	8. 886
1965	National Bureau of Standards, sample at 25° C	8. 885

The density of cubic metaboric acid calculated from the NBS lattice constant is 2.489 g/cm^3 at 25 °C.

References

[1] M. V. Kilday and E. J. Prosen, Heats of solution, transition, and formation of three crystalline forms of metaboric acid, J. Res. NBS **68A** (Phys. and Chem.) No. 1, 127–137 (1964).

[2] W. H. Zachariasen, The crystal structure of cubic metaboric acid, Acta Cryst. **16**, 380–384 (1963).

Neodymium Arsenate, $NdAsO_4$ (monoclinic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of neodymium arsenate was precipitated at NBS from a water solution of arsenic pentoxide and neodymium trichloride. It was heated 1 hr at 930 °C. Spectrographic analysis showed the following major nonrare-earth impurities: 0.01 to 0.1 percent antimony and 0.001 to 0.01 percent each of aluminum, calcium, iron, lead, and silicon. Rare-earth impurities were less than 0.1 percent of total rare-earth content.

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

The *d*-values of the three strongest lines are 3.129, 2.941, and 3.331 Å.

Structural data. Schwarz [1] in 1963 determined that neodymium arsenate has the huttonite structure, the space group C_{2h}^5—$P2_1/n$ (No. 14), and 4($NdAsO_4$) per unit cell.

Lattice constants

		a	b	c	β
		Å	Å	Å	
1965	National Bureau of Standards, sample at 25 °C	6. 897 ± 0. 001	7. 094 ± 0. 001	6. 6849 ± 0. 0007	104°54. 0′ ± 0. 7′

The density of neodymium arsenate calculated from the NBS lattice constants is 5.950 g/cm^3 at 25 °C.

Reference

[1] H. Schwarz, Über die Chromate (V) der Seltenen Erden, III Neodymchromat (V), $NdCrO_4$, Z. Anorg. Allgem. Chem. **322**, 129 (1963).

Neodymium Arsenate, $NdAsO_4$ (monoclinic)—Continued

hkl	Internal Standard Ag, a=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
$\bar{1}01$	5. 378	5
110	4. 860	10
011	4. 774	11
$\bar{1}11$	4. 287	11
101	4. 137	4
111	3. 573	8
020	3. 546	14
200	3. 331	57
002	3. 227	7
120	3. 129	100
210, $\bar{2}11$	3. 017	21
$\bar{1}12$	2. 958	34
012	2. 941	68
121, $\bar{2}02$	2. 691	24
211, $\bar{2}12$	2. 516	17
112	2. 484	14
220, $\bar{2}21$	2. 428	6
$\bar{1}22$	2. 397	5
$\bar{3}01$	2. 289	<2
130	2. 230	14
$\bar{1}03$, 031	2. 221	
$\bar{3}11$	2. 180	6
221, $\bar{2}22$	2. 145	7
$\bar{1}13$, 310	2. 120	3
131	2. 053	<2
$\bar{3}12$	2. 013	<2
212	1. 986	27
301	1. 952	2
230, $\bar{2}31$	1. 928	4
$\bar{1}32$	1. 913	25
320, 311	1. 882	15

hkl	Internal Standard Ag, a=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
023	1. 842	3
$\bar{3}22$	1. 807	17
040	1. 773	9
132	1. 765	19
140	1. 713	8
400, $\bar{4}02$	1. 666	10
$\bar{2}04$, $\bar{1}14$	1. 626	5
410, $\bar{4}12$	1. 622	10
004	1. 614	4
312, $\bar{3}23$	1. 601	3
213, $\bar{2}14$	1. 586	5
014	1. 575	4
$\bar{3}32$	1. 570	4
240, $\bar{2}41$	1. 566	
$\bar{1}42$, 232	1. 557	2
$\bar{1}24$	1. 512	4
322	1. 491	<2
$\bar{2}42$, 223	1. 480	4
340, 051	1. 386	2
124, 043	1. 369	6
$\bar{1}34$	1. 365	6
$\bar{3}42$	1. 355	2
332	1. 350	7
034	1. 333	<2
204	1. 325	7
412, $\bar{4}14$	1. 322	
$\bar{1}15$	1. 311	<2

Neodymium Vanadate, $NdVO_4$ (tetragonal)

Powder data card. No. 6–0217, Milligan, Watt, and Rachford [1] 1949.

Additional published patterns. None.

NBS sample. The sample of neodymium vanadate was prepared at NBS by adding a hot solution of sodium orthovanadate to a hot acidic solution of neodymium chloride. After the sample was dried at 110 °C for 1 hr, it was heated for 20 min at 700 °C to improve the crystallinity. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon and 0.001 to 0.01 percent each of aluminum, calcium, copper, and magnesium. Rare-earth impurities were less than 0.1 percent of total rare-earth content.

The color of the sample was pale blue. The indices of refraction could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are 3.664, 2.732, and 1.881 Å

Structural data. Milligan, Watt, and Rachford [1] in 1949 determined that neodymium vanadate has the zircon structure, the space group D_{4h}^{19}—$I4_1/amd$ (No. 141) and $4(NdVO_4)$ per unit cell.

Lattice constants

		a	c
		Å	Å
1949	Milligan, Watt, and Rachford [1]-------	7. 31	6. 42
1965	National Bureau of Standards, sample at 25 °C-----------	7. 3290 ±0. 0003	6. 4356 ±0. 0006

The density of neodymium vanadate calculated from the NBS lattice constants is 4.979 g/cm^3 at 25 °C.

Reference

[1] W. O. Milligan, L. M. Watt and H. H. Rachford, X-ray diffraction studies on heavy metal orthovanadates, J. Phys. Chem. **53**, 227–234 (1949).

hkl	Internal Standard W, a=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	I
	Å	
101	4. 835	31
200	3. 664	100
211	2. 921	11
112	2. 732	73
220	2. 590	19
202	2. 419	5
301	2. 284	16
103	2. 059	10
321	1. 938	12
312	1. 881	57
400	1. 8325	16
213	1. 7951	5
411	1. 7131	2
420	1. 6391	13
303	1. 6122	3
004	1. 6086	6
332	1. 5219	16
204	1. 4733	13
501	1. 4293	6
224	1. 3670	12
512	1. 3121	12
440	1. 2954	5
600	1. 2214	5
404	1. 2086	6
215	1. 1977	5
611	1. 1840	3
532	1. 1704	10
620	1. 1584	5
424	1. 1481	10
325	1. 0874	2
613, 116	1. 0504	6
640	1. 0163	4
543, 444	1. 0094	4
552	0. 9867	5
633, 316	. 9734	6
624	. 9404	6
732	. 9220	3
723, 336	. 9113	2
660	. 8637	3
653, 516	. 8596	9

Potassium Acid Phthalate, $C_6H_4(COOH)(COOK)$ (orthorhombic)

Powder data card. No. 1–0020, Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of potassium acid phthalate was obtained from J. T. Baker Chemical Co., Phillipsburg, N.J. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, sodium, and rubidium.

Potassium Acid Phthalate, $C_6H_4(COOH)(COOK)$ (orthorhombic)—Continued

Lattice constants

		a	*b*	*c*
		Å	Å	Å
1957	Okaya and Pepinsky [2]	9. 61	13. 26	6. 47
1963	Bearden and Huffman [3]	9. 62	13. 3164	6. 47
1965	National Bureau of Standards, sample at 25 °C	9. 607	13. 312	6. 475

The sample is colorless and optically negative. The refractive indices are

$N_\alpha=1.500$, $N_\beta=1.653$, $N_\gamma=1.660$, $2V\cong10°$.

The *d*-values of the three strongest lines are 13.32, 4.982, and 4.030 Å.

Structural data. Okaya and Pepinsky [2] in 1957 reported that potassium acid phthalate has the space group* D_2^3—$P2_122_1$ (No. 18) with $4[C_6H_4(COOH)(COOK)]$ per unit cell.

The density of potassium acid phthalate calculated from the NBS lattice constants is 1.638 g/cm^3 at 25 °C.

hkl	Internal Standard Ag, *a*=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
010	13. 32	100
110	7. 80	2
020	6. 651	1
111	4. 982	36
200	4. 802	4
030	4. 438	<1
121	4. 179	14
130	4. 030	20
220	3. 894	4
211	3. 705	9
131	3. 423	6
221	3. 338	12
002	3. 240	2
012, 140	3. 145	14
112	2. 990	18
231, 022	2. 912	12
320	2. 886	5
141	2. 830	4
122	2. 787	6
202	2. 684	2
050	2. 663	10
321, 212	2. 632	6
032	2. 615	6
150	2. 566	2
132, 241	2. 522	7
222	2. 488	2
331	2. 410	4
151	2. 386	6
142	2. 257	4
411, 060	2. 219	2
251	2. 191	2
160	2. 161	2
242	2. 090	2
161	2. 050	6
152	2. 010	4
203	1. 969	3
351	1. 953	2
440	1. 946	1
261	1. 924	<1
133, 070, 510	1. 902	1
170, 441	1. 866	<1
062	1. 829	<1
233	1. 800	<1
162	1. 797	1
171	1. 792	1

References

[1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Anal. Chem. **10,** 457–512 (1938).

[2] Y. Okaya and R. Pepinsky, The crystal structure of ammonium acid phthalate, Acta Cryst. **10,** 324–328 (1957).

[3] A. J. Bearden and F. N. Huffman, Precision measurement of the cleavage plane grating spacing of potassium acid phthalate, Rev. Sci. Instr. **34,** No. 11, 1233–1234 (1963).

[4] Y. Okaya, The crystal structure of potassium acid phthalate, KC_6H_4COOH-COOK, Acta Cryst. **19,** 879 (1965).

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*Okaya [4] in 1965 reported that the revised space group is C^5_{2v}–Pca2, (No. 29).

Praseodymium Arsenate, $PrAsO_4$ (monoclinic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of praseodymium arsenate was precipitated at NBS from a water solution of arsenic pentoxide and praseodymium trichloride. It 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, iron, magnesium, lead, and silicon. Rare-earth impurities were less than 0.1 percent of total rare-earth content.

The color of the sample was light green. The indices of refraction could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are 3.141, 2.953, and 3.349 Å.

Structural data. Schwarz [1] in 1963 reported that praseodymium arsenate is isostructural with huttonite with the space group C_{2h}^5—$P2_1/n$ (No. 14) and $4(PrAsO_4)$ per unit cell.

The density of praseodymium arsenate calculated from the NBS lattice constants is 5.804 g/cm³ at 25 °C.

hkl	Internal Standard Ag, a=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
$\bar{1}01$	5.404	5
110	4.878	12
011	4.799	11
$\bar{1}11$	4.304	12
101	4.158	5
111	3.591	8
020	3.560	19
200	3.349	60
002	3.246	8
120	3.141	100
210, $\bar{2}11$	3.031	24
$\bar{1}12$	2.967	40
012	2.953	82
$\bar{2}02$	2.701	29
$\bar{2}12$	2.525	22
112	2.497	16
220, $\bar{2}21$	2.440	8
$\bar{1}22$	2.405	8
$\bar{3}01$	2.299	4
$\bar{1}03$, 031	2.231	23
$\bar{3}11$	2.188	10
$\bar{2}22$, 221	2.155	9
122	2.134	2
$\bar{1}13$, 310	2.130	5
131	2.061	4
$\bar{3}12$	2.021	6
212	1.997	39
301	1.962	4
230, $\bar{2}31$	1.935	11
103, $\bar{1}32$	1.920	35
311, $\bar{1}23$, 320	1.892	18
023	1.848	6
$\bar{3}22$	1.814	25
$\bar{3}03$	1.802	2
222	1.797	2
$\bar{2}23$	1.793	3
231	1.785	4
040	1.7794	8
132	1.7726	30
140	1.7202	13
$\bar{4}11$	1.6828	2
$\bar{4}02$	1.6729	13
410	1.6300	14
$\bar{1}33$, 330	1.6265	16
004	1.6231	12
312	1.6101	5
014	1.5823	5
$\bar{3}32$	1.5761	8
240, $\bar{2}41$	1.5722	9
$\bar{1}42$	1.5632	2
$\bar{1}24$	1.5185	7
$\bar{4}22$	1.5140	5
322	1.4994	3
223, 241	1.4871	8
$\bar{3}14$	1.4758	5
$\bar{4}31$	1.3995	5
$\bar{1}43$, 340	1.3922	6
303	1.3871	5
124, $\bar{1}51$	1.3767	11
$\bar{1}34$	1.3709	10
$\bar{3}42$	1.3602	6
332	1.3568	12

Reference

[1] H. Schwarz, Über die Chromate (V) der Seltenen Erden, II. Praseodymchromat (V) $PrCrO_4$, Z. Anorg. Allgem. Chem. **322,** 15–24 (1963).

Lattice constants

		a	b	c	β
		Å	Å	Å	
1965	National Bureau of Standards, sample at 25 °C--------	6.929 ±0.001	7.119 ±0.001	6.715 ±0.001	104°48.2′ ±0.6′

Samarium Arsenate, $SmAsO_4$ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of samarium arsenate was prepared at NBS from a water solution of samarium trichloride and arsenic pentoxide. The sample was heated to 900 °C for 20 hrs to sharpen the pattern. Spectrographic analysis showed the following major nonrare-earth impurities: 0.1 to 1.0 percent silicon: 0.01 to 0.1 percent aluminum; and 0.001 to 0.01 percent each of calcium, iron, and magnesium. Rare-earth impurities were less than 0.1 percent of total rare-earth content.

The sample had a cream color. The indices of refraction could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are 3.594, 2.708, and 1.853 Å.

Structural data. Durif and Forrat [1] in 1957 determined that samarium arsenate has the zircon structure with the space group D_{4h}^{19}—$I4_1/amd$ (No. 141) and 4($SmAsO_4$) per unit cell.

Lattice constants

		a	c
		Å	Å
1957	Durif and Forrat [1]---	7.20	6.40
1965	National Bureau of Standards, sample at 25 °C-----------	7.1865 ±0.0004	6.3999 ±0.0005

The density of samarium arsenate calculated from NBS lattice constants is 5.813 g/cm³ at 25 °C.

hkl	Internal Standard Ag, a=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	I
	Å	
101	4.784	14
200	3.594	100
211	2.869	7
112	2.708	69
220	2.540	19
202	2.390	4
301	2.244	10
103	2.045	6
321	1.904	5
312	1.853	49
400	1.7967	16
213	1.7778	2
411	1.6817	2
420	1.6068	11
004	1.6004	10
332	1.4973	12
204	1.4617	10
501	1.4020	2
224	1.3539	8
512	1.2901	12
440	1.2709	2
600	1.1980	5
404	1.1949	7
503	1.1922	5
215	1.1894	3
532	1.1504	6
620	1.1362	3
424	1.1341	6
116	1.0439	6
206	1.0225	1
640	0.9965	1
444	.9948	1
552	.9686	2
316	.9655	2
604	.9586	1
624	.9263	5
732	.9054	4
336	.9029	2
820	.8712	1
516	.8504	6
644	.8458	1

Reference

[1] A. Durif and F. Forrat, Sur quelques arséniates des terres rares à structure zircon, Compt. Rend. **245,** 1636–38 (1957).

Samarium Oxide, Sm_2O_3 (cubic)

Powder data cards. None. Nos. 9–201, 11–412, and 13–244 are for the monoclinic B form of samarium oxide.

Additional published patterns. Zachariasen [1] 1927.

NBS sample. The sample of samarium oxide was obtained from the Lindsay Chemical Co., West Chicago, Ill. The cubic form was obtained when the sample was heated at 800 °C for 19 hrs. The analysis by Lindsay Chemical Co. showed the rare-earth impurities to be less than 0.1 percent of total rare-earth content.

The sample was cream colored. The index of refraction is about 1.97.

The *d*-values of the three strongest lines are 3.155, 1.9317, and 2.731 Å.

Structural data. Zachariasen [1] in 1927 determined that the C-modification of samarium oxide has the manganese dioxide structure, the space group T_h^7—Ia3 (No. 206) with 16(Sm_2O_3) per unit cell.

Lattice constants

		Å
1925	Goldschmidt, Barth, and Ulrich [2]	10. 87
1927	Zachariasen [1]	10. 89
1939	Bommer [3]	10. 915
1954	Templeton and Dauber [4]	10. 932
1954	Brauer and Gradinger [5]	10. 928
1965	National Bureau of Standards, sample at 25 °C	10. 927

The density of samarium oxide calculated from NBS lattice constant is 7.100 g/cm³ at 25 °C.

hkl	Internal Standards W, *a*=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å		
	d	*I*	*a*
	Å		Å
211	4. 460	11	10. 925
222	3. 155	100	10. 929
321	2. 920	4	10. 926
400	2. 731	33	10. 924
411	2. 575	8	10. 925
420	2. 444	1	10. 930
332	2. 330	4	10. 928
510	2. 143	7	10. 927
521	1. 995	2	10. 927
440	1. 9317	40	10. 929
530	1. 8739	4	10. 927
600	1. 8212	1	10. 927
611	1. 7723	5	10. 925
541	1. 6857	4	10. 925
622	1. 6474	29	10. 928
631	1. 6111	7	10. 927
444	1. 5776	8	10. 930
710	1. 5454	2	10. 928
640	1. 5154	2	10. 928
721	1. 4871	2	10. 928
732	1. 3880	3	10. 929
800	1. 3663	4	10. 930
811	1. 3450	4	10. 927
831	1. 2703	3	10. 928
662	1. 2536	6	10. 929
840	1. 2218	5	10. 928
921	1. 1785	3	10. 929
930	1. 1521	4	10. 930
844	1. 1152	6	10. 927
941	1. 1040	<1	10. 929
10·2·0	1. 0714	3	10. 926
10·2·2	1. 0516	4	10. 928
10·3·1	1. 0418	4	10. 926
871	1. 0234	1	10. 927
10·4·0	1. 0145	3	10. 926
10·3·3	1. 0060	1	10. 929
11·2·1	0. 9736	3	10. 929
880	. 9660	2	10. 929
10·6·2	. 9236	2	10. 928
12·0·0	. 9106	2	10. 927
12·1·1	. 9043	2	10. 927
11·5·2	. 8921	1	10. 926
12·4·2	. 8532	2	10. 926
Average value of last five lines			10. 927

References

[1] W. H. Zachariasen, The crystal structure of the modification C of the sesquioxides of the rare-earth metals and of indium and thallium, Norsk Geol. Tidsskr. **9,** 310–316 (1927).

[2] V. M. Goldschmidt, T. Barth, and F. Ulrich, Geochemische Verteilungsgesetze der Elemente IV,—Zur Krystallstruktur der Oxyde der selten Erdmetalle Skrifter Norske Videnskaps-Akad. Oslo I Mat. Naturv. Kl. (1925).

[3] H. Bommer, Die Gitterkonstanten der C-Formen der Oxyde der seltenen Erdmetalle, Z. Anorg. Allgem. Chem. **241,** 273–280 (1939).

[4] D. H. Templeton and C. H. Dauben, Lattice parameters of some rare-earth compounds and a set of crystal radii, J. Am. Chem. Soc. **76,** 5237–5239 (1954).

[5] I. G. Brauer and H. Gradinger, Über heterotype Mischphasen bei Seltenerdoxyden, Z. Anorg. Allgem. Chem. **276,** 209–226 (1954).

Scandium Arsenate, $ScAsO_4$ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of scandium arsenate was prepared at NBS from a water solution of arsenic pentoxide and scandium trichloride. It was heated 30 min at 900 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of antimony, silicon, and vanadium; and 0.001 to 0.01 percent each of aluminum, chromium, copper, iron, magnesium, lead and tin.

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

The *d*-values of the three strongest lines are 3.354, 2.569, and 1.742 Å.

Structural data. No reference to the structure of scandium arsenate was found, but it is apparently isostructural with yttrium arsenate with the space group D_{4h}^{19}—$I4_1/amd$ (No. 141) and $4(ScAsO_4)$ per unit cell.

Lattice constants

		a	*c*
		Å	*Å*
1965	National Bureau of Standards, sample at 25 °C	6.7101 ±0.0001	6.1126 ±0.0002

The density of scandium arsenate calculated from the NBS lattice constants is 4.437 g/cm³ at 25 °C.

hkl	Internal Standards W, *a*=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	A	
101	4.516	10
200	3.354	100
211	2.693	22
112	2.569	48
220	2.371	11
202	2.259	7
301	2.100	<1
312	1.742	40
213	1.6854	4
400	1.6777	10
411	1.5727	3
004	1.5283	3
420	1.5008	7
332	1.4048	12
204	1.3908	7
323	1.3744	3
501	1.3111	<1
224	1.2851	4
314	1.2400	2
521	1.2210	2
512	1.2090	5
105	1.2032	3
440	1.1864	2
404	1.1299	3
600	1.1186	3
532	1.0771	5
424	1.0709	6
620	1.0611	2
541	1.0332	1
116	0.9960	3
444	.9370	1
640	.9305	3
316	.9184	3
552	.9062	4
604	.9025	2
624	.8715	4
336	.8565	1
732	.8466	5
800	.8388	1
811	.8246	<1
615	.8190	<1
820, 307	.8137	1
516	.8056	6
644	.7948	3
660	.7909	1
327	.7905	

Strontium Boron Oxide, SrB_4O_7 (orthorhombic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of strontium boron oxide was prepared at NBS from strontium carbonate and boric acid. It was heated to 1,000 °C, ground, and then alternately reheated and reground several times. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of barium, calcium, and silicon; and 0.001 to 0.01 percent each of aluminum, iron, and magnesium.

hkl	Internal Standard W, a=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	I
	Å	
020	5.35	24
100	4.43	4
110	4.10	29
011	3.940	31
101	3.061	28
111	2.942	13
130	2.778	43
031	2.729	51
040	2.677	15
121	2.657	100
131	2.324	<1
140	2.292	17
200	2.214	26
210	2.168	2
002	2.118	30
220	2.046	11
141	2.015	63
022	1.969	13
201	1.962	16
211	1.929	20
051	1.911	8
230	1.881	25
221	1.842	3
122	1.7990	2
060	1.7846	5
231	1.7187	8
240	1.7060	4
132	1.6839	7
042	1.6609	4
241	1.5818	1
142	1.5549	4
161	1.5419	8
202	1.5301	6
212	1.5147	1
222	1.4708	5
251, 170	1.4461	6
071	1.4385	3
152	1.4252	6
232	1.4059	2
013	1.3990	<1
260	1.3893	3
311	1.3817	3
171	1.3677	5
062	1.3644	
321	1.3481	6
103	1.3444	3
080	1,3384	5
242	1.3280	4
261	1.3198	3
033	1.3122	3
123, 162	1.3040	7
340	1.2919	7
270, 133	1.2584	<1
252	1.2450	1
341	1.2360	2
181	1.2264	3
350	1.2150	2
271	1.2062	2
312	1.2026	4
172	1.1940	4
213	1.1825	3
053	1.1784	4
223, 262	1.1616	3
091, 280	1.1456	3
082	1.1313	3
233	1.1288	4
342	1.1030	3
361	1.0982	3
420	1.0837	<1
163	1.0739	3
0·10·0, 401	1.0710	<1
411	1.0652	1
352	1.0540	1
421	1.0498	2
253	1.0402	2
024	1.0379	2
371	1.0300	1
114	1.0247	2
303	1.0198	<1
291	1.0173	<1
313	1.0152	2
124, 1·10·1	1.0107	4
282	1.0076	4
323, 362	1.0016	1
441	0.9942	<1
263	.9899	1
134	.9892	
044	.9843	1
412	.9766	1
381, 422	.9650	2

Strontium Boron Oxide, SrB_4O_7 (orthorhombic)—Continued

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

The *d*-values of the three strongest lines are 2.657, 2.015, and 2.729 Å.

Structural data. Block, Perloff, and Weir [1] in 1964 determined that strontium boron oxide has the space group C_{2v}^7—Pnm2_1 (No. 31) and 2(SrB_4O_7) per unit cell.

Lattice constants

		a	*b*	*c*
		Å	Å	Å
1964	Block, Perloff, and Weir [1]	4.431	10.706	4.237
1965	National Bureau of Standards, sample at 25 °C	4.4263 ±0.0002	10.7074 ±0.0005	4.2338 ±0.0002

The density of strontium boron oxide calculated from the NBS lattice constants is 4.019 g/cm³ at 25 °C.

Reference

[1] S. Block, A. Perloff, and C. E. Weir, The crystallography of some M^{+2} borates, Acta Cryst. **17**, 314 (1964).

Tin Arsenide, SnAs (cubic)

Powder data cards. None.

Additional published patterns. Willott and Evans [1] 1934.

NBS sample. The sample of tin arsenide was prepared at NBS in a solid state reaction by heating a mixture of arsenic and tin in an evacuated Pyrex tube at 500 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent lead, and 0.001 to 0.01 percent each of aluminum, antimony, bismuth, copper, indium, iron, magnesium, nickel, and silicon.

The sample was a gray opaque powder.

The *d*-values of the three strongest lines are 2.862, 2.024, and 1.652 Å.

Structural data. Goldschmidt [2] in 1928 determined that tin arsenide has the sodium chloride structure, the space group O_h^5—Fm3m (No. 225) and 4(SnAs) per unit cell.

hkl	Internal Standard W, *a*=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å		
	d	*I*	*a*
	Å		Å
111	3.306	13	5.725
200	2.862	100	5.725
220	2.024	55	5.725
311	1.726	4	5.723
222	1.652	17	5.724
400	1.4310	8	5.724
331	1.3129	2	5.723
420	1.2800	16	5.724
422	1.1684	10	5.724
511	1.1015	<1	5.724
440	1.0120	2	5.725
531	0.9676	1	5.724
600	.9540	6	5.724
620	.9052	4	5.7247
622	.8630	4	5.7244
444	.8263	1	5.7248
711	.8017	<1	5.7252
640	.7939	4	5.7250
Average value of last five lines			5.7248

Lattice constants

		Å
1928	Goldschmidt [2]	5.720
1934	Willott and Evans [1]	5.692
1935	Hägg and Hybinette [3]	5.728
1965	National Bureau of Standards, sample at 25 °C	5.7248

The density of tin arsenide calculated from the NBS lattice constant is 6.854 g/cm³ at 25 °C.

References

[1] W. H. Willott and E. J. Evans, X-ray investigation of the arsenic-tin system of alloys, Phil. Mag. **18**, 114 (1934).

[2] V. M. Goldschmidt, Atomic distances in metals, Z. Physik. Chem. (Leipzig) **133**, 397 (1928).

[3] G. Hägg and A. G. Hybinette, X-ray studies on the systems Sn-Sb and Sn-As, Phil. Mag. **20**, 913 (1935).

Ytterbium Arsenate, $YbAsO_4$ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of ytterbium arsenate was precipitated at NBS from a water solution of arsenic pentoxide and ytterbium trichloride. It was dried 1 hr at 880 °C. Spectrographic analysis showed the following major nonrare-earth impurities: 0.01 to 0.1 percent each of antimony and titanium and 0.001 to 0.01 percent each of aluminum, calcium, iron, nickel, lead, and silicon. Rare-earth impurities were less than 0.1 percent of total rare-earth content.

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

The *d*-values of the three strongest lines are 3.486, 2.6375, and 1.8004 Å.

Structural data. Durif and Forrat [1] in 1957 determined that ytterbium arsenate has the zircon structure with the space group D_{4h}^{19}—$I4_1/amd$ (No. 141) and 4($YbAsO_4$) per unit cell.

Lattice constants

		a	c
		Å	Å
1957	Durif and Forrat [1]	6. 99	6. 24
1965	National Bureau of Standards, sample at 25 °C	6. 9716 ±0. 0002	6. 2437 ±0. 0003

The density of ytterbium arsenate calculated from the NBS lattice constants is 6.828 g/cm^3 at 25 °C.

hkl	Internal Standard W, a=3.1648 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	I
	Å	
101	4. 652	22
200	3. 486	100
211	2. 788	5
112	2. 6375	74
220	2. 4648	24
202	2. 3258	3
301	2. 1781	10
103	1. 9939	7
321	1. 8468	7
312	1. 8004	56
400	1. 7424	16
213	1. 7308	3
411	1. 6316	1
420	1. 5587	15
332	1. 4541	14
204	1. 4250	11
501	1. 3604	2
224	1. 3188	8
512	1. 2524	11
440	1. 2322	3
105	1. 2289	
404	1. 1625	7
503	1. 1582	
611	1. 1271	<1
532	1. 1166	7
424	1. 1029	12
325	1. 0491	<1
631	1. 0250	<1
116	1. 0187	3
613	1. 0039	<1
444, 640	0. 9669	5
543	. 9647	3
721	. 9464	<1
552	. 9403	9
604	. 9321	2
633	. 9302	2
624	. 9004	5
703	. 8984	3
732	. 8784	5
800	. 8715	<1
820	. 8456	<1
516	. 8282	5
644	. 8220	5
536	. 7849	7

Reference

[1] A. Durif and F. Forrat, Sur quelques arséniates des terres rares à structure zircon, Compt. Rend. **245**, 1636–38 (1957).

Zinc Antimony Oxide, $ZnSb_2O_4$ (tetragonal)

Powder data cards. No. 4–0563, Stahl [1] 1943. No. 1–0678 is probably $ZnO{\cdot}Sb_2O_5$ and not $ZnO{\cdot}Sb_2O_3$.

Additional published patterns. None.

NBS sample. The sample of zinc antimony oxide was prepared at NBS from zinc oxide and antimony trioxide. The mixture was wrapped in gold foil and sealed in a nitrogen filled quartz tube. It was heated to 700 °C for ¾ of an hour. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of arsenic, magnesium, lead, and silicon.

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

The *d*-values of the three strongest lines are 3.206, 2.694, and 1.9509 Å.

Structural data. Stahl [1] in 1943 determined that zinc antimony oxide has the space group D_{4h}^{13}—P4/mbc (No. 135) with 4($ZnSb_2O_4$) per unit cell.

hkl	Internal Standard W, *a*=4.0861 Å; temp. 25 °C Cu λ 1.5405 Å	
	d	*I*
	Å	
110	6. 021	8
200	4. 261	17
210	3. 811	1
211	3. 206	100
220	3. 011	22
002	2. 964	10
310	2. 694	29
112	2. 662	11
202	2. 434	19
212	2. 341	7
400	2. 129	1
410	2. 066	2
330	2. 008	6
312	1. 995	3
411	1. 9509	29
420	1. 9042	6
213	1. 7552	14
402	1. 7296	6
430	1. 7033	<1
332	1. 6625	19
511	1. 6075	<1
520	1. 5815	<1
521	1. 5283	6
440	1. 5056	1
004	1. 4833	4
432	1. 4775	3
530	1. 4607	7
512	1. 4551	3
413	1. 4283	8
600	1. 4192	5
610	1. 4000	1
620	1. 3469	1
224, 540	1. 3302	<1
532	1. 3104	3
541	1. 2980	6
602	1. 2805	3
523	1. 2350	4
622	1. 2264	4
334	1. 1933	<1
424	1. 1704	<1
721	1. 1477	2
215	1. 1327	4
730	1. 1184	2
712	1. 1159	3
543	1. 1035	2
731	1. 0989	<1
642	1. 0972	1
650	1. 0904	1
651	1. 0728	1
800	1. 0648	<1
444, 810	1. 0565	1
811	1. 0400	5
820	1. 0328	<1
415, 713	1. 0288	1
604	1. 0258	1
653	1. 0232	<1
821	1. 0174	<1
425, 723	1. 0068	2
660	1. 0037	2
751	0. 9765	1
822	. 9754	<1
206	. 9633	<1
840	. 9523	2
662	. 9508	1
525	. 9493	1
910	. 9405	1
841	. 9400	1
752	. 9390	1
813	. 9318	3
644, 920	. 9239	<1
921	. 9128	<1
930	. 8977	1
406, 912	. 8966	<1
851	. 8925	3
336	. 8870	2
753	. 8852	2
932	. 8593	4
10·0·0	. 8517	1
10·0·1	. 8432	<1
10·1·1	. 8390	2

Zinc Antimony Oxide, ZnSb$_2$O$_4$ (tetragonal)—Continued

Lattice constants

		a	*c*
		Å	Å
1943	Stahl [1]	8. 508	5. 932
1965	National Bureau of Standards, sample at 25 °C	8. 5168 ±0. 0002	5. 9331 ±0. 0003

The density of zinc antimony oxide calculated from the NBS lattice constants is 5.754 g/cm^3 at 25 °C.

Reference

[1] S. Stahl, The crystal structure of ZnSb$_2$O$_4$, Arkiv Kemi, **Bd. 17B** No. 5, (1943–44).

CALCULATED POWDER PATTERNS

Antimony Cerium, CeSb (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [8] 1937.

Structural data. Iandelli and Botti [8] in 1937 determined that antimony cerium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(CeSb) per unit cell. The atoms occupy the special positions:

Ce: 0 0 0
Sb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1937	Iandelli and Botti [8]	6. 412
1963	Kuz'min and Nikitina [32]	6. 41

The lattice constant used in this calculated pattern is a=6.412 Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.21, 2.27, and 1.434 Å.

The calculated density is 6.598 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 70	<1
200	3. 21	100
220	2. 27	69
311	1. 933	<1
222	1. 851	23
400	1. 603	10
331	1. 471	<1
420	1. 434	27
422	1. 309	19
511	1. 234	<1
440	1. 133	6
531	1. 084	<1
600	1. 069	12
620	1. 014	8
622	0. 967	8
444	. 925	2
711	. 898	<1
640	. 889	7
642	. 857	14
731	. 835	<1
800	. 802	2

Antimony Dysprosium, DySb (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that antimony dysprosium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(DySb) per unit cell. The atoms occupy the special positions:

Dy: 0 0 0
Sb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=6.153 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.08, 2.18, and 1.376 Å.

The density of antimony dysprosium calculated from the constant of Brixner is 8.104 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.55	4
200	3.08	100
220	2.18	68
311	1.855	2
222	1.776	22
400	1.538	10
331	1.412	<1
420	1.376	26
422	1.256	19
511	1.184	<1
440	1.088	6
531	1.040	<1
600	1.026	13
620	0.973	9
533	.938	<1
622	.928	8
444	.888	3
711	.862	<1
640	.853	8
642	.822	16
731	.801	<1

Antimony Erbium, ErSb (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that antimony erbium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(ErSb) per unit cell. The atoms occupy the special positions:

Er: 0 0 0
Sb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=6.106 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.05, 2.16, and 1.365 Å.

The density of antimony erbium calculated from the constant of Brixner is 8.432 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.53	4
200	3.05	100
220	2.16	68
311	1.841	2
222	1.763	22
400	1.526	10
331	1.401	<1
420	1.365	26
422	1.246	19
511	1.175	<1
440	1.079	6
531	1.032	<1
600	1.018	13
620	0.965	9
533	.931	<1
622	.921	9
444	.881	3
711	.855	<1
640	.847	8
642	.816	17
731	.795	<1

Antimony Gadolinium, GdSb (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that antimony gadolinium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(GdSb) per unit cell. The atoms occupy the special positions:

Gd: 0 0 0
Sb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=6.217 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.11, 2.20, and 1.390 Å.

The density of antimony gadolinium calculated from the constant of Brixner is 7.712 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.59	3
200	3.11	100
220	2.20	69
311	1.874	1
222	1.795	23
400	1.554	10
331	1.426	<1
420	1.390	26
422	1.269	19
511	1.196	<1
440	1.099	6
531	1.051	<1
600	1.036	12
620	0.983	9
533	.948	<1
622	.937	8
444	.897	3
711	.870	<1
640	.862	8
642	.831	16
731	.809	<1

Antimony Lanthanum, LaSb (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti, [8] 1937.

Structural data. Iandelli and Botti [8] in 1937 determined that antimony lanthanum is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(LaSb) per unit cell. The atoms occupy the special positions:

La: 0 0 0
Sb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constant

		Å
1937	Iandelli and Botti [8]	6.488
1963	Kuz'min and Nikitina [32]	6.49

The lattice constant used in this calculated pattern is a=6.488 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.24, 2.29, and 1.451 Å.

The calculated density is 6.339 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.75	<1
200	3.24	100
220	2.29	69
311	1.956	<1
222	1.873	23
400	1.622	10
331	1.488	<1
420	1.451	27
422	1.324	19
440	1.147	6
600	1.081	12
620	1.026	8
622	0.978	8
444	.936	2
640	.900	7
642	.867	13
800	.811	2
820	.787	16

Antimony Neodymium, NdSb (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti, [9] 1937.

Structural data. Iandelli and Botti [9] in 1937 determined that antimony neodymium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(NdSb) per unit cell. The atoms occupy the special positions:

Nd: 0 0 0
Sb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1937	Iandelli and Botti [9]	6. 322
1963	Kuz'min and Nikitina [32]	6. 32

The lattice constant used in this calculated pattern is a=6.322 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.16, 2.24, and 1.414 Å.

The calculated density is 6.992 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 65	1
200	3. 16	100
220	2. 24	69
311	1. 906	<1
222	1. 825	23
400	1. 580	10
331	1. 450	<1
420	1. 414	26
422	1. 290	19
511	1. 217	<1
440	1. 118	6
531	1. 069	<1
600	1. 054	12
620	1. 000	9
533	0. 964	<1
622	. 953	8
444	. 912	3
711	. 885	<1
640	. 877	7
642	. 845	15
731	. 823	<1
800	. 790	2

Antimony Praseodymium, PrSb (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [8] 1937.

Structural data. Iandelli and Botti [8] in 1937 determined that antimony praseodymium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(PrSb) per unit cell. The atoms occupy the special positions:

Pr: 0 0 0
Sb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1937	Iandelli and Botti [8]	6. 366
1963	Kuz'min and Nikitina [32]	6. 37

The lattice constant used in this calculated pattern is a=6.366 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.18, 2.25, and 1.423 Å.

The calculated density is 6.762 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 68	1
200	3. 18	100
220	2. 25	69
311	1. 919	<1
222	1. 838	23
400	1. 592	10
331	1. 460	<1
420	1. 423	26
422	1. 299	19
511	1. 225	<1
440	1. 125	6
531	1. 076	<1
600	1. 061	12
620	1. 007	9
533	0. 971	<1
622	. 960	8
444	. 919	3
711	. 891	<1
640	. 883	7
642	. 851	14
731	. 829	<1
800	. 796	2

Antimony Scandium, SbSc (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that antimony scandium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(SbSc) per unit cell. The atoms occupy the special positions:

Sb: 0 0 0
Sc: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=5.859 Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 2.93, 2.07, and 3.38 Å.

The density of antimony scandium calculated from the constant of Brixner is 5.505 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 38	39
200	2. 93	100
220	2. 07	65
311	1. 767	16
222	1. 691	21
400	1. 465	9
331	1. 344	6
420	1. 310	23
422	1. 196	16
511	1. 128	4
440	1. 036	5
531	0. 990	5
600	. 976	12
620	. 926	9
533	. 893	2
622	. 883	8
444	. 846	3
711	. 820	4
640	. 812	9
642	. 783	21

Antimony Thorium, SbTh (cubic)

Calculated Pattern

Ferro [22] in 1956 determined that antimony thorium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(SbTh) per unit cell. The atoms occupy the special positions:

Sb: 0 0 0
Th: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Ferro [22] reports the lattice constant a=6.318 Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.16, 2.23, and 1.413 Å.

The density of antimony thorium calculated from the constant of Ferro is 9.317 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 65	16
200	3. 16	100
220	2. 23	69
311	1. 905	7
222	1. 824	23
400	1. 580	10
331	1. 449	3
420	1. 413	27
422	1. 290	20
511	1. 216	2
440	1. 117	6
531	1. 068	2
600	1. 053	13
620	0. 999	9
533	. 963	<1
622	. 952	9
444	. 912	3
711	. 885	2
640	. 876	8
642	. 844	16
731	. 823	3
800	. 790	2

Antimony Thulium, SbTm (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that antimony thulium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(SbTm) per unit cell. The atoms occupy the special positions:

Sb: 0 0 0
Tm: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

Brixner [30] reports the lattice constant a=6.083 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.04, 2.15, and 1.360 Å.

The density of antimony thulium calculated from the constant of Brixner is 8.577 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.51	5
200	3.04	100
220	2.15	68
311	1.834	2
222	1.756	22
400	1.521	10
331	1.396	<1
420	1.360	26
422	1.242	18
511	1.171	<1
440	1.075	6
531	1.028	<1
600	1.014	13
620	0.962	9
533	.928	<1
622	.917	9
444	.878	3
711	.852	<1
640	.844	9
642	.813	17
731	.792	<1

Antimony Ytterbium, SbYb (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that antimony ytterbium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(SbYb) per unit cell. The atoms occupy the special positions:

Sb: 0 0 0
Yb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=5.922 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.96, 2.09, and 1.324 Å.

The density of antimony ytterbium calculated from the constant of Brixner is 9.427 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.42	6
200	2.96	100
220	2.09	68
311	1.786	2
222	1.710	22
400	1.480	10
331	1.359	<1
420	1.324	26
422	1.209	19
511	1.140	<1
440	1.047	6
531	1.001	<1
600	0.987	13
620	.936	10
533	.903	<1
622	.893	9
444	.855	3
711	.829	<1
640	.821	9
642	.791	21

Antimony Yttrium, SbY (cubic)

Calculated Pattern

Domange, Flahaut, Guittard and Loriers [27] in 1958 determined that antimony yttrium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(SbY) per unit cell. The atoms occupy the special positions:

Sb: 0 0 0
Y: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=6.163 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.08, 2.18, and 1.378 Å.

The density of antimony yttrium calculated from the constant of Brixner is 5.977 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 56	4
200	3. 08	100
220	2. 18	67
311	1. 858	2
222	1. 779	2
400	1. 541	10
331	1. 414	<1
420	1. 378	25
422	1. 258	18
511	1. 186	<1
440	1. 089	5
531	1. 042	<1
600	1. 027	12
620	0. 974	8
553	. 940	<1
622	. 929	8
444	. 890	2
711	. 863	<1
640	. 855	8
642	. 824	15
731	. 802	<1

Bismuth Cerium, BiCe (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti, [10] 1937.

Structural data. Iandelli and Botti [10] in 1937 determined that bismuth cerium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(BiCe) per unit cell. The atoms occupy the special positions:

Bi: 0 0 0
Ce: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

The lattice constant used in this calculated pattern is a=6.500 Å, as reported by Iandelli and Botti [10].

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.25, 2.30, and 1.453 Å.

The calculated density is 8.443 g/cm^2.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 75	7
200	3. 25	100
220	2. 30	71
311	1. 960	3
222	1. 876	24
400	1. 625	11
331	1. 491	1
420	1. 453	28
422	1. 327	20
511	1. 251	<1
440	1. 149	6
531	1. 099	<1
600	1. 083	13
620	1. 028	9
533	0. 991	<1
622	. 980	8
444	. 938	3
711	. 910	<1
640	. 901	7
642	. 869	15
731	. 846	1
800	. 812	2
733	. 794	<1
820	. 788	17

Bismuth Dysprosium, BiDy (cubic)

Calculated Pattern

Structural data. Kuz'min and Nikitina [32] in 1963 determined that bismuth dysprosium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(BiDy) per unit cell. The atoms occupy the special positions:

Bi: 0 0 0
Dy: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

The lattice constant used in this calculated pattern is a=6.20 Å, as reported by Kuz'min and Nikitina [32].

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.10, 2.19, and 1.39 Å.

The calculated density is 10.35 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.58	3
200	3.10	100
220	2.19	70
311	1.87	1
222	1.79	23
400	1.55	10
331	1.42	<1
420	1.39	28
422	1.27	20
511	1.19	<1
440	1.10	6
531	1.05	<1
600	1.03	13
620	0.980	10
533	.945	<1
622	.935	9
444	.895	3
711	.868	<1
640	.860	8
642	.829	17
731	.807	<1

Bismuth Erbium, BiEr (cubic)

Calculated Pattern

Structural data. Kuz'min and Nikitina [32] in 1963 determined that bismuth erbium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(BiEr) per unit cell. The atoms occupy the special positions:

Bi: 0 0 0
Er: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

The lattice constant used in this calculated pattern is a=6.22 Å, as reported by Kuz'min and Nikitina [32].

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.11, 2.20, and 1.39 Å.

The calculated density is 10.38 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.59	2
200	3.11	100
220	2.20	70
311	1.88	1
222	1.80	23
400	1.56	10
331	1.43	<1
420	1.39	28
422	1.27	20
511	1.20	<1
440	1.10	6
531	1.05	<1
600	1.04	13
620	0.983	10
533	.949	<1
622	.938	9
444	.898	3
711	.871	<1
640	.863	9
642	.831	18
731	.810	<1

Bismuth Holmium, BiHo (cubic)

Calculated Pattern

Additional published pattern. Bruzzone [31] 1961.

Structural data. Bruzzone [31] in 1961 determined that bismuth holmium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(BiHo) per unit cell. The atoms occupy the special positions:

Bi: 0 0 0
Ho: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1961	Bruzzone [31]	6.228
1963	Kuz'min and Nikitina [32]	6.23

The lattice constant used in this calculated pattern is a=6.228 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.11, 2.20, and 1.393 Å.

The calculated density is 10.280 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.60	2
200	3.11	100
220	2.20	70
311	1.878	1
222	1.798	24
400	1.557	10
331	1.429	<1
420	1.393	28
422	1.271	20
511	1.199	<1
440	1.101	6
531	1.053	<1
600	1.038	13
620	0.985	10
533	.950	<1
622	.939	9
444	.899	3
711	.872	<1
640	.864	8
642	.832	17
731	.811	<1

Bismuth Lanthanum, BiLa (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [10] 1937.

Structural data. Iandelli and Botti [10] in 1937 determined that bismuth lanthanum is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(BiLa) per unit cell. The atoms occupy the special positions:

Bi: 0 0 0
La: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1937	Iandelli and Botti [10]	6.578
1963	Kuz'min and Nikitina [32]	6.58

The lattice constant used in this calculated pattern is a=6.578 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.29, 2.33, and 1.471 Å.

The calculated density is 8.118 g/cm^2.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.80	7
200	3.29	100
220	2.33	72
311	1.983	3
222	1.899	24
400	1.644	11
331	1.509	1
420	1.471	29
422	1.343	21
511	1.266	1
440	1.163	6
531	1.112	1
600	1.096	13
620	1.040	9
533	1.003	<1
622	0.992	8
444	.949	3
711	.921	<1
640	.912	7
642	.879	14
731	.856	1
800	.822	2
733	.804	<1
820	.798	16

Bismuth Neodymium, BiNd (cubic)

Calculated Pattern

Structural data. Iandelli [23] in 1956 determined that bismuth neodymium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(BiNd) per unit cell. The atoms occupy the special positions:

Bi: 0 0 0
Nd: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1956	Iandelli [23]	6. 424
1963	Kuz'min and Nikitina [32]	6. 42

The lattice constant used in this calculated pattern is a=6.424 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.21, 2.27, and 1.436 Å.

The calculated density is 8.849 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 71	6
200	3. 21	100
220	2. 27	70
311	1. 937	3
222	1. 854	24
400	1. 606	11
331	1. 474	1
420	1. 436	28
422	1. 311	20
511	1. 236	<1
440	1. 136	6
531	1. 086	<1
600	1. 071	13
620	1. 016	9
533	0. 980	<1
622	. 968	8
444	. 927	3
711	. 900	<1
640	. 891	8
642	. 858	15
731	. 836	<1
800	. 803	2
733	. 785	<1

Bismuth Praseodymium, BiPr (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [10] 1937.

Structural data. Iandelli and Botti [10] in 1937 determined that bismuth praseodymium is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(BiPr) per unit cell. The atoms occupy the special positions:

Bi: 0 0 0
Pr: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1937	Iandelli and Botti [10]	6. 461
1963	Kuz'min and Nikitina [32]	6. 46

The lattice constant used in this calculated pattern is a=6.461 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.23, 2.28, and 1.445 Å.

The calculated density is 8.616 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 73	6
200	3. 23	100
220	2. 28	71
311	1. 948	3
222	1. 865	24
400	1. 615	11
331	1. 482	1
420	1. 445	28
422	1. 319	20
511	1. 243	<1
440	1. 142	6
531	1. 092	<1
600	1. 077	13
620	1. 022	9
533	0. 985	<1
622	. 974	8
444	. 933	3
711	. 905	<1
640	. 896	8
642	. 863	15
731	. 841	<1
800	. 808	2
733	. 789	<1
820	. 784	18

Bismuth Telluride, BiTe (cubic)

Calculated Pattern

Semiletov [18] in 1954 determined that bismuth telluride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(BiTe) per unit cell. The atoms occupy the special positions:

Bi: 0 0 0
Te: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Semiletov [18] reports the lattice constant a=6.47 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.24, 2.29, and 1.45 Å.

The density of bismuth telluride calculated from the constant of Semiletov is 8.25 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 74	11
200	3. 24	100
220	2. 29	70
311	1. 95	5
222	1. 87	24
400	1. 62	11
331	1. 48	2
420	1. 45	28
422	1. 32	20
511	1. 25	1
440	1. 14	6
531	1. 10	2
600	1. 08	13
620	1. 02	9
533	0. 987	<1
622	. 975	8
444	. 934	3
711	. 906	1
640	. 897	7
642	. 865	15
731	. 842	2
800	. 809	2
733	. 790	<1
820	. 785	17

Calcium Telluride, CaTe (cubic)

Calculated Pattern

Additional published pattern. Oftedal [2] 1927.

Structural data. Oftedal [2] in 1927 determined that calcium telluride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(CaTe) per unit cell. The atoms occupy the special positions:

Ca: 0 0 0
Te: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1927	Oftedal [2]	6. 358
1939	Senff and Klemm [12]	6. 354

The lattice constant used in this calculated pattern is the average value a=6.356 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.18, 2.25, and 3.67 Å.

The calculated density is 4.337 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 67	46
200	3. 18	100
220	2. 25	68
311	1. 917	20
222	1. 835	22
400	1. 590	10
331	1. 459	7
420	1. 422	25
422	1. 298	17
511	1. 224	5
440	1. 124	5
531	1. 075	5
600	1. 060	11
620	1. 005	8
533	0. 970	2
622	. 958	7
444	. 918	2
711	. 890	4
640	. 882	7
642	. 850	13
731	. 828	6
800	. 795	2

Cerium Arsenide, CeAs (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [8] 1937.

Structural data. Iandelli and Botti [8] in 1937 determined that cerium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(CeAs) per unit cell. The atoms occupy the special positions:

Ce: 0 0 0
As: ½ ½ ½.

The lattice constant used in this calculated pattern is a=6.072 Å, as reported by Iandelli and Botti [8].

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.04, 2.15, and 1.358 Å.

The calculated density is 6.380 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.51	17
200	3.04	100
220	2.15	67
311	1.831	7
222	1.753	22
400	1.518	9
331	1.393	3
420	1.358	25
422	1.239	17
511	1.169	2
440	1.073	6
531	1.026	2
600	1.012	12
620	0.960	9
533	.926	<1
622	.915	8
444	.876	3
711	.850	2
640	.842	8
642	.811	16
731	.791	3

Cerium Nitride, CeN (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [7] 1937.

Structural data. Iandelli and Botti [7] in 1937 determined that cerium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(CeN) per unit cell. The atoms occupy the special positions:

Ce: 0 0 0
N: ½ ½ ½.

The lattice constant used in this calculated pattern is a=5.021 Å, as reported by Iandelli and Botti [7].

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.90, 2.51, and 1.775 Å.

The calculated density is 8.087 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2.90	100
200	2.51	72
220	1.775	44
311	1.514	35
222	1.449	13
400	1.255	6
331	1.152	13
420	1.123	16
422	1.025	12
511	0.966	11
440	.888	5
531	.849	16
600	.837	13
620	.794	11

Cerium Phosphide, CeP (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [6] 1937.

Structural data. Iandelli and Botti [6] in 1937 determined that cerium phosphide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(CeP) per unit cell. The atoms occupy the special positions:

Ce: 0 0 0
P: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

The lattice constant used in this calculated pattern is $a=5.909$ Å, as reported by Iandelli and Botti [6].

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 2.95, 3.41, and 209 Å.

The calculated density is 5.508 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
111	3. 41	78
200	2. 95	100
220	2. 09	66
311	1. 782	32
222	1. 706	21
400	1. 477	9
331	1. 356	11
420	1. 321	24
422	1. 206	18
511	1. 137	8
440	1. 045	6
531	0. 999	9
600	. 985	13
620	. 934	9
533	. 901	4
622	. 891	9
444	. 853	3
711	. 827	8
640	. 819	9
642	. 790	20

Cobalt Iodide, CoI$_2$ (hexagonal)

Calculated Pattern

Ferrari and Giorgi [4] in 1929 determined that cobalt iodide is isomorphous with cadmium iodide with the space group D_{3d}^3—$P\bar{3}m1$ (No. 164) and 1(CoI$_2$) per unit cell. The atoms occupy the special positions:

Co: 0 0 0
I: $\frac{1}{3}\ \frac{2}{3}\ u;\ \frac{2}{3}\ \frac{1}{3}\ \bar{u}$ with $u=0.25$.

Ferrari and Giorgi [4] report the lattice constants $a=3.97$ Å and $c=6.66$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.06, 2.39 and 1.98 Å.

The density of cobalt iodide calculated from the constants of Ferrari and Giorgi is 5.712 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
001	6. 66	9
100	3. 44	6
002	3. 33	15
101	3. 06	100
102	2. 39	32
003	2. 22	<1
110	1. 98	24
111	1. 90	2
103	1. 86	20
200	1. 72	<1
112	1. 71	10
004, 201	1. 66	17
202	1. 53	6
104	1. 50	<1
113	1. 48	<1
203	1. 36	6
005	1. 33	<1
210	1. 30	<1
114, 211	1. 28	19
105	1. 24	4
212	1. 21	5
204	1. 20	<1
300	1. 15	3
301	1. 13	<1
213	1. 12	6
115, 006	1. 11	<1
302	1. 08	2

Dysprosium Arsenide, DyAs (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that dysprosium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(DyAs) per unit cell. The atoms occupy the special positions:

Dy: $0\ 0\ 0$
As: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

Brixner [30] reports the lattice constant a=5.780 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.89, 2.04, and 3.34 Å.

The density of dysprosium arsenide calculated from the constant of Brixner is 8.166 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.34	25
200	2.89	100
220	2.04	65
311	1.743	10
222	1.669	21
400	1.445	9
331	1.326	4
420	1.292	24
422	1.180	17
511	1.112	3
440	1.022	6
531	0.977	3
600	.963	13
620	.914	10
533	.881	1
622	.871	9
444	.834	3
711	.809	3
640	.802	10

Dysprosium Nitride, DyN (cubic)

Calculated Pattern

Klemm and Winkelmann [24] in 1956 determined that dysprosium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(DyN) per unit cell. The atoms occupy the special positions:

Dy: $0\ 0\ 0$
N: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

Klemm and Winkelmann [24] report the lattice constant a=4.905 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.83, 2.45, and 1.734 Å.

The density of dysprosium nitride calculated from the constant of Klemm and Winkelmann is 9.934 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2.83	100
200	2.45	69
220	1.734	42
311	1.479	36
222	1.416	13
400	1.226	6
331	1.125	13
420	1.097	16
422	1.001	13
511	0.944	12
440	.867	5
531	.829	18
600	.818	14

Dysprosium Telluride, DyTe (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that dysprosium telluride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(DyTe) per unit cell. The atoms occupy the special positions:

Dy: 0 0 0
Te: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=6.092 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.05, 2.15, and 1.362 Å.

The density of dysprosium telluride calculated from the constant of Brixner is 8.522 g/cm^3.

Calculated Pattern
Copper λ

hkl	d	Peak height
		I
	Å	
111	3.52	3
200	3.05	100
220	2.15	68
311	1.837	1
222	1.759	22
400	1.523	10
331	1.398	<1
420	1.362	26
422	1.244	18
511	1.172	<1
440	1.077	6
531	1.030	<1
600	1.015	12
620	0.963	9
533	.929	<1
622	.918	9
444	.879	3
711	.853	<1
640	.845	8
642	.814	18
731	.793	<1

Erbium Arsenide, ErAs (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that erbium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(ErAs) per unit cell. The atoms occupy the special positions:

Er: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=5.732 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.87, 2.03, and 3.31 Å.

The density of erbium arsenide calculated from the constant of Brixner is 8.541 g/cm^3.

Calculated Pattern
Copper λ

hkl	d	Peak height
		I
	Å	
111	3.31	27
200	2.87	100
220	2.03	66
311	1.728	11
222	1.655	21
400	1.433	9
331	1.315	4
420	1.282	24
422	1.170	18
511	1.103	3
440	1.013	6
531	0.969	4
600	.955	13
620	.906	10
533	.874	2
622	.864	10
444	.827	3
711	.803	4
640	.795	11

Erbium Nitride, ErN (cubic)

Calculated Pattern

Klemm and Winkelmann [24] in 1956 determined that erbium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(ErN) per unit cell. The atoms occupy the special positions:

Er: 0 0 0
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Klemm and Winkelmann [24] report the lattice constant a=4.839 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.79, 2.42, and 1.711 Å.

The density of erbium nitride calculated from the constant of Klemm and Winkelmann is 10.63 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2. 79	100
200	2. 42	68
220	1. 711	41
311	1. 459	35
222	1. 397	13
400	1. 210	6
331	1. 110	14
420	1. 082	16
422	0. 988	13
511	. 931	13
440	. 855	6
531	. 818	19
600	. 806	15

Erbium Telluride, ErTe (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that erbium telluride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(ErTe) per unit cell. The atoms occupy the special positions:

Er: 0 0 0
Te: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=6.063 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.03, 2.14, and 1.356 Å.

The density of erbium telluride calculated from the constant of Brixner is 8.787 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 50	4
200	3. 03	100
220	2. 14	68
311	1. 828	2
222	1. 750	23
400	1. 516	10
331	1. 391	<1
420	1. 356	26
422	1. 238	18
511	1. 167	<1
440	1. 072	6
531	1. 025	<1
600	1. 010	13
620	0. 959	9
533	. 925	<1
622	. 914	9
444	. 875	3
711	. 849	<1
640	. 841	8
642	. 810	18
731	. 789	<1

Europium Nitride, EuN (cubic)

Calculated Pattern

Klemm and Winkelmann [24] in 1956 determined that europium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(EuN) per unit cell. The atoms occupy the special positions:

Eu: 0 0 0
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Klemm and Winkelmann [24] report the lattice constant $a=5.014$ Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.89, 2.51, and 1.773 Å.

The density of europium nitride calculated from the constant of Klemm and Winkelmann is 8.745 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2.89	100
200	2.51	69
220	1.773	43
311	1.512	36
222	1.447	33
400	1.254	6
331	1.150	13
420	1.121	16
422	1.023	12
511	0.965	12
440	.886	5
531	.848	16
600	.836	13
620	.793	11

Europium Oxide, EuO (cubic)

Calculated Pattern

Structural data. Eick, Baenziger, and Eyring [21] in 1956 determined that europium oxide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(EuO) per unit cell. Atoms occupy the special positions:

Eu: 0 0 0
O: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

The lattice constant used in this calculated pattern is $a=5.1439$ Å, as reported by Eick, Baenziger, and Eyring [21].

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.970, 2.572, and 1.819 Å.

The calculated density is 8.196 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2.970	100
200	2.572	77
220	1.819	47
311	1.551	37
222	1.485	15
400	1.286	6
331	1.180	14
420	1.150	17
422	1.050	13
511	0.990	12
440	.909	5
531	.869	16
600	.857	12
620	.813	11
533	.784	9

Gadolinium Arsenide, GdAs (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that gadolinium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(GdAs) per unit cell. The atoms occupy the special positions:

Gd: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant $a=5.854$ Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.93, 2.07, and 1.309 Å.

The density of gadolinium arsenide calculated from the constant of Brixner is 7.687 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.38	23
200	2.93	100
220	2.07	66
311	1.765	9
222	1.690	21
400	1.464	9
331	1.343	4
420	1.309	25
422	1.195	17
511	1.127	3
440	1.035	6
531	0.990	3
600	.976	13
620	.926	9
533	.893	1
622	.883	9
444	.845	3
711	.820	3
640	.812	9
642	.782	22

Gadolinium Nitride, GdN (cubic)

Calculated Pattern

Klemm and Winkelmann [24] in 1956 determined that gadolinium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(GdN) per unit cell. The atoms occupy the special positions:

Gd: 0 0 0
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Klemm and Winkelmann [24] report the lattice constant $a=4.999$ Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.89, 2.50, and 1.767 Å.

The density of gadolinium nitride calculated from the constant of Klemm and Winkelmann is 9.105 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2.89	100
200	2.50	69
220	1.767	42
311	1.507	35
222	1.443	13
400	1.250	6
331	1.147	13
420	1.118	16
422	1.020	12
511	0.962	12
440	.884	5
531	.845	16
600	.833	13
620	.790	11

Germanium Iodide, GeI_2 (hexagonal)

Calculated Pattern

Powell and Brewer [11] in 1938 determined that germanium iodide is isomorphous with cadmium iodide with the space group D_{3d}^3—$P\bar{3}m1$ (No. 164) and $1(GeI_2)$ per unit cell. The atoms occupy the special positions:

Ge: 0 0 0
I: $\frac{1}{3}\ \frac{2}{3}\ u;\ \frac{2}{3}\ \frac{1}{3}\ \bar{u}$ with u=0.25.

Powell and Brewer [11] report the lattice constants a=4.14 Å and c=6.80 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.17, 2.47, and 2.07 Å.

The density of germanium iodide calculated from the constants of Powell and Brewer is 5.369 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
001	6.80	12
100	3.59	4
002	3.40	12
101	3.17	100
102	2.47	35
003	2.27	<1
110	2.07	26
111	1.98	2
103	1.92	20
200	1.79	<1
112	1.77	9
201	1.73	14
004	1.70	4
202	1.59	8
104	1.54	<1
113	1.53	<1
203	1.41	6
005, 210	1.36	<1
211	1.33	10
114	1.31	10
105	1.27	4
212	1.26	6
204	1.23	<1
300	1.20	3
301	1.18	<1
213	1.16	6
115	1.14	<1
006, 302	1.13	2
205, 106	1.08	5

Holmium Nitride, HoN (cubic)

Calculated Pattern

Klemm and Winkelmann [24] in 1956 determined that holmium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(HoN) per unit cell. The atoms occupy the special positions:

Ho: 0 0 0
N: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

Klemm and Winkelmann [24] report the lattice constant a=4.874 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.81, 2.44, and 1.723 Å.

The density of holmium nitride calculated from the constant of Klemm and Winkelmann is 10.26 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
111	2.81	100
200	2.44	68
220	1.723	41
311	1.470	35
222	1.407	13
400	1.218	6
331	1.118	14
420	1.090	16
422	0.995	12
511	.938	12
440	.862	5
531	.824	18
600	.812	14

Holmium Selenide, HoSe (cubic)

Calculated Pattern

Additional published pattern. Bruzzone [31] 1961.

Structural data. Bruzzone [31] in 1961 determined that holmium selenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(HoSe) per unit cell. The atoms occupy the special positions:

Ho: 0 0 0
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

The lattice constant used in this calculated pattern is a=5.680 Å, as reported by Bruzzone [31].

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.84, 2.01, and 1.270 Å.

The calculated density is 8.840 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
111	3. 28	23
200	2. 84	100
220	2. 01	66
311	1. 713	9
222	1. 640	21
400	1. 420	9
331	1. 303	3
420	1. 270	25
422	1. 159	18
511	1. 093	3
440	1. 004	6
531	0. 960	3
600	. 947	14
620	. 898	10
533	. 866	1
622	. 856	10
444	. 820	3
711	. 795	3
640	. 788	11

Iron Bromide, FeBr$_2$ (hexagonal)

Calculated Pattern

Ferrari and Giorgi [3] in 1929 determined that iron bromide is isomorphous with cadmium iodide with the space group D_{3d}^3—P$\bar{3}$m1 (No. 164) and 1(FeBr$_2$) per unit cell. The atoms occupy the special positions:

Fe: 0 0 0
Br: $\frac{1}{3}$ $\frac{2}{3}$ u; $\frac{2}{3}$ $\frac{1}{3}$ $\bar{u}$ with u=0.25.

Ferrari and Giorgi [3] report the lattice constants a=3.748 Å and c=6.183 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.87, 2.24, and 1.87 Å.

The density of iron bromide calculated from the constants of Ferrari and Giorgi is 4.761 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
001	6. 18	19
100	3. 25	2
002	3. 09	10
101	2. 87	100
102	2. 24	38
003	2. 06	<1
110	1. 87	25
111	1. 79	3
103	1. 74	18
200	1. 62	<1
112	1. 60	7
201	1. 57	12
004	1. 55	4
202	1. 437	7
104	1. 396	<1
113	1. 387	1
203	1. 275	6
005	1. 237	<1
210	1. 227	<1
211	1. 203	9
114	1. 192	9
105	1. 156	4
212	1. 140	6
204	1. 119	<1
300	1. 082	3

Iron Iodide, FeI_2 (hexagonal)

Calculated Pattern

Ferrari and Giorgi [4] in 1929 determined that iron iodide is isomorphous with cadmium iodide with the space group D_{3d}^3—P$\bar{3}$m1 (No. 164) and 1(FeI_2) per unit cell. The atoms occupy the special positions:

Fe: 0 0 0
I: $\frac{1}{3}\,\frac{2}{3}\,u;\ \frac{2}{3}\,\frac{1}{3}\,\bar{u}$ with $u=0.25$.

Ferrari and Giorgi [4] report the lattice constants $a=4.05$ Å and $c=6.76$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.11, 2.43, and 2.02 Å.

The density of iron iodide calculated from the constants of Ferrari and Giorgi is 5.354 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
001	6.76	8
100	3.51	6
002	3.38	15
101	3.11	100
102	2.43	32
003	2.25	<1
110	2.02	24
111	1.94	1
103	1.90	20
200	1.75	<1
112	1.74	11
201	1.70	14
004	1.69	4
202	1.56	6
104	1.52	<1
113	1.51	<1
203	1.38	6
210	1.33	<1
211, 114	1.30	19
105	1.26	4
212	1.23	5
204	1.22	<1
300	1.17	3
301	1.15	<1
213	1.14	6
006	1.13	<1
115	1.12	<1
302	1.10	2

Lanthanum Arsenide, LaAs (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [8] 1937.

Structural data. Iandelli and Botti [8] in 1937 determined that lanthanum arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(LaAs) per unit cell. The atoms occupy the special positions:

La: 0 0 0
As: $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$.

The lattice constant used in this calculated pattern is $a=6.137$ Å, as reported by Iandelli and Botti [8].

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.07, 2.17, and 1.372 Å.

The calculated density is 6.144 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.54	15
200	3.07	100
220	2.17	67
311	1.850	7
222	1.772	22
400	1.534	10
331	1.408	3
420	1.372	25
422	1.253	18
511	1.181	2
440	1.085	5
531	1.037	2
600	1.023	12
620	0.970	9
533	.936	<1
622	.925	8
444	.886	3
711	.859	2
640	.851	8
642	.820	16
731	.799	3

Lanthanum Nitride, LaN (cubic)

Calculated Pattern

Additional published patterns. Iandelli and Botti [7] 1937, and Young and Ziegler [15] 1952.

Structural data. Iandelli and Botti [7] in 1937 determined that lanthanum nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(LaN) per unit cell. The atoms occupy the special positions:

La: 0 0 0
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1937	Iandelli and Botti [7]	5.286
1952	Young and Ziegler [15]	5.295
1956	Klemm and Winkelmann [24]	5.30
1963	Lyutaya and Samsonov [33]	5.302

The lattice constant used in this calculated pattern is the average value $a = 5.30$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.06, 2.65, and 1.87 Å.

The calculated density is 6.822 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.06	100
200	2.65	74
220	1.87	46
311	1.60	37
222	1.53	14
400	1.32	6
331	1.22	14
420	1.19	16
422	1.08	12
511	1.02	11
440	0.937	5
531	.896	14
600	.883	11
620	.838	9
533	.808	7
622	.799	10

Lanthanum Selenide, LaSe (cubic)

Calculated Pattern

Structural data. Iandelli [20] in 1955 determined that lanthanum selenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(LaSe) per unit cell. The atoms occupy the special positions:

La: 0 0 0
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1955	Iandelli [20]	6.063
1959	Guittard and Benacerraf [28]	6.060

The lattice constant used in this calculated pattern is the average value $a = 6.062$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.03, 2.14, and 1.356 Å.

The calculated density is 6.496 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.50	14
200	3.03	100
220	2.14	68
311	1.828	6
222	1.750	22
400	1.516	10
331	1.391	2
420	1.356	25
422	1.238	18
511	1.167	1
440	1.072	6
531	1.025	2
600	1.010	12
620	0.959	9
533	.925	<1
622	.914	8
444	.875	3
711	.849	1
640	.841	8
642	.810	17
731	.789	2

Lutetium Nitride, LuN (cubic)

Calculated Pattern

Klemm and Winkelmann [24] in 1956 determined that lutetium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4 (LuN) per unit cell. The atoms occupy the special positions:

Lu: 0 0 0
N: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

Klemm and Winkelmann [24] report the lattice constant a=4.766 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.75, 2.38, and 1.685 Å.

The density of lutetium nitride calculated from the constant of Klemm and Winkelmann is 11.59 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2. 75	100
200	2. 38	67
220	1. 685	40
311	1. 437	35
222	1. 376	12
400	1. 192	5
331	1. 093	14
420	1. 066	16
422	0. 973	13
511	. 917	13
440	. 843	6
531	. 806	20
600	. 794	16

Magnesium Bromide, $MgBr_2$ (hexagonal)

Calculated Pattern

Ferrari and Giorgi [3] in 1929 determined that magnesium bromide is isomorphous with cadmium iodide with the space group D_{3d}^3—P$\bar{3}$m1 (No. 164) and 1($MgBr_2$) per unit cell. The atoms occupy the special positions:

Mg: 0 0 0
Br: $\frac{1}{3}\ \frac{2}{3}\ u$; $\frac{2}{3}\ \frac{1}{3}\ \bar{u}$ with u=0.25.

Ferrari and Giorgi [3] report the lattice constants a=3.822 Å and c=6.269 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.93, 2.28, and 1.91 Å.

The density of magnesium bromide calculated from the constants of Ferrari and Giorgi is 3.855 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
001	6. 27	4
100	3. 31	11
002	3. 13	19
101	2. 93	100
102	2. 28	25
003	2. 09	<1
110	1. 91	21
111	1. 83	<1
103	1. 77	18
200	1. 65	1
112	1. 63	12
201	1. 60	13
004	1. 57	3
202	1. 464	5
104	1. 416	1
113	1. 410	<1
203	1. 297	6
210	1. 251	<1
211	1. 227	9
114	1. 212	8
105	1. 172	4
212	1. 162	4
204	1. 138	<1
300	1. 103	3

Manganese Bromide, $MnBr_2$ (hexagonal)

Calculated Pattern

Ferrari and Giorgi [3] in 1929 determined that manganese bromide is isomorphous with cadmium iodide with the space group D_{3d}^3—$P\bar{3}m1$ (No. 164) and 1($MnBr_2$) per unit cell. The atoms occupy the special positions:

Mn: 0 0 0
Br: $\frac{1}{3}\ \frac{2}{3}\ u;\ \frac{2}{3}\ \frac{1}{3}\ \bar{u}$ with $u=0.25$.

Ferrari and Giorgi [3] report the lattice constants $a=3.828$ Å and $c=6.200$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 2.92, 2.26, and 1.91 Å.

The density of manganese bromide calculated from the constants of Ferrari and Giorgi is 4.532 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
001	6.20	17
100	3.32	2
002	3.10	10
101	2.92	100
102	2.26	36
003	2.07	<1
110	1.91	26
111	1.83	3
103	1.75	18
200	1.66	<1
112	1.63	7
201	1.60	13
004	1.55	4
202	1.462	7
113, 104	1.404	1
203	1.293	6
210	1.253	<1
005	1.240	<1
211	1.228	9
114	1.205	9
212, 105	1.162	9
204	1.132	<1
300	1.105	3
301	1.088	<1

Manganese Iodide, MnI_2 (hexagonal)

Calculated Pattern

Ferrari and Giorgi [4] in 1929 determined that manganese iodide is isomorphous with cadmium iodide with the space group D_{3d}^3—$P\bar{3}m1$ (No. 164) and 1(MnI_2) per unit cell. The atoms occupy the special positions:

Mn: 0 0 0
I: $\frac{1}{3}\ \frac{2}{3}\ u;\ \frac{2}{3}\ \frac{1}{3}\ \bar{u}$ with $u=0.25$.

Ferrari and Giorgi [4] report the lattice constants $a=4.17$ Å and $c=6.83$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.19, 2.48, and 2.08 Å.

The density of magnanese iodide calculated from the constants of Ferrari and Giorgi is 4.984 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
001	6.83	7
100	3.61	7
002	3.42	15
101	3.19	100
102	2.48	30
003	2.28	<1
110	2.08	25
111	1.99	1
103	1.93	20
200	1.81	<1
112	1.78	12
201	1.75	14
004	1.71	4
202	1.60	6
104, 113	1.54	1
203	1.41	6
005, 210	1.36	<1
211	1.34	10
114	1.32	9
105	1.28	4
212	1.27	5
204	1.24	<1
300	1.20	3
301	1.19	<1
213	1.17	6
115, 006, 302	1.14	2
106, 205	1.09	3

Neodymium Arsenide, NdAs (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [9] 1937.

Structural data. Iandelli and Botti [9] in 1937 determined that neodymium arsenide is isomorphous with sodium chloride, with the space group O_h^5—Fm3m (No. 225) and 4(NdAs) per unit cell. The atoms occupy the special positions:

Nd: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

The lattice constant used in this calculated pattern is a=5.970 Å, as reported by Iandelli and Botti [9].

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.98, 2.11, and 1.335 Å.

The calculated density is 6.841 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
111	3.45	19
200	2.98	100
220	2.11	67
311	1.800	8
222	1.723	22
400	1.492	10
331	1.370	3
420	1.335	24
422	1.219	18
511	1.149	2
440	1.055	6
531	1.009	2
600	0.995	12
620	.944	9
533	.910	1
622	.900	8
444	.862	3
711	.836	2
640	.828	9
642	.798	18

Neptunium Nitride, NpN (cubic)

Calculated Pattern

Zachariasen [14] in 1949 determined that neptunium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(NpN) per unit cell. The atoms occupy the special positions:

Np: 0 0 0
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Zachariasen [14] reports the lattice constant a=4.897 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.83, 2.45, and 1.731 Å.

The density of neptunium nitride calculated from the constant of Zachariasen is 14.20 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
111	2.83	100
200	2.45	62
220	1.731	39
311	1.476	36
222	1.414	12
400	1.224	5
331	1.123	14
420	1.095	15
422	1.000	12
511	0.942	13
440	.866	5
531	.828	19
600	.816	14

Plutonium Arsenide, PuAs (cubic)

Calculated Pattern

Gorum [26] in 1957 determined that plutonium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(PuAs) per unit cell. The atoms occupy the special positions:

Pu: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Gorum [26] reports the lattice constant a=5.855 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.93, 2.07, and 3.38 Å.

The density of plutonium arsenide calculated from the constant of Gorum is 10.487 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 38	50
200	2. 93	100
220	2. 07	68
311	1. 765	21
222	1. 690	23
400	1. 464	10
331	1. 343	8
420	1. 309	26
422	1. 195	19
511	1. 127	6
440	1. 035	6
531	0. 990	7
600	. 976	14
620	. 926	10
533	. 893	3
622	. 883	10
444	. 845	3
711	. 820	6
640	. 812	10
642	. 782	24

Plutonium Phosphide, PuP (cubic)

Calculated Pattern

Gorum [26] in 1957 determined that plutonium phosphide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(PuP) per unit cell. The atoms occupy the special positions:

Pu: 0 0 0
P: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Gorum [26] reports the lattice constant a=5.644 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.26, 2.82, and 1.995 Å.

The density of plutonium phosphide calculated from the constant of Gorum is 10.08 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 26	100
200	2. 82	86
220	1. 995	58
311	1. 702	41
222	1. 629	19
400	1. 411	8
331	1. 295	15
420	1. 262	22
422	1. 152	16
511	1. 086	11
440	0. 998	6
531	. 954	13
600	. 941	13
620	. 892	10
533	. 861	6
622	. 851	10
444	. 815	3
711	. 790	14
640	. 783	12

Plutonium Telluride, PuTe (cubic)

Calculated Pattern

Gorum [26] in 1957 determined that plutonium telluride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(PuTe) per unit cell. The atoms occupy the special positions:

Pu: 0 0 0
Te: ½ ½ ½.

Gorum [26] reports the lattice constant a=6.183 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.09, 2.19, and 1.383 Å.

The density of plutonium telluride calculated from the constant of Gorum is 10.385 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.57	18
200	3.09	100
220	2.19	70
311	1.864	8
222	1.785	23
400	1.546	10
331	1.418	3
420	1.383	28
422	1.262	20
511	1.190	2
440	1.093	6
531	1.045	2
600	1.030	13
620	0.978	10
533	.943	1
622	.932	9
444	.892	3
711	.866	2
640	.857	9
642	.826	18
731	.805	3

Potassium Hydroxide, KOH, at 300 °C (cubic)

Calculated Pattern

Structural data. Teichert and Klemm [13] in 1939 determined that potassium hydroxide at 300 °C is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(KOH) per unit cell. The atoms occupy the special positions:

K: 0 0 0
O: ½ ½ ½
H: undefined.

The lattice constant used in this calculated pattern is a=5.79 Å, as reported by Teichert and Klemm [13].

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.90, 2.05, and 3.34 Å.

The calculated density is 1.920 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.34	25
200	2.90	100
220	2.05	56
311	1.75	10
222	1.67	16
400	1.45	6
331	1.33	4
420	1.29	15
422	1.18	10
511	1.11	3
440	1.02	3
531	0.979	3
600	.965	7
620	.915	5
533	.883	2
622	.873	5
444	.836	2
711	.811	4
640	.803	6

Praseodymium Arsenide, PrAs (cubic)

Calculated Pattern

Additional published pattern. Iandelli and Botti [8] 1937.

Structural data. Iandelli and Botti [8] in 1937 determined that praseodymium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(PrAs) per unit cell. The atoms occupy the special positions:

Pr: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

The lattice constant used in this calculated pattern is a=6.009 Å, as reported by Iandelli and Botti [8].

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.00, 2.12, and 1.344 Å.

The calculated density is 6.607 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 47	18
200	3. 00	100
220	2. 12	67
311	1. 812	8
222	1. 735	22
400	1. 502	10
331	1. 379	3
420	1. 344	25
422	1. 227	18
511	1. 156	2
440	1. 062	6
531	1. 016	2
600	1. 002	12
620	0. 950	9
533	. 916	1
622	. 906	8
444	. 867	3
711	. 841	2
640	. 833	8
642	. 803	18
731	. 782	4

Praseodymium Sulfide, PrS (cubic)

Calculated Pattern

Structural data. Iandelli [20] in 1955 determined that praseodymium sulfide is isomorphous with sodium chloride, with the space group O_h^5—Fm3m (No. 225) and 4(PrS) per unit cell. The atoms occupy the special positions:

Pr: 0 0 0
S: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Lattice constants

		Å
1955	Iandelli [20]	5. 739
1956	Picon and Patrie [25]	5. 747

The lattice constant used in this calculated pattern is the average value a=5.743 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.87, 3.31, and 2.03 Å.

The calculated density is 6.065 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 31	75
200	2. 87	100
220	2. 03	65
311	1. 730	30
222	1. 657	21
400	1. 435	9
331	1. 317	11
420	1. 283	24
422	1. 171	17
511	1. 104	8
440	1. 015	6
531	0. 970	9
600	. 956	13
620	. 907	10
533	. 875	4
622	. 865	10
444	. 828	3
711	. 804	9
640	. 796	11

Samarium Arsenide, SmAs (cubic)

Calculated Pattern

Iandelli [23] in 1956 determined that samarium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(SmAs) per unit cell. The atoms occupy the special positions:

Sm: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Iandelli [23] reports the lattice constant $a=5.921$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 2.96, 2.09, and 1.324 Å.

The density of samarium arsenide calculated from the constant of Iandelli is 7.208 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.42	21
200	2.96	100
220	2.09	67
311	1.785	9
222	1.709	22
400	1.480	9
331	1.358	3
420	1.324	25
422	1.209	18
511	1.140	2
440	1.047	6
531	1.001	3
600	0.987	13
620	.936	9
533	.903	1
622	.893	9
444	.855	3
711	.829	2
640	.821	9
642	.791	19

Scandium Arsenide, ScAs (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that scandium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(ScAs) per unit cell. The atoms occupy the special positions:

Sc: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant $a=5.487$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 2.74, 1.940, and 1.227 Å.

The density of scandium arsenide calculated from the constant of Brixner is 4.820 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.17	12
200	2.74	100
220	1.940	62
311	1.654	4
222	1.584	19
400	1.372	8
331	1.259	2
420	1.227	21
422	1.120	15
511	1.056	1
440	0.970	5
531	.927	1
600	.914	12
620	.868	9
533	.837	<1
622	.827	9
444	.792	3

Sodium Hydroxide, NaOH at 300 °C (cubic)

Calculated Pattern

Structural data. West [5] in 1935 determined that sodium hydroxide at 300 °C is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) with 4(NaOH) per unit cell. The atoms occupy the special positions:

Na: 0 0 0
O: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$
H: undefined.

The lattice constant used in this calculated pattern is a=5.01 Å, as reported by West [5].

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.50, 1.77, and 1.45 Å.

The calculated density is 2.112 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
111	2.89	1
200	2.50	100
220	1.77	52
311	1.51	3
222	1.45	14
400	1.25	5
331	1.15	1
420	1.12	12
422	1.02	9
511	0.964	<1
440	.886	3
531	.847	<1
600	.835	7
620	.792	6

Strontium Telluride, SrTe (cubic)

Calculated Pattern

Goldschmidt [1] in 1926 determined that strontium telluride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(SrTe) per unit cell. The atoms occupy the special positions:

Sr: 0 0 0
Te: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Goldschmidt [1] reports the lattice constant a=6.660 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.33, 2.35, and 1.489 Å.

The density of strontium telluride calculated from the constant of Goldschmidt is 4.839 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
111	3.85	5
200	3.33	100
220	2.35	69
311	2.01	2
222	1.923	23
400	1.665	10
331	1.528	<1
420	1.489	27
422	1.359	19
511	1.282	<1
440	1.177	6
531	1.126	<1
600	1.110	11
620	1.053	8
533	1.016	<1
622	1.004	7
444	0.961	2
711	.933	<1
640	.924	6
642	.890	12
731	.867	<1
800	.832	2
733	.814	<1
820	.808	13
822	.785	10

Terbium Nitride, TbN (cubic)

Calculated Pattern

Klemm and Winkelmann [24] in 1956 determined that terbium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(TbN) per unit cell. The atoms occupy the special positions:

Tb: $0\ 0\ 0$
N: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

Klemm and Winkelmann [24] report the lattice constant a=4.933 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.85, 2.47, and 1.744 Å.

The density of terbium nitride calculated from the constant of Klemm and Winkelmann is 9.568 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2.85	100
200	2.47	69
220	1.744	42
311	1.487	36
222	1.424	13
400	1.233	6
331	1.132	14
420	1.103	16
422	1.007	12
511	0.949	12
440	.872	5
531	.834	17
600	.822	13

Thorium Arsenide, ThAs (cubic)

Calculated Pattern

Ferro [19] in 1955 determined that thorium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(ThAs) per unit cell. The atoms occupy the special positions:

Th: $0\ 0\ 0$
As: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

Ferro [19] reports the lattice constant a=5.972 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.99, 2.11, and 3.45 Å.

The density of thorium arsenide calculated from the constant of Ferro is 9.572 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.45	47
200	2.99	100
220	2.11	68
311	1.801	20
222	1.724	23
400	1.493	10
331	1.370	8
420	1.335	26
422	1.219	19
511	1.149	6
440	1.056	6
531	1.009	6
600	0.995	13
620	.944	10
533	.911	3
622	.900	10
444	.862	3
711	.836	5
640	.828	10
642	.798	20

Thulium Arsenide, TmAs (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that thulium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(TmAs) per unit cell. The atoms occupy the special positions:

Tm: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=5.711 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.86, 2.02, and 3.30 Å.

The density of thulium arsenide calculated from the constant of Brixner is 8.695 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.30	27
200	2.86	100
220	2.02	65
311	1.722	11
222	1.649	21
400	1.428	9
331	1.310	4
420	1.277	24
422	1.166	17
511	1.099	3
440	1.010	6
531	0.965	4
600	.952	13
620	.903	10
533	.871	2
622	.861	10
444	.824	3
711	.800	4
640	.792	11

Thulium Nitride, TmN (cubic)

Calculated Pattern

Klemm and Winkelmann [24] in 1956 determined that thulium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(TmN) per unit cell. The atoms occupy the special positions:

Tm: 0 0 0
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Klemm and Winkelmann [24] report the lattice constant a=4.809 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.78, 2.40, and 1.700 Å.

The density of thulium nitride calculated from the constant of Klemm and Winkelmann is 10.93 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2.78	100
200	2.40	67
220	1.700	40
311	1.450	35
222	1.388	12
400	1.202	5
331	1.103	14
420	1.075	16
422	0.982	13
511	.925	13
440	.850	6
531	.813	19
600	.802	15

Thulium Telluride, TmTe (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that thulium telluride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(TmTe) per unit cell. The atoms occupy the special positions:

Tm: 0 0 0
Te: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

Brixner [30] reports the lattice constant $a=6.042$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.02, 2.14, and 1.351 Å.

The density of thulium telluride calculated from the constant of Brixner is 8.929 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 49	4
200	3. 02	100
220	2. 14	67
311	1. 822	2
222	1. 744	22
400	1. 510	10
331	1. 386	<1
420	1. 351	26
422	1. 233	18
511	1. 163	<1
440	1. 068	6
531	1. 021	<1
600	1. 007	13
620	0. 955	9
533	. 921	<1
622	. 911	9
444	. 872	3
711	. 846	<1
640	. 838	9
642	. 807	18
731	. 787	<1

Titanium Sulfide, TiS_2 (hexagonal)

Calculated Pattern

Jeannin and Bénard [29] in 1959 determined that titanium sulfide is isomorphous with cadmium iodide with the space group D_{3d}^3—P$\bar{3}$m1 (No. 164) and 1(TiS_2) per unit cell. The atoms occupy the special positions:

Ti: 0 0 0
S: $\frac{1}{3}\ \frac{2}{3}\ u$; $\frac{2}{3}\ \frac{1}{3}\ \bar{u}$ with $u=0.25$.

Jeannin and Bénard [29] report the lattice constants $a=3.4049$ Å and $c=5.6912$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 2.62, 5.69, and 2.05 Å.

The density of titanium sulfide calculated from the constants of Jeannin and Bénard is 3.255 g/cm³.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
001	5. 69	55
100	2. 95	2
002	2. 85	2
101	2. 62	100
102	2. 05	47
003	1. 90	2
110	1. 70	23
111	1. 63	7
103	1. 60	15
200	1. 474	<1
112	1. 461	<1
201	1. 427	9
004	1. 423	4
202	1. 309	8
104	1. 281	<1
113	1. 267	2
203	1. 164	5
005	1. 138	<1
210	1. 114	<1
211	1. 094	7
114	1. 092	9

Uranium Telluride, UTe (cubic)

Calculated Pattern

Ferro [16] in 1954 determined that uranium telluride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(UTe) per unit cell. The atoms occupy the special positions:

U: 0 0 0
Te: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Ferro [16] reports the lattice constant a=6.163 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 3.08, 2.18, and 1.378 Å.

The density of uranium telluride calculated from the constant of Ferro is 10.374 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
111	3.56	17
200	3.08	100
220	2.18	70
311	1.858	8
222	1.779	23
400	1.541	10
331	1.414	3
420	1.378	27
422	1.258	19
511	1.186	2
440	1.089	6
531	1.042	2
600	1.027	13
620	0.974	10
533	.940	1
622	.929	9
444	.890	3
711	.863	2
640	.855	9
642	.824	18
731	.802	3

Ytterbium Arsenide, YbAs (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that ytterbium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(YbAs) per unit cell. The atoms occupy the special positions:

Yb: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=5.698 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.85, 2.01, and 3.29 Å.

The density of ytterbium arsenide calculated from the constant of Brixner is 8.902 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height *I*
	Å	
111	3.29	29
200	2.85	100
220	2.01	66
311	1.718	12
222	1.645	21
400	1.424	9
331	1.307	4
420	1.274	24
422	1.163	18
511	1.097	3
440	1.007	6
531	0.963	4
600	.950	13
620	.901	10
533	.869	2
622	.859	10
444	.822	3
711	.798	4
640	.790	11

Ytterbium Nitride, YbN (cubic)

Calculated Pattern

Klemm and Winkelmann [24] in 1956 determined that ytterbium nitride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(YbN) per unit cell. The atoms occupy the special positions:

Yb: 0 0 0
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Klemm and Winkelmann [24] report the lattice constant a=4.786 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.76, 2.39, and 1.692 Å.

The density of ytterbium nitride calculated from the constant of Klemm and Winkelmann is 11.33 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	2.76	100
200	2.39	66
220	1.692	40
311	1.443	35
222	1.382	12
400	1.196	5
331	1.098	14
420	1.070	16
422	0.977	13
511	.921	13
440	.846	6
531	.809	20
600	.798	16

Yttrium Arsenide, YAs (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that yttrium arsenide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(YAs) per unit cell. The atoms occupy the special positions:

Y: 0 0 0
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$.

Brixner [30] reports the lattice constant a=5.786 Å.

No temperature correction was included.

The calculated d-values of the three strongest lines are 2.89, 2.05, and 1.294 Å.

The density of yttrium arsenide calculated from the constant of Brixner is 5.617 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3.34	2
200	2.89	100
220	2.05	63
311	1.745	<1
222	1.670	20
400	1.446	9
331	1.327	<1
420	1.294	22
422	1.181	16
511	1.114	<1
440	1.023	5
531	0.978	<1
600	.964	12
620	.915	9
533	.882	<1
622	.872	8
444	.835	3
711	.810	<1
640	.802	9

Yttrium Telluride, YTe (cubic)

Calculated Pattern

Brixner [30] in 1960 determined that yttrium telluride is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(YTe) per unit cell. The atoms occupy the special positions:

Y: $0\ 0\ 0$
Te: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

Brixner [30] reports the lattice constant $a = 6.095$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 3.05, 2.15, and 1.363 Å.

The density of yttrium telluride calculated from the constant of Brixner is 6.351 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 52	5
200	3. 05	100
220	2. 15	67
311	1. 838	2
222	1. 759	22
400	1. 524	9
331	1. 398	<1
420	1. 363	25
422	1. 244	17
511	1. 173	<1
440	1. 077	5
531	1. 030	<1
600	1. 016	12
620	0. 964	8
533	. 929	<1
622	. 919	8
444	. 880	3
711	. 853	<1
640	. 845	8
642	. 814	16
731	. 794	<1

Zirconium Phosphide, ZrP (cubic)

Calculated Pattern

Schönberg [17] in 1954 determined that zirconium phosphide is isomorphous with sodium chloride with the space group O_h^5—Fm3m (No. 225) and 4(ZrP) per unit cell. The atoms occupy the special positions:

Zr: $0\ 0\ 0$
P: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$.

Schönberg [17] reports the lattice constant $a = 5.27$ Å.

No temperature correction was included.

The calculated *d*-values of the three strongest lines are 2.63, 1.86, and 3.04 Å.

The density of zirconium phosphide calculated from the constant of Schönberg is 5.54 g/cm^3.

Calculated Pattern
Copper λ

hkl	*d*	Peak height
		I
	Å	
111	3. 04	51
200	2. 63	100
220	1. 86	61
311	1. 59	18
222	1. 52	19
400	1. 32	8
331	1. 21	6
420	1. 18	21
422	1. 07	16
511	1. 01	5
440	0. 931	6
531	. 890	6
600	. 878	14
620	. 833	11
533	. 803	3
622	. 794	12

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CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONOGRAPH 25, SECTIONS 1, 2, 3, AND 4 [5]

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

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONOGRAPH 25, SECTIONS 1, 2, 3, AND 4—Continued

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m—Monograph 25.
A mineral name in ( ) indicates a synthetic sample.

m—Monograph 25.
A mineral name in ( ) indicates a synthetic sample.

m—Monograph 25.
A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONOGRAPH 25, SECTIONS 1, 2, 3, AND 4—Continued

m—Monograph 25.
A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONOGRAPH 25, SECTIONS 1, 2, 3, AND 4—Continued

m—Monograph 25.
A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE MINERAL INDEX

CUMULATIVE MINERAL INDEX—Continued

* Natural mineral.
m—Monograph 25.

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