NBS CIRCULAR 539

VOLUME 7

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

The National Bureau of Standards

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Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, Nancy T. Gilfrich, and Marlene I. Cook



National Bureau of Standards Circular 539

Volume 7, Issued September 27, 1957

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Errata

Vol. 1. Page 56, to Cerie Oxide, add mineral name (cerianite). Page 71, table 43, hkl 633 should be 533.
Vol. 2. Page 26, d-value in last column of 1.225 should be 1.238. Page 30, in Lattice constants table, "b" should be "e".
Vol. 3. Page 35, see structure change for HgO, Acta Cryst. 9, 685 (1956), in which "a" is doubled.
Vol. 6. Page 8, under Structural data, delete 3[(NH₄)₂GeF₄] per unit rhombohedral cell. Page 27, under Structural data, delete 3[Mg(OH)₂] per unit rhombohedral cell. Page 41, under Structural data, space ground D2s bould read D²², delete 3[K5GeF₄) per Page 41, under Structural data, space group $D^{3}z$ should read $D^{33}z$ -, delete $3(K_{2}GeF_{6})$ per unit rhombohedral cell.

Page 48, under Structural data, delete 3(Rb2PtF6) per unit rhombohedral cell.

Standard X-ray Diffraction Powder Patterns

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

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Vol. 7—Data for 53 Substances

Howard E. Swanson, Nancy T. Gilfrich,¹ and Marlene I. Cook¹

Fifty-three standard X-ray diffraction powder patterns are presented. Fourth-six are to replace sixty-two patterns already represented in the X-ray Powder Data File, and seven are for substances not previously represented. The X-ray Powder Data File is a compilation of diffraction patterns from all sources and is used for the identification of unknown crystalline materials by matching spacing and intensity measurements. In this Circular, compar-ison is made of all powder diffraction data available for each of the substances reported. The patterns were made with a Geiger counter X-ray diffractometer, using samples of high purity. The *d*-values were assigned Miller indices determined by comparison with cal-culated interplanar spacings and from space group considerations. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible.

Included are X-ray data for the following fifty-three substances: $AlCl_3 \cdot 6H_2O$, NH_4NO_3 , $(NH_4)_2C_2O_4 \cdot H_2O$, NH_4ClO_4 , $BaMOO_4$, BaS, $BaWO_4$, $CdCO_3$, CdSe, $CaCrO_4$, $Ca(NO_3)_2$, CaS, Cs_2SO_4 , $AuSb_2$, $AuSb_1$, LaF_3 , LaOCl, $PbMoO_4$, $PbWO_4$, $LiIO_3$, $LiNO_3$, $MgCO_3$, $MgSO_4 \cdot 7H_2O$, MgS, $MnCO_3$, Hg_2Br_2 , HgSe, $NiSO_4 \cdot 6H_2O$, $KBrO_3$, KCNO, K_2TiF_6 , KIO_4 , $KMnO_4$, RbBr, $AgClO_3$, Ag_2MoO_4 , Ag_2SO_4 , $NaIO_3$, $NaIO_4$, $NaCIO_4$, $SrMoO_4$, SrS, $SrWO_4$, NH_3SO_3 , TeO_2 , TIBr, TI_3PO_4 , $TIPO_4$, SnTe, $CO(NH_2)_2$, Zn_2SiO_4 , $ZnSO_4$, and $Zr(SO_4)_2 \cdot 4H_2O$.

INTRODUCTION

The National Bureau of Standards in its program² for the revision and evaluation of published X-ray data for the X-ray Powder Data File presents data for 53 compounds. This paper is the seventh of the series of "Standard X-ray Dif-fraction Powder Patterns." These patterns are recommended to replace 62 cards now in the file. The patterns for 7 compounds not represented in the file have been added. These compounds are gold tin, lanthanum oxychloride, sodium metaperiodate, strontium molybdate, thallium(I) phosphate, thallium(III) phosphate, and zirconium sulfate tetrahydrate.

The experimental procedure and general plan of these reports have not changed from that of the previous volumes of the NBS Circular.³ The basic technique is described and discussed in the same order that is followed in presenting the data for each compound in the body of this volume.

ASTM cards. Each section of this Circular contains a table listing the file card numbers, the three strongest lines, the radiations used, and the literature references for each card. Cards listed in the 1955 index to the Powder Data File [1]⁴ are included in the table.

Additional published patterns. Literature references and radiation data for patterns that had not been published as ASTM cards are listed. These patterns are included in the tables of dvalues and intensities.

NBS sample. Many of the samples used to make the NBS patterns were special preparations (of exceptionally high purity) obtained or pre-pared only in small quantities. The purity of each sample was determined by spectrographic or chemical analysis. The limit of detection for the alkali elements is 0.05 percent for the NBS spectrographic analysis. Unless otherwise noted, the spectrographic analysis was done at NBS after any recrystallization or heat treatment. A phase-purity check was made on the nonopaque materials during the refractive index determina-Another excellent check of phase-purity tion. was provided by the X-ray pattern itself as it was indexed by comparison with theoretical *d*-values. Treating the sample by appropriate annealing, recrystallizing, or heating in a hydrothermal bomb improved the quality of most of the patterns.

At least two intensity patterns were prepared to check reproducibility of measured values. Samples that gave satisfactory intensity patterns showed a particle-size average well within the range of 5 to 10 microns, as suggested by Alexander, Klug, and Kummer [2]. A special cell with one open end was used for making intensity measurements. An intensity sample was prepared by clamping a flat piece of glass temporarily over the surface of this holder, and, while it was held in a perpendicular position, the sample was drifted in from the open end. The glass was then carefully removed so that the surface of the sample could be exposed to

Fellow of the Joint Committee on Chemical Analysis by Powder Diffraction Methods at the National Bureau of Standards.
 ² 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 Materials, the American Crystallographic Association, the British Institute of Physics, and the National Association of Corrosion Engineers. Additional financial support is provided by the National Bureau of Standards.
 ³ Other volumes were published as follows: Vol. 1 and Vol. 2, June 1953; Vol. 3, June 1954; Vol. 4, March 1955; Vol. 5, October 1955, and Vol. 6, September 1956.
 ⁴ Figures in brackets indicate the literature references at the end of each

⁴ Figures in brackets indicate the literature references at the end of each section of this paper.

the X-ray beam. For a few powder samples 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 intensity values of each pattern were measured as peak height above background and are expressed as percentages of the strongest line.

Additional patterns are obtained for d-value measurements. These specimens were prepared by packing, into a shallow holder, a sample containing approximately 5 weight percent of tungsten powder that served as an internal standard. The lattice constant of tungsten at 25° C is 3.1648 A, as determined by Jette and Foote [3]. All of the NBS patterns are made at 25° C by using filtered copper radiation $(K_{\alpha 1})$, having a wavelength of 1.5405 A.

Interplanar spacings and intensity measurements. Interplanar spacing data presented in the tables were converted to angstrom units as internationally defined in 1946 [4]. The conversions were from Bragg angle data, from d-values in kX units using the factor 1.00202, or from *d*-values based on wavelengths given in other than kX units. In each case the type of conversion made is indicated. The wavelength values in the tables of *d*-values and intensities are given in angstrom units, whereas the wavelengths listed under the first section of each report are the original values taken from the literature. The table of patterns contains data based on the original work rather than that data reported on the ASTM cards.

Intensities taken from the literature, when numerically evaluated, were given the following abbreviations: s, strong; m, medium; w, weak; D, diffuse; db, doublet; and v, very.

Structural data. Although the NBS lattice constants of cubic materials were calculated for each d-value, the constant reported is that obtained by averaging the last five lines because of the greater accuracy of measurement in the largeangle part of the pattern. The unit-cell values for each noncubic substance were determined by

means of a least-squares calculation made by the SEAC from the latter half of the pattern, using those *d*-values for which there was only one possible Miller index. The number of significant figures reported in the NBS pattern is limited by the quality of each sample and by its structural symmetry.

Published unit-cell data were converted to angstrom units in the same manner as were the published *d*-values. When cell values based upon more than one cell configuration have been taken from the literature, corrections that were made to make them comparable have been indicated. The limits of error generally published with unitcell data have not been included in the table because the number of determinations, and their accuracy and variations were such that a statistical evaluation would be unjustified.

The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter and are based upon atomic weights reported by E. Wichers [5] in 1956 and the Avogadro number (6.0240×10^{23}) reported by Straumanis [6] in 1954. The refractive index measurements were made in white light by grain immersion methods, using oils standardized in sodium light.

- [1] Cumulative alphabetical and grouped numerical index
- [1] Committee and grouped and grouped interfact match of X-ray diffraction data, American Society for Testing Materials. Philadelphia, Pa. (1955).
 [2] 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, 702–752 (1949) 742-753 (1948).
- [3] E. R. Jette and F. Foote, Precision determination of lattice constants, J. Chem. Phys. 3, 605-616 (1935).
- [4] Anonymous, The conversion factor for kX units to angstrom units, J. Sci. Inst. 24, 27 (1947).
 [5] E. Wichers, Report of the Committee on Atomic Weights of the American Chemical Society, J. Am. Chem. Soc. 78, 3235 (1956).
- [6] M. E. Straumanis, Remark concerning the absolute value of Avagadro's number, Phys. Rev. 95, 566 (1954).

Aluminum Chloride Hexahydrate (chloralluminite), AlCl₃·6H₂O (trigonal)

ASTM Cards

Card number	Index lines	Radiation	Source
 1-0682	3. 29 2. 30 2. 05	Molybde- num	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of aluminum chloride hexahydrate was obtained from the Johnson Matthey Co., Ltd., London. Their spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of calcium, copper, magnesium, silicon, and sodium.

The sample is colorless and optically negative with the refractive indices $N_0=1.560$ and $N_e=1.506$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel have been converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel. National Bureau of Stand- ards.	113, 122 113	321 122	134 321

Lattice constants. Andress and Carpenter [2] in 1934 determined that aluminum chloride hexahydrate has chromium chloride hexahydratetype structure, the space group $D_{3d}^6-R\overline{3}c$, and $2(AlCl_3\cdot 6H_2O)$ per unit rhombohedral cell or $6(AlCl_3\cdot 6H_2O)$ per unit hexagonal cell.

The unit-cell measurements reported by Andress and Carpenter have been converted from rhombohedral to hexagonal values and from kX to angstrom units for comparison with the NBS values.

		a	с
$1934 \\ 1957$	Andress and Carpenter[2]_ National Bureau of Standards.	$A \\ 11.78 \\ 11.831$	A 11. 84 11. 910 at 25°C

The density of aluminum chloride hexahydrate calculated from the NBS lattice constants is 1.666 at 25° C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1957 National J of Stand Cu, 1.5405	7 Bureau lards A, 25° C
	d	Ι	d	Ι
$110 \\ 012 \\ 202 \\ 211 \\ 300$	$\begin{matrix} A \\ 6. \ 0 \\ 5. \ 2 \\ 3. \ 90 \\ 3. \ 70 \\ 3. \ 42 \end{matrix}$	$17 \\ 20 \\ 13 \\ 27 \\ 11$	$\begin{matrix} A \\ 5, 95 \\ 5, 14 \\ 3, 89 \\ 3, 68 \\ 3, 416 \end{matrix}$	$26 \\ 26 \\ 40 \\ 37 \\ 25$
$113 \\ 122 \\ 220 \\ 131 \\ 312$	$\left. \begin{array}{c} 3. \ 30 \\ 2. \ 96 \\ 2. \ 76 \\ 2. \ 57 \end{array} \right.$	$100 \\ 12 \\ 11 \\ 40$	$\left\{\begin{array}{c} 3.\ 297\\ 3.\ 246\\ 2.\ 949\\ 2.\ 764\\ 2.\ 565\end{array}\right.$	$100 \\ 57 \\ 13 \\ 40 \\ 27$
$321 \\ 232 \\ 134 \\ 125 \\ 006$	$\left.\begin{array}{c} 2. \ 30 \\ 2. \ 18 \\ 2. \ 05 \\ \end{array}\right\} \\ \left.\begin{array}{c} 1. \ 99 \end{array}\right.$	53 27 53 8	$\begin{array}{c} 2.\ 308\\ 2.\ 188\\ 2.\ 056\\ \left\{\begin{array}{c} 2.\ 030\\ 1.\ 985\end{array}\right.$	$48 \\ 15 \\ 20 \\ 8 \\ 6$
$\begin{array}{c} 413 \\ 404 \\ 422 \\ 511 \\ 152 \end{array}$	$\left. \begin{array}{c} 1.94 \\ -1.82 \\ 1.76 \end{array} \right $	27 8 27	$\left\{\begin{array}{c} 1.948\\ 1.941\\ 1.842\\ 1.818\\ 1.758\end{array}\right.$	$\begin{array}{c}14\\15\\1\\3\\9\end{array}$
$\begin{array}{c} 054 \\ 235 \\ 226 \\ 244 \\ 514 \end{array}$	$\left. \begin{array}{c} 1.\ 68 \\ 1.\ 65 \\ \end{array} \right.$	13 11 	$\left\{\begin{array}{ccc} 1.\ 688\\ 1.\ 673\\ 1.\ 648\\ 1.\ 623\\ 1.\ 5664\end{array}\right.$	$\begin{array}{c}1\\4\\<1\\<1\end{array}$
$161 \\ 523 \\ 416 \\ 440 \\ 434$	$\left. \begin{array}{c} -1.51 \\ 1.478 \end{array} \right\}$	$\frac{11}{17}$	$\left\{\begin{array}{c} 1.5487\\ 1.5158\\ 1.4839\\ 1.4801\\ 1.4660\end{array}\right.$	$2 \\ 2 \\ 2 \\ 3 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ $
$155 \\ 072 \\ 621 \\ 336 \\ 262$	$ 1. 415 \\ 1. 383 $	$\frac{11}{13}$	$\begin{array}{c} 1.\ 4566\\ 1.\ 4215\\ 1.\ 4106\\ 1.\ 3996\\ 1.\ 3819 \end{array}$	$\begin{matrix} 1\\ < 1\\ < 1\\ < 1\\ < 1\end{matrix}$
$327 \\ 170 \\ 318 \\ 354 \\ 713$	$ \begin{array}{r} 1.358\\ 1.319\\ \hline 1.293 \end{array} $	<u>5</u> 9 <u>5</u> -	$\begin{array}{c} 1.\ 3789\\ 1.\ 3573\\ 1.\ 3184\\ 1.\ 3139\\ 1.\ 2843 \end{array}$	$\overset{<1}{\underset{<1}{\overset{1}{\underset{>}{\overset{1}{\atop}}}}}$
$526 \\ 633 \\ 722$	1. 227	13	$\begin{array}{c} 1.\ 2648 \\ 1.\ 2274 \\ 1.\ 2247 \end{array}$	$<^1_{\substack{3\\2}}$

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457–512 (1938).
 K. R. Andress and C. Carpenter, Kristallhydrate. II.
- [2] K. R. Andress and C. Carpenter, Kristallhydrate. II. Die Struktur von Chromiumchlorid und Aluminumchlorid hexahydrat, Z. Krist. 87, 446-463 (1934).

ASTM cards

· · · · · · · · · · · · · · · · · · ·				
	Card numbers	Index lines	Radiation	Source
	1-0809	$\begin{array}{c} 3.\ 09\\ 2.\ 72\\ 2.\ 25 \end{array}$	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
	3-1239	(a)	(a)	West [2] 1932.

* No powder data.

A pattern of the cubic form of NH_4NO_3 made at 150° C is on ASTM card 4–0605.

Additional published patterns. None.

NBS sample. The sample of ammonium nitrate was obtained from Johnson, Matthey & Co., Ltd., London. Their spectrographic analysis showed less than 0.0001 percent silver as the only impurity.

The sample is colorless and optically negative with the indices of refraction $N\alpha = 1.411$, $N\beta = 1.612$, $N\gamma = 1.635$, and $2V \cong 35^{\circ}$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel- National Bureau of Stand- ards.	$\begin{array}{c} 111\\111\end{array}$	020 020	112, 210 011

Structural data. West [2] in 1932 determined that the orthorhombic form of ammonium nitrate has the space group D_{2h}^{13} -Pnmm, and 2(NH₄NO₃) per unit cell. Ammonium nitrate is used as a structure-type. This form is the IV modification which is stable from -18° to $+32^{\circ}$ C [3]. Four other structures have been recognized by Hendricks, Posnjak, and Kracek [3].

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

References

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
- [2] C. D. West, The crystal structure of rhombic ammonium nitrate, J. Am. Chem. Soc. 54, 2256-2260 (1932).
- [3] S. B. Hendricks, E. Posnjak, and F. C. Kracek, Molecular rotation in the solid state. The variation of the crystal structure of ammonium nitrate with temperature, J. Am. Chem. Soc. 54, 2766-2786 (1932).

Lattice constants

		a	b	с
1932 1932 1957	West [2] Hendricks, Posnjak, and Kracek [3]. National Bureau of Standards.	A 4. 938 4. 97 4. 942	$\begin{array}{c} A \\ 5. \ 449 \\ 5. \ 46 \\ 5. \ 438 \end{array}$	A 5. 744 5. 76 5. 745 at 25° C

The density of ammonium nitrate calculated from the NBS lattice constants is 1.728 at 25° C.

Ammonium Nitrate (form IV) (ammonia-niter), NH₄NO₃ (orthorhombic)

	1	938	195	7
hkl	Hanawalt, Rinn, and Frevel		National Bureau of Standards	
	Mo, 0.7107 A		Cu, 1.5405 A, 25° C	
	d	Ι	d	Ι
$100 \\ 011 \\ 110 \\ 111 \\ 002$	$\begin{array}{c} A \\ 4.94 \\ 3.96 \\ \hline 3.10 \\ 2.87 \end{array}$		$\begin{array}{c} A \\ 4.95 \\ 3.96 \\ 3.66 \\ 3.087 \\ 2.879 \end{array}$	$45 \\ 67 \\ 1 \\ 100 \\ 10$
$\begin{array}{c} 020 \\ 102 \\ 120 \\ 112 \\ 210 \end{array}$	$ \begin{array}{c} 2.73\\ 2.48\\ 2.38\\ 2.25 \end{array} $	75 13 10 75	$\left\{\begin{array}{c} 2.\ 722\\ 2.\ 485\\ 2.\ 380\\ \left\{\begin{array}{c} 2.\ 260\\ 2.\ 249\end{array}\right.\right.$	$75 \\ 10 \\ 8 \\ 44 \\ 1$
$211 \\ 022 \\ 122 \\ 103 \\ 212$	2. 10 1. 97 1. 83 1. 78	5 5 5 6	$\begin{array}{c} 2. \ 094 \\ 1. \ 978 \\ 1. \ 835 \\ 1. \ 786 \\ 1. \ 769 \end{array}$	$\overset{2}{\overset{4}{\overset{1}{\overset{4}{\overset{4}{\overset{2}{\overset{1}{\overset{4}{\overset{2}{\overset{1}{\overset{2}{\overset{1}{\overset{2}{\overset{2}{\overset{2}{2$
$\begin{array}{c} 031 \\ 131 \\ 310 \\ 303 \\ 123 \end{array}$	$\begin{array}{c} 1.\ 73\\ 1.\ 63\\ 1.\ 57\\ 1.\ 51\\ 1.\ 498 \end{array}$	$5 \\ 9 \\ 10 \\ 10 \\ 10 \\ 10$	$\begin{array}{c} 1.\ 730\\ 1.\ 631\\ 1.\ 578\\ 1.\ 513\\ 1.\ 492 \end{array}$	355 51 2
$ \begin{array}{r} 132 \\ 230 \\ 004 \\ 302 \\ 312 \end{array} $	$ \left. \begin{array}{c} 1. \ 467 \\ 1. \ 433 \\ \end{array} \right. $	15 5	$\begin{cases} 1. 464 \\ 1. 461 \\ 1. 434 \\ 1. 423 \\ 1. 383 \end{cases}$	$\stackrel{1}{\stackrel{2}{\stackrel{<}{_{\scriptstyle 1}}}}_{\stackrel{1}{\stackrel{\scriptstyle 1}{_{\scriptstyle 1}}}}$
104			1. 380	1

Ammonium Oxalate Monohydrate (oxammite), (NH₄)₂C₂O₄·H₂O (orthorhombic)

ASTM cards

Cards numbers	Index lines	Radiation	Source
1-0825	$\begin{array}{c} 3.\ 06\\ 2.\ 67\\ 3.\ 81 \end{array}$	Molyb- denum	Hanawalt, Rinn, and Frevel [1] 1938.
5-0192*	$\begin{array}{c} 6. \ 37 \\ 2. \ 88 \\ 2. \ 68 \end{array}$		Winchell and Ben- oit [2] 1951.

*This ASTM card was deleted in the 1955 index.

Additional published patterns. None.

NBS sample. The sample of ammonium oxalate monohydrate was obtained from the Baker Chemical Co., New Jersey. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of calcium and silicon; and 0.0001 to 0.001 percent each of aluminum and magnesium.

The sample is colorless and optically negative with the indices of refraction $N\alpha = 1.434$, $N\beta =$ 1.549, N $\gamma = 1.591$, and 2V $\simeq 60^{\circ}$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel- Winchell and Benoit	$021 \\ 211 \\ 211 \\ 211$	$211 \\ 230 \\ 110$	$\begin{array}{c} 001 \\ 110 \\ 021 \end{array}$

Structural data. Hendricks and Jefferson [3] in 1936 determined that ammonium oxalate monohydrate had the space group $D_2^3 - P2_12_12$ and $2[(NH_4)_2C_2O_4 H_2O]$ per unit cell. Ammonium oxalate monohydrate is used as the structure-type.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice	constants
1.4 0000000	00100001010

		1		1
		a	b	c
		1		4
1926	Wood [4]	8.08	10,36	3.83
1936	Hendricks and Jeffer-	8.06	10. 29	3. 83
	son [3].			
1957	National Bureau of	8. 035	10.31	3.801 at
	Standards.			$25^{\circ}\mathrm{C}$

The density of ammonium oxalate monohydrate calculated from the NBS lattice constants is 1.498 at 25° C.

hkl	193 Hanav Rinn, Frev Mo, 0.7	8 valt, and vel 107 A	19 Winche Ben	51 ell and oit	194 Natio Burea Stand Cu, 1.5 25°	57 onal au of lards 405 A, C
	d	Ι	d	Ι	d	1
$ \begin{array}{r} 110 \\ 020 \\ 120 \\ 200 \\ 001 \end{array} $	$\begin{array}{c} A \\ 6.3 \\ 5.1 \\ \hline \\ 3.82 \end{array}$	60 10 80	$\begin{array}{c} A \\ 6.46 \\ \hline \\ 3.83 \end{array}$	80 70	$\begin{matrix} A \\ 6. 32 \\ 5. 15 \\ 4. 23 \\ 4. 02 \\ 3. 80 \end{matrix}$	$99 \\ 37 \\ 10 \\ 3 \\ 72$
$210 \\ 011 \\ 101 \\ 111 \\ 130$	3.583.443.27	$\begin{array}{c} 10\\10\\60\\\end{array}$	3.49 3.29	60	$\begin{array}{c} 3.\ 74\\ 3.\ 564\\ 3.\ 437\\ 3.\ 256\\ 3.\ 158 \end{array}$	$9 \\ 15 \\ 16 \\ 60 \\ 3$
$\begin{array}{c} 021 \\ 121 \end{array}$	3.07 2.87 2.77	$100 \\ 80 \\ 10$	3. 07 2. 88	60 60	3. 057 2. 858	$\begin{array}{c} 95 \\ 60 \end{array}$
$211 \\ 230 \\ 310$	$\left. \begin{array}{c} 2.68\\ 2.59 \end{array} \right\}$	100 60	2. 68 2. 62	100B 100B	$\begin{array}{c} 2. \ 666 \\ \{2. \ 606 \\ 2. \ 592 \end{array}$	$\begin{array}{c}100\\50\\43\end{array}$
$140 \\ 131 \\ 320 \\ 240 \\ 311$	$\left. \begin{array}{c} 2. \ 43 \\ 2. \ 36 \\ \hline 2. \ 14 \end{array} \right.$	60 60 <u>30</u> -	$2. 47 \\ 2. 40 \\ \hline 2. 16$	60B 60B 	$\begin{cases} 2. \ 453 \\ 2. \ 429 \\ 2. \ 374 \\ 2. \ 169 \\ 2. \ 142 \end{cases}$	$33 \\ 27 \\ 26 \\ 7 \\ 23$
$330 \\ 141 \\ 321 \\ 400 \\ 420$	2. 01 1. 86	$\frac{1}{20}$	2. 02 1. 89	30 40B	$\begin{array}{c} 2.\ 113\\ 2.\ 061\\ 2.\ 014\\ 2.\ 008\\ 1.\ 871 \end{array}$	$1 \\ 2 \\ 10 \\ 1 \\ 6$
$331 \\ 250 \\ 112 \\ 022 \\ 151$	1. 82	20	1.84	40B	$\begin{array}{c} 1. \ 846 \\ 1. \ 836 \\ 1. \ 822 \\ 1. \ 784 \\ 1. \ 768 \end{array}$	
$\begin{array}{c} 411 \\ 122 \\ 430 \\ 212 \\ 160 \end{array}$			1.75 1.69	20 	$\begin{array}{c} 1.\ 750\\ 1.\ 739\\ 1.\ 735\\ 1.\ 696\\ 1.\ 680 \end{array}$	1 1 1 1 1
$341 \\ 061 \\ 161 \\ 232$	}				$\begin{array}{c} 1.\ 668\\ 1.\ 565\\ 1.\ 536\end{array}$	$\begin{array}{c} 1 \\ 1 \\ 3 \end{array}$
142^{232}	, 				1. 502	2
$501 \\ 441 \\ 332$					$\begin{array}{c} 1.\ 483 \\ 1.\ 463 \\ 1.\ 413 \end{array}$	$ \frac{2}{3} 2 $

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- tion in $(NH_4)_2C_2O_4$ ·H₂O and the structure of the oxalate group, J. Chem. Phys. 4, 102-107 (1936). [4] J. F. Wood, The crystal structure of some oxalates,
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Ammonium Perchlorate, NH₄ClO₄ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0315	$\begin{array}{c} 4.\ 61\\ 3.\ 60\\ 3.\ 25 \end{array}$	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

ASTM card 2-0232 gives a cubic pattern for NH₄ClO₄ at 243° C.

Additional published patterns. None.

NBS sample. The sample of ammonium perchlorate was obtained from the City Chemical Corp., New York, N. Y. Spectographic analysis showed the following impurities: 0.0001 to 0.001 percent each of aluminum, calcium, magnesium, and silicon.

The sample is colorless and optically positive with the refractive indices $N\alpha = 1.481$, $N\beta = 1.483$, $N\gamma = 1.487$, and $2V \simeq 70^{\circ}$.

Interplanar spacings and intensity measure-ments. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel National Bureau of Standards	011 011	$\begin{array}{c} 210\\ 210\end{array}$	$\begin{array}{c} 211\\ 211\end{array}$

Structural data. Büssem and Herrmann [2] in 1930 determined that ammonium perchlorate has barium sulfate-type structure, the space group D¹⁶_{2h}-Pnma, and 4(NH₄ClO₄) per unit cell. According to Herrmann and Ilge [3] and Braekken and Harang [4], the cubic form of ammoniun perchlorate is stable above 240° C.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice con	ıstan	ts
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		a	b	с
		A	A	A
1928	Bussem and Herr- mann [5].	9.24	5. 81	7. 43
1932	Gottfried and Schus- terius [6].	9. 221	5.828	7.464
1957	National Bureau of Standards.	9. 231	5. 813	7.453 at 25° C.

The density of ammonium perchlorate calculated from the NBS lattice constants is 1.951 at 25° C.

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J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).

hkl	1933 Hanawalt, and Fr Mo, 0.71	8 , Rinn, evel 107 A	1957 National D of Stand Cu, 1.5405	7 Bureau lards A, 25° C
	d	Ι	d	I
$101 \\ 011 \\ 201 \\ 002 \\ 210$	$\begin{array}{c} A \\ 5.8 \\ 4.62 \\ 3.94 \\ 3.71 \\ 3.61 \end{array}$	$16 \\ 100 \\ 30 \\ 30 \\ 60$	$\begin{array}{c} A \\ 5.\ 80 \\ 4.\ 58 \\ 3.\ 922 \\ 3.\ 724 \\ 3.\ 611 \end{array}$	$26 \\ 100 \\ 43 \\ 33 \\ 61$
$102 \\ 211 \\ 112 \\ 202 \\ 121 \\ 212$	$\left.\begin{array}{c} 3.\ 26\\ 2.\ 98\\ 2.\ 91\\ \end{array}\right\}$	$ \begin{array}{r} 60 \\ 60 \\ $	3. 455 3. 249 2. 970 2. 899 2. 595	$9\\51\\42\\26\\29$
$311 \\ 302 \\ 221 \\ 400 \\ 122$			2. 552 2. 374 2. 334 2. 305 2. 243	$ \begin{array}{c} 3 \\ 3 \\ 1 \\ 3 \\ 1 \end{array} $
$\begin{array}{r} 401 \\ 312 \\ 222 \\ 213 \\ 402 \end{array}$	2. 21	35 	2. 205 2. 191 2. 054 2. 047 1. 961	$^{12}_{16} < ^{1}_{1} \\ ^{3}_{1}$
$303 \\ 412 \\ 123 \\ 313 \\ 421$	1. 85	 20 	1. 933 1. 859 1. 850 1. 834 1. 756	$1 \\ 12 \\ 12 \\ 4 \\ < 1$
$114 \\ 403 \\ 132 \\ 323 \\ 232$	$ \left. \begin{array}{c}\\ 1. \ 68\\ 1. \ 60 \end{array} \right. \right\} $	25 2	1. 742 1. 690 1. 611	2 11 3
$124 \\ 600 \\ 314 \\ 431 \\ 513$)] 1. 54 1. 45 	 2 8 	$1.546 \\ 1.538 \\ 1.4562 \\ 1.4361$	$1 \\ 3 \\ 5 \\ 2$
$602 \\ 414 \\ 324 \\ 432 \\ 333$	$ 1. 395 \\ 1. 365 $	$\frac{1}{6}$	$\begin{array}{c} 1.\ 4217\\ 1.\ 4076\\ 1.\ 3977\\ 1.\ 3792\\ 1.\ 3680 \end{array}$	$\begin{array}{c}1\\1\\4\\1\\2\end{array}$
$134 \\ 523 \\ 504$	$\begin{array}{c}\\ 1. 314\\ 1. 214 \end{array}$	$\frac{4}{2}$	$\begin{array}{c} 1. \ 3287 \\ 1. \ 3206 \\ 1. \ 3112 \end{array}$	2 1 1

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- [5] W.
- 67, 405–408 (1928).
 [6] C. Gottfried and C. Schusterius, Die Struktur von Kaliumund Ammoniumperchlorat, Z. Krist. 84, 65-73 (1932).

ASTM cards

Card number	Index lines	Radiation	Source
2-0449	3. 36 2. 79 2. 10	Molyb- denum.	General Electric Co., Wembley, England.

Additional published patterns

Source	Radiation	Wavelength
Zambonini and Levi [1] 1925.	Copper	Κα

NBS sample. The sample of barium molybdate was precipitated from solutions of barium chloride and sodium molybdate. The sample was annealed at 600° C for 2 hours to sharpen the diffraction pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, iron, potassium, lead, and silicon; 0.001 to 0.01 percent each of aluminum, copper, magnesium, strontium, and thallium; and 0.0001 to 0.001 percent each of silver, chromium, cesium, lithium, manganese, and tin.

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

Interplanar spacings and intensity measurements. The *d*-values reported by the General Electric Co., England, were converted from kX to angstrom units and the *d*-values of the Zambonini and Levi pattern were calculated from reported Bragg angle data.

Pattern	1	2	3
General Electric Co., England Zambonini and Levi National Bureau of Standards	$112 \\ 112 \\ 112 \\ 112$	$200 \\ 204 \\ 204$	$204 \\ 116 \\ 200$

Structural data. Vegard and Refsum [2] in 1928 determined that barium molybdate has calcium tungstate-type structure, the space group $C_{4n}^4-I4_1/a$, and $4(BaMoO_4)$ per unit cell.

The "a" measurement reported by Zambonini and Levi was multiplied by $2/\sqrt{2}$ and the "a" measurement of Vegard and Refsum was multiplied by the $\sqrt{2}/2$. The "c" measurement of Zambonini and Levi was doubled. All of the unit-cell measurements were converted from kX to angstrom units for comparison with the NBS values.

Barium Molybdate, BaMoO₄ (tetragonal)

hkl	General Elec. Co., Wembley, Eng. Mo, 0.7107 A		1925 Zambonini and Levi Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	Ι	d	Ι	d	Ι
$101 \\ 112 \\ 004 \\ 200 \\ 202$	A 3. 37 3. 21 2. 80	$ \begin{array}{r} \overline{100}\\ 40\\ 50\\ \end{array} $	A 3. 26 3. 15 2. 72	vs vw w	$\begin{array}{c} A \\ 5. 11 \\ 3. 357 \\ 3.202 \\ 2. 789 \\ 2. 557 \end{array}$	$2 \\ 100 \\ 20 \\ 24 \\ 3$
$114 \\ 211 \\ 105 \\ 213 \\ 204$	$ \begin{array}{r} \overline{2.45} \\ 2.33 \\ \overline{2.10} \end{array} $	$ \begin{bmatrix} 10 \\ 10 \\ $	 2. 08	 S	2. 4866 2. 4492 2. 3293 2. 1537 2. 1035	$ \begin{array}{r} 3 \\ 2 \\ 3 \\ 30 \end{array} $
$220 \\ 116 \\ 312 \\ 224 \\ 008$	1. 97 1. 88 1. 70 1. 68	$30 \\ 40 \\ 40 \\ 30 \\$	1.863 1.693 1.679	s s m	$\begin{array}{c} 1. \ 9721 \\ 1. \ 8779 \\ 1. \ 7007 \\ 1. \ 6797 \\ 1. \ 6024 \end{array}$	$10 \\ 18 \\ 23 \\ 12 \\ 2$
$\begin{array}{r} 400 \\ 208 \\ 316 \\ 332 \\ 404 \end{array}$	1. 39 1. 36 1. 28	$ \begin{array}{c} 10 \\ - 20 \\ 10 \\ \end{array} $	1. 392 1. 364 1. 290	m ms m	$\begin{array}{c} 1.\ 3946\\ 1.\ 3899\\ 1.\ 3606\\ 1.\ 2885\\ 1.\ 2795 \end{array}$	$2 \\ 7 \\ 10 \\ 3 \\ 3$
$\begin{array}{r} 420 \\ 228 \\ 1 \cdot 1 \cdot 10 \\ 424 \\ 336 \end{array}$	1. 24 	10 	$ \begin{array}{c} 1. \ 252 \\ \hline 1. \ 170 \\ 1. \ 126 \end{array} $	m ms mw	$\begin{array}{c} 1.\ 2478\\ 1.\ 2444\\ 1.\ 2195\\ 1.\ 1631\\ 1.\ 1201 \end{array}$	$\begin{array}{c}3\\5\\4\\4\\4\end{array}$
$512 \\ 0.0.12 \\ 408 \\ 3.1.10 \\ 2.0.12$		 	$ \begin{array}{c} 1. \ 085 \\ \overline{1. \ 043} \\ \overline{0. \ 991} \end{array} $	s vw w	$\begin{array}{c} 1.\ 0788\\ 1.\ 0688\\ 1.\ 0523\\ 1.\ 0373\\ 0.\ 9978 \end{array}$	$ \begin{array}{c} 4 \\ 5 \\ 3 \\ 2 \\ 4 \end{array} $
$\begin{array}{r} 440 \\ 428 \\ 516 \\ 532 \\ 444 \end{array}$	} 		. 983 . 952 	w ms	$\left\{\begin{array}{c} .9865\\ .9846\\ .9741\\ .9465\\ .9427\end{array}\right.$	2 3 3 2 3
$2 \cdot 2 \cdot 12 \\ 600 \\ 3 \cdot 3 \cdot 10 \\ 604 \\ 1 \cdot 1 \cdot 14$. 901 . 890	mw vw	. 9395 . 9301 . 9181 . 8930 . 8920	$\overset{2}{\overset{1}{\overset{1}{\overset{3}{\overset{1}{\overset{1}{\overset{1}{\overset{3}{\overset{1}{1$
620					. 8823	1
$\frac{622}{536}$	}				. 8735	4
$\begin{array}{c} 624 \\ 4{\cdot}0{\cdot}12 \end{array}$. 858 . 847	m w	.8508 .8484	$ < \frac{1}{3}$
$448 \\ 5 \cdot 1 \cdot 10$. 840	m 	. 8401 . 8324	$\begin{array}{c} 2\\ 4\end{array}$

Lattice constants

-		a	c
$1925 \\ 1928 \\ 1957$	Zambonini and Levi [3] Vegard and Refsum [2] National Bureau of Standards.	$\begin{matrix} A \\ 5. \ 61 \\ 5. \ 567 \\ 5. \ 5802 \end{matrix}$	A 12. 89 12. 781 12. 821 at 25° C.

The density of barium molybdate calculated from the NBS lattice constants is 4.945 at 25° C.

References

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Barium Sulfide, BaS (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0757	$\begin{array}{c} 3. \ 18 \\ 2. \ 25 \\ 3. \ 67 \end{array}$	Molyb- denum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Holgersson [2] 1923	Copper	Kα

NBS sample. The sample of barium sulfide was obtained from the Baker Chemical Co., Phillipsburgh, N. J. The sample was annealed for 7 hours at 900° C in an argon atmosphere. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of strontium and tin; 0.01 to 0.1 percent each of aluminum, calcium, and silicon; 0.001 to 0.01 percent of copper; and 0.0001 to 0.001 percent each of boron, chromium, iron, potassium, lithium, magnesium, and lead.

The sample is colorless. The refractive index is too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measure-ments. The *d*-values reported by Hanawalt, Rinn, and Frevel have been converted from kX to angstrom units. The *d*-values of the Holgersson pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel Holgersson National Bureau of Standards	$200 \\ 200 \\ 200 \\ 200$	$220 \\ 220 \\ 220 \\ 220$	$111 \\ 420 \\ 111$

Structural data. Holgersson [2] in 1923 determined that barium sulfide has sodium chloridetype structure, the space group O_b^5 -Fm3m, and 4(BaS) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

$1923 \\ 1927 \\ 1956 \\ 1957$	Holgersson [2] Goldschmidt [3] Güntert and Faessler [4] National Bureau of Stand- ards.	A 6.359 6.381 6.3877 at 21 ° C 6.386 at 25 ° C

The density of barium sulfide calculated from the NBS lattice constant is 4.320 at 25° C.

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- [2] S. Holgersson, Die Struktur der Sulfide von Mg, Ca, Sr, und Ba, Z. anorg. u. allgem. Chem. 126, 179–192
- (1923).
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- [4] O. J. Güntert and A. Faessler, Präzisionsbestimmung der Gitterkonstaten der Erdalkalisulfide MgS, CaS, SrS und BaS, Z. Krist. 107, 357-361 (1956).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		revel 1923 Holgersson Cu, 1.5418 A		on 3 A	1957 National Bureau of Standards Cu, 1.5405 A, 25° C			
	d	I	a	d	Ι	a	d	Ι	a
111 200 220 311	$\begin{array}{c} A \\ 3. 68 \\ 3. 19 \\ 2. 25 \\ \hline 1. 91 \end{array}$	$53 \\ 100 \\ 83 \\ \bar{40}$	$\begin{array}{c} A \\ 6.37 \\ 6.38 \\ 6.36 \\ \hline 6.33 \\ \hline 6.33 \\ \end{array}$	$\begin{array}{c} A\\ 3.\ 65\\ 3.\ 16\\ 2.\ 24\\ 2.\ 08\\ 1.\ 90 \end{array}$	w vs vs s m	$\begin{array}{c} A \\ 6.32 \\ 6.32 \\ 6.34 \\ \hline 6.30 \end{array}$	$\begin{array}{c} A \\ 3.688 \\ 3.194 \\ 2.258 \\ \hline 1.9258 \\ \hline \end{array}$	$\begin{array}{r} 72\\100\\80\\ \overline{40}\end{array}$	$\begin{array}{c} A \\ 6.388 \\ 6.388 \\ 6.387 \\ \hline 6.387 \\ \hline \end{array}$
$222 \\ 400 \\ 331 \\ 420 \\ 422$	$1.83 \\ 1.59 \\ 1.463 \\ 1.424 \\ 1.302$	$27 \\ 15 \\ 11 \\ 45 \\ 25$	$\begin{array}{c} 6.34\\ 6.36\\ 6.377\\ 6.368\\ 6.378\end{array}$	$ \begin{array}{r} 1.82 \\ \hline 1.46 \\ 1.42 \\ 1.30 \end{array} $	s m vs vs	6. 30 6. 36 6. 35 6. 37	$\begin{array}{c} 1.8433\\ 1.5970\\ 1.4652\\ 1.4285\\ 1.3037\end{array}$	$27 \\ 14 \\ 12 \\ 33 \\ 22$	6. 384 6. 388 6. 387 6. 388 6. 388 6. 387
$511 \\ 440 \\ 531 \\ 600 \\ 620$	$\begin{array}{c} 1.\ 227\\ 1.\ 127\\ 1.\ 078\\ 1.\ 063\\ 1.\ 007 \end{array}$	$10 \\ 5 \\ 5 \\ 8 \\ 4$	$\begin{array}{c} 6. \ 376 \\ 6. \ 375 \\ 6. \ 378 \\ 6. \ 378 \\ 6. \ 369 \end{array}$	$\begin{array}{c} 1. \ 22 \\ 1. \ 125 \\ 1. \ 073 \\ 1. \ 060 \\ 1. \ 006 \end{array}$	m m s m	$\begin{array}{c} 6. & 34 \\ 6. & 364 \\ 6. & 348 \\ 6. & 360 \\ 6. & 363 \end{array}$	$\begin{array}{c} 1. \ 2291 \\ 1. \ 1286 \\ 1. \ 0801 \\ 1. \ 0641 \\ 1. \ 0094 \end{array}$	$ \begin{array}{c} 10 \\ 6 \\ 8 \\ 13 \\ 9 \end{array} $	$\begin{array}{c} 6. \ 387 \\ 6. \ 384 \\ 6. \ 381 \\ 6. \ 385 \\ 6. \ 384 \end{array}$
$533 \\ 622 \\ 444 \\ 711 \\ 640$	0. 962 . 893 . 885	$-\frac{1}{4}$	$\begin{array}{c} -6.\ 381\\ \hline 6,\ 377\\ \hline 6.\ 381 \end{array}$	$\begin{array}{c} 0.\ 9592\\ .\ 9180\\ .\ 8914\\ .\ 8819 \end{array}$	s w m m	$\begin{array}{c} 6. \ 363 \\ 6. \ 360 \\ 6. \ 366 \\ 6. \ 359 \end{array}$	$\begin{array}{c} 0. \ 9734 \\ . \ 9627 \\ . \ 9217 \\ . \ 8941 \\ . \ 8856 \end{array}$	${\overset{5}{\overset{8}{<}}_{\overset{1}{6}}_{7}}$	$\begin{array}{c} 6. \ 383 \\ 6. \ 386 \\ 6. \ 386 \\ 6. \ 385 \\ 6. \ 386 \end{array}$
$642 \\ 731 \\ 800$. 853 . 831	5 1 	6. 383 6. 383	. 8503 . 8288 . 7958	vs s w	$\begin{array}{c} 6. & 363 \\ 6. & 366 \\ 6. & 366 \end{array}$.8534 .8313 .7984	$\overset{12}{\overset{8}{<1}}$	$\begin{array}{c} 6. \ 386 \\ 6. \ 385 \\ 6. \ 387 \end{array}$
Average of last five lines 6.381		6. 381			6. 364			6. 386	

Barium Sulfide, BaS (cubic)

Barium Tungstate BaWO₄ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
· 1-0658	$\begin{array}{c} 3. \ 34 \\ 2. \ 08 \\ 1. \ 70 \end{array}$	Molybde- num.	New Jersey Zinc Co.

Additional published patterns

Source	Radiation	Wavelength
Navarro and Palacios [1] 1929.	Chromium	Kα

NBS sample. The sample of barium tungstate was precipitated from solutions of barium chloride and sodium tungstate. It was annealed at 800° C for 2 hours to sharpen the diffraction pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, potassium, sodium, and silicon; 0.001 to 0.01 percent each of silver, copper, iron, lithium, magnesium, manganese, and antimony.

The sample is colorless. The index of refraction could not be determined by the usual liquid grain immersion method as the sample was too fine.

Interplanar spacings and intensity measurements. The *d*-values of the Navarro and Palacios pattern were calculated from Bragg angle data, and the *d*-values reported by the New Jersey Zinc Co. were converted from kX to angstrom units. The pattern reported by Navarro and Palacios did not include intensity measurements. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
New Jersey Zinc Co National Bureau of Standards	$\begin{array}{c} 112\\112\end{array}$	$\begin{array}{c} 204 \\ 204 \\ 204 \end{array}$	$\begin{array}{c} 312\\ 312\end{array}$

Structural data. Navarro and Palacios [2] in 1929 determined that barium tungstate has calcium tungstate-type structure, the space group C_{4h}^6 -I4₁/a, and 4(BaWO₄) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice	constants
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		a	с
1928 1931 1931 1932 1957	Vegard and Refsum [3] Navarro and Palacios [2]. Aanerud [4] Jimenez [5] National Bureau of Standards.	$\begin{array}{c} A \\ 5.\ 60 \\ 5.\ 65 \\ 5.\ 60 \\ 5.\ 65 \\ 5.\ 6134 \end{array}$	A 12. 71 12. 72 12. 74 12. 72 12. 72 12. 720 at 25° C.

The density of barium tungstate calculated from the NBS lattice constants is 6.382 at 25° C.

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- 21-32 (1931).
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Barium Tungstate, BaWO₄ (tetragonal)

hkl	New Jersey Zine Co. Mo, 0.7107 A		1929 Navarro and Palacios Cr, 2.291 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	Ι	d	Ι	d	Ι
$101 \\ 112 \\ 004 \\ 200 \\ 114$	$\begin{array}{c} A \\ 5.\ 05 \\ 3.\ 34 \\ 3.\ 14 \\ 2.\ 78 \\ \end{array}$	4 100 30 26 -	A 3. 39 3. 20 2. 82 2. 48	- - - -	$\begin{array}{c} A\\ 5.\ 13\\ 3.\ 367\\ 3.\ 178\\ 2.\ 805\\ 2.\ 483\end{array}$	$7\\100\\23\\31\\1$
$211 \\ 204 \\ 220 \\ 116 \\ 215$	2. 08 1. 97 1. 85 		2.111.991.8801.787		2. 464 2. 104 1. 985 1. 870 1. 787	$2 \\ 33 \\ 14 \\ 24 \\ 1$
312 206 224 008	$ \begin{array}{r} 1. \ 68 \\ 1. \ \overline{67} \\ 1. \ 58 \\ \end{array} $	50 10 4 -	$ \begin{array}{r} 1. 706 \\ 1. \overline{685} \\ 1. \overline{485} \end{array} $		1. 710 1. 6908 1. 6836 1. 5898	$32 \\ 2 \\ 16 \\ 3 \\$
$\begin{array}{c} 400 \\ 208 \\ 316 \\ 332 \\ 404 \end{array}$	$ \begin{array}{c} 1.\ 37\\ 1.\ 35\\ 1.\ 28 \end{array} \right\} $		 {		$\begin{array}{c} 1.\ 4037\\ 1.\ 3835\\ 1.\ 3611\\ 1.\ 2955\\ 1.\ 2840 \end{array}$	$4 \\ 7 \\ 13 \\ 7 \\ 6$
$\begin{array}{r} 420 \\ 228 \\ 1 \cdot 1 \cdot 10 \\ 424 \\ 336 \end{array}$	$\begin{array}{c} 1.\ 25\\ 1.\ 23\\ 1.\ 20\\ 1.\ 16\\ 1.\ 12 \end{array}$			- - -	$\begin{array}{c} 1.\ 2553\\ 1.\ 2411\\ 1.\ 2114\\ 1.\ 1677\\ 1.\ 1226 \end{array}$	$5 \\ 7 \\ 4 \\ 6 \\ 3$
$512 \\ 0.0.12 \\ 408 \\ 3.1.10 \\ 440$	$ \begin{array}{r} 1.08 \\ \overline{1.05} \\ 1.03 \\ \end{array} $	10 -6 10 -			$\begin{array}{c} 1.\ 0849\\ 1.\ 0603\\ 1.\ 0523\\ 1.\ 0340\\ 0.\ 9927 \end{array}$	$\stackrel{3}{\stackrel{2}{\underset{3}{\overset{3}{1}}}}$
2.0.12 428 516 532 444					$\begin{array}{c} . \ 9915 \\ . \ 9852 \\ . \ 9771 \\ . \ 9520 \\ . \ 9473 \end{array}$	$ \begin{array}{c} 1 \\ 3 \\ 2 \\ 3 \\ 2 \\ 2 \end{array} $
$\begin{array}{r} 600 \\ 2\cdot 2\cdot 12 \\ 3\cdot 3\cdot 10 \\ 604 \\ 620 \end{array}$					$\begin{array}{r} .9358\\ .9350\\ .9171\\ .8978\\ .8877\end{array}$	$2 \\ 3 \\ 2 \\ 3 \\ 2 \\ 2$
$ \begin{array}{r} 1 \cdot 1 \cdot 14 \\ 536 \\ 624 \\ 4 \cdot 0 \cdot 12 \\ 448 \end{array} $. 8856 . 8766 . 8550 . 8460 . 8419	35 33 33 33
$5.1.10 \\ 4.2.12 \\ 3.1.14 \\ 608 \\ 712$. 8325 . 8099 . 8088 . 8065 . 7879	$ \begin{array}{c} 4 \\ 1 \\ 4 \\ 3 \\ 7 \end{array} $

Cadmium Carbonate (otavite), CdCO₃ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0907	$2.94 \\3.77 \\1.83$	Molyb- denum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [2] 1928	Copper	

NBS sample. The sample of cadmium carbonate was obtained from the Fisher Scientific Co., New York, N. Y. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of chromium, nickel, and lead; and 0.0001 to 0.001 percent each of calcium, copper, iron, magnesium, and silicon.

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

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel have been converted from kX to angstrom units and the *d*-values of the Zachariasen pattern have been calculated from Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel.	104	012	018, 116
Zachariasen National Bureau of Standards.	$\left \begin{array}{c}104\\104\end{array}\right $	018, 116 012	$112 \\ 110$

Structural data. Wyckoff [3] in 1920 determined the structure of the calcite group. Zachariasen [2] in 1928 found that cadmium carbonate has calcite-type structure, the space group $D_{3d}^{6}-R\overline{3}c$ with $2(CdCO_{3})$ per unit rhombohedral

cell or $6(CdCO_3)$ per unit hexagonal cell. Two unit-cell measurements have been con-verted from the rhombohedral to the hexagonal cell values and from kX to angstrom units for comparison with the NBS values.

		a	с
$1928 \\ 1947 \\ 1957$	Zachariasen [2] Vegard [4] National Bureau of Standards.	$\begin{matrix} A \\ 4. \ 923 \\ 5. \ 014 \\ 4. \ 930 \end{matrix}$	$\begin{matrix} A \\ 16. \ 28 \\ 16. \ 37 \\ 16. \ 27 \\ at \ 25^{\circ} \ C \end{matrix}$

The density of cadmium carbonate calculated from the NBS lattice constants is 4.980 5° at 2C.

hkl	1938 Hanaw Rinn, a Frev Mo, 0.71	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1928 Zachariasen Cu,		7 onal u of ards 405 A, C
	d	Ι	d	Ι	d	Ι
$\begin{array}{c} 012 \\ 104 \\ 006 \\ 110 \\ 113 \end{array}$	$ \begin{array}{c} A\\ 3.78\\ 2.95\\ \hline 2.47\\ 2.23\\ \end{array} $	$ \begin{array}{r} 80 \\ 100 \\ 50 \\ 3 \end{array} $	$\begin{array}{c} A \\ 3.\ 65 \\ 2.\ 85 \\ 2.\ 65 \\ 2.\ 40 \\ 2.\ 20 \end{array}$	$50 \\ 100 \\ 10-20 \\ 50 \\ 5 \end{bmatrix}$	$\begin{array}{c} A\\ 3.\ 78\\ 2.\ 95\\ 2.\ 72\\ 2.\ 46\\ 2.\ 245\end{array}$	$78 \\ 100 \\ 3 \\ 35 \\ 7$
$202 \\ 024 \\ 018 \\ 116 \\ 122$	$2.06 \\ 1.88 \\ 1.83 \\ 1.58$	$45 \\ 33 \\ 80 \\ 40$	$\begin{array}{c} 2.\ 02\\ 1.\ 85\\ \{1.\ 80\\ 1.\ 78\\ 1.\ 55 \end{array}$		$\begin{array}{c} 2.\ 066\\ 1.\ 890\\ \{1.\ 838\\ 1.\ 825\\ 1.\ 582 \end{array}$	$27 \\ 14 \\ 23 \\ 34 \\ 15$
1.0.10 214 208 300 0.0.12	1.501.4731.4221.358	$17 \\ 5 \\ 15 \\ 5 \\ 5$	$\begin{array}{c} 1. \ 49 \\ 1. \ 47 \\ 1. \ 44 \\ 1. \ 39 \\ 1. \ 33 \end{array}$	$\begin{array}{c} 20 \\ 50 \\ 20 - 30 \\ 40 \\ 20 \end{array}$	$\begin{array}{c} 1.\ 522\\ 1.\ 500\\ 1.\ 473\\ 1.\ 423\\ 1.\ 357 \end{array}$	$\begin{array}{c} 4\\11\\5\\7\\2\end{array}$
$0.2.10 \\ 128 \\ 306 \\ 220 \\ 1.1.12$	$1. 297 \\ \Big\} 1. 263 \\ 1. 232 \\ 1. 192 \\$	5 17 5 8	$1. 27 \\ 1. 24 \\ 1. 20 \\ 1. 17$	20-30 50 20 40	$ \begin{array}{c} 1.\ 293 \\ \{1.\ 263 \\ 1.\ 260 \\ 1.\ 232 \\ 1.\ 189 \end{array} $	$3 \\ 6 \\ 3 \\ 2 \\ 4$
$312 \\ 2 \cdot 1 \cdot 10 \\ 134 \\ 226 \\ 042$	$1.\ 144 \\ 1.\ 122 \\$	8 8	$\begin{array}{c} 1. \ 15 \\ 1. \ 13 \\ 1. \ 12 \\ 1. \ 10 \\ 1. \ 02 \end{array}$	$ \begin{array}{r} 30 \\ 30 \\ 30-40 \\ 30 \\ 30 \\ 30 \end{array} $	$\begin{array}{c} 1.\ 171\\ 1.\ 146\\ 1.\ 137\\ 1.\ 121\\ 1.\ 057 \end{array}$	3 4 5 5 <1
$404 \\ 318 \\ 1 \cdot 1 \cdot 15 \\ 3 \cdot 0 \cdot 12 \\ 232$	$ \Big\} 1. \ 024 \\ 0. \ 978 \\$	8 7	1. 01 0. 979 . 970 . 959	$50 \\ 20 \\ 40 \\ 30$	$\begin{cases} 1.\ 032 \\ 1.\ 0231 \\ 0.\ 9900 \\ .\ 9825 \\ .\ 9725 \end{cases}$	$ \begin{smallmatrix} 3 \\ 4 \\ 1 \\ 2 \\ < 1 \end{smallmatrix}$
${ \begin{array}{c} 1\cdot 3\cdot 10 \\ 324 \\ 048 \\ 140 \\ 413 \end{array} }$. 944	7	.947 .941 .933 .920 .911	$10 \\ 20 \\ 40 \\ 40 \\ 20$	$\begin{array}{c} . \ 9571 \\ . \ 9522 \\ . \ 9446 \\ . \ 9310 \\ . \ 9191 \end{array}$	$\begin{array}{c} \displaystyle \stackrel{\scriptstyle <}{\underset{\scriptstyle 1}{\overset{\scriptstyle 1}{\underset{\scriptstyle <}{\overset{\scriptstyle 1}{\underset{\scriptstyle 1}{\atop 1}{\atop 1}}}}}}}}}}$
$2 \cdot 2 \cdot 12 \\ 4 \cdot 0 \cdot 10 \\ 238 \\ 416$	 } . 882	7	. 902 	30 	.9126 .8928 .8814	$\stackrel{\leq 1}{\stackrel{\scriptstyle <}{\stackrel{\scriptstyle \sim}{\stackrel{\scriptstyle \sim}{}}{\stackrel{\scriptstyle \sim}{\stackrel{\scriptstyle \sim}{\stackrel{\scriptstyle \sim}{\stackrel{\scriptstyle \sim}{}}{\stackrel{\scriptstyle \sim}{\stackrel{\scriptstyle \sim}{\stackrel{\scriptstyle \sim}{\stackrel{\scriptstyle \sim}{}}{\stackrel{\scriptstyle \sim}{\stackrel{\scriptstyle \sim}{}}{ }{}}}}}}}}}}}}$

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
 W. H. Zachariasen, Untersuchungen über die Kristall-struktur von Sesquioxyden und Vervindungen ABO₃, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. 1928, No. 4 (1928).
 R. W. G. Wyckoff, The crystal structures of some car-bonates of the calcite group Am J. Sci 50, 317-360
- bonates of the calcite group, Am. J. Sci. 50, 317-360 (1920).[4] L. Vegard, Investigation into the structure and prop-
- erties of solid matter with the help of X-rays, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. 1947, No. 2 (1947).

Cadmium Selenide, CdSe (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
2-0330	3. 74 2. 16 3. 31		General Electric Co., Wembley, England.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [1] 1926	Copper	Kα

NBS sample. The sample of cadmium selenide was obtained from the Mallinckrodt Chemical Works, New York, N. Y. It was annealed at 200° C in an argon atmosphere. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of calcium, copper, iron, and manganese; and 0.0001 to 0.001 percent each of aluminum, magnesium, nickel, lead, silicon, and tin.

The sample is black and opaque.

Interplanar spacings and intensity measurements. The *d*-values of the Zachariasen pattern were calculated from Bragg angle data. The *d*values of the General Electric Co., England, pattern were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
General Electric Co., England Zachariasen National Bureau of Standards	$100 \\ 110 \\ 100$	$110 \\ 100 \\ 110$	$101 \\ 112 \\ 101$

Structural data. Zachariasen [1] in 1926 determined that cadmium selenide has wurtzitetype structure with the space group C_{6v}^4 -P6₃mc and 2(CdSe) per unit cell. Goldschmidt [2] in 1926 reported a cubic form of cadmium selenide, which is formed by passing hydrogen selenide through a boiling solution of cadmium sulfate.

The unit-cell measurements reported by Zachariasen and by Goldschmidt were converted from kX to angstrom units for comparison with the NBS values.

References

- W. H. Zachariasen, Über die Kristallstrukturen der Selenide von Beryllium, Zink, Cadmium und Quecksilber, Z. physik. Chem. 124, 436–448 (1926).
- silber, Z. physik. Chem. 124, 436–448 (1926).
 [2] V. M. Goldschmidt, Geochemische Verteilungsgesetze der Elemente; VII, Die Gesetze der Krystallochemie, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. 1926, No. 2 (1926).

Lattice constants

		a	с
1926 1926 1957 [.]	Goldschmidt [2] Zachariasen [1] National Bureau of Standards.	A 4. 31 4. 31 4. 299	A 7. 03 7. 02 7.010 at 25° C.

The density of cadmium selenide calculated from the NBS lattice constants is 5.663 at 25° C.

hkl	General Electric Co., England		192 Zachar Cu, 1.54	6 iasen 418 A	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι	d	Ι	d	Ι	
$100 \\ 002 \\ 101 \\ 102 \\ 110$	$\begin{array}{c} A\\ 3.\ 74\\ 3.\ 52\\ 3.\ 305\\ 2.\ 563\\ 2.\ 157\end{array}$	$100 \\ 80 \\ 90 \\ 40 \\ 100$	$\begin{array}{c} A\\ 3.\ 74\\ 3.\ 49\\ 3.\ 30\\ 2.\ 57\\ 2.\ 160\end{array}$	$ \begin{array}{r} 80 \\ 30 \\ 60 \\ 20 \\ 100 \end{array} $	$\begin{array}{c} A\\ 3.\ 72\\ 3.\ 51\\ 3.\ 290\\ 2.\ 554\\ 2.\ 151\end{array}$	$100 \\ 70 \\ 75 \\ 36 \\ 85$	
$103 \\ 200 \\ 112 \\ 201 \\ 202$	$\begin{array}{c} 1. \ 988 \\ 1. \ 866 \\ 1. \ 839 \\ 1. \ 807 \\ 1. \ 649 \end{array}$	$70 \\ 30 \\ 80 \\ 20 \\ 30$	$\begin{array}{c} 1. \ 989 \\ 1. \ 872 \\ 1. \ 842 \\ 1. \ 812 \\ 1. \ 649 \end{array}$	$70 \\ 20 \\ 80 \\ 20 \\ 10$	$\begin{array}{c} 1.\ 980\\ 1.\ 863\\ 1.\ 834\\ 1.\ 800\\ 1.\ 645 \end{array}$	$70 \\ 12 \\ 51 \\ 11 \\ 8$	
$203 \\ 210 \\ 211 \\ 105 \\ 212$	1. 459 1. 409 1. 383 1. 315	$50 \\ 30 \\ 30 \\ 40 \\$	1. 460 1. 411 1. 384 1. 315	70 20 30 50 	$\begin{array}{c} 1.\ 456\\ 1.\ 407\\ 1.\ 380\\ 1.\ 3120\\ 1.\ 3059 \end{array}$	$20 \\ 8 \\ 8 \\ 13 \\ 5$	
$ \begin{array}{r} 300 \\ 301 \\ 213 \\ 302 \\ 205 \end{array} $	1. 244	30 	$ \begin{array}{c} 1. 245 \\ \overline{1. 209} \\ 1. 174 \\ 1. 123 \end{array} $	$ \begin{array}{r} 40 \\ \bar{70} \\ 40 \\ 40 \\ 40 \end{array} $	$\begin{array}{c} 1.\ 2411\\ 1.\ 2218\\ 1.\ 2055\\ 1.\ 1700\\ 1.\ 1201 \end{array}$		
$106 \\ 220 \\ 310 \\ 222 \\ 116$			1. 078 1. 031	40 80 	$\begin{array}{c} 1.\ 1144\\ 1.\ 0748\\ 1.\ 0327\\ 1.\ 0273\\ 1.\ 0267\end{array}$	$egin{array}{c} 2 \\ 6 \\ 3 \\ 6 \\ 4 \end{array}$	
$\begin{array}{c} 311 \\ 215 \\ 312 \\ 313 \\ 400 \end{array}$			0. 997 . 948	80 80	$\begin{array}{c} 1.\ 0219\\ 0.\ 9932\\ .\ 9906\\ .\ 9446\\ .\ 9307 \end{array}$	29666< <1	
$\begin{array}{c} 401 \\ 402 \\ 216 \\ 207 \\ 008 \end{array}$	}				. 9226 . 8992 . 8820 . 8761	<1 <1 <1 <1	
$ \begin{array}{c} 403 \\ 320 \\ 306 \\ 315 \end{array} $. 8648 . 8542 . 8508 . 8314	3 1 2 5	

Calcium Chromate, CaCrO₄ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0516	$\begin{array}{c} 3.\ 63\\ 2.\ 70\\ 1.\ 86 \end{array}$	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Clouse [2] 1932	Molyb- denum	Kα

NBS sample. The sample of calcium chromate was prepared at NBS by melting CaCl₂ with K_2CrO_4 and washing. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of barium, strontium, vanadium, and zirconium; and 0.0001 to 0.001 percent each of aluminum, copper, potassium, magnesium, manganese, and silicon.

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

Interplanar spacings and intensity measure-ments. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The *d*-values of the Clouse pattern were calculated from Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel Clouse National Bureau of Standards	$200 \\ 200 \\ 200 \\ 200$	$112 \\ 312 \\ 112$	$312 \\ 112 \\ 312$

Structural data. Clouse [3] in 1930 determined that calcium chromate has zirconium silicate-type structure, the space group D_{4h}¹⁹-I4₁/amd with $4(CaCrO_4)$ per unit cell.

The unit-cell measurements reported by Clouse were converted from kX to angstrom units for comparison with the NBS values.

References

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
- [2] J. H. Clouse, Investigations on the X-ray crystal structures of CaCrO₄, CaCrO₄·H₂O, and structures of CaCrO₄, CaCrO₄, CaCrO₄, 20, and CaCrO₄·2H₂O, Z. Krist. 83, 161–171 (1932).
 [3] J. H. Clouse, On the crystal structure of calcium chromate, CaCrO₄, Z. Krist. 76, 285–286 (1930).

Lattice constants

$ 1930 \\ 1932 \\ 1957 $	Clouse [3] Clouse [2] National Bureau of	a 7. 11 7. 26 7. 242	c A 6.20 6.35 6.290 at
1957	Standards.	7, 242	6.290 at 25° C.

The density of calcium chromate calculated from the NBS lattice constants is 3.142 at 25° C

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		19381932Hanawalt, Rinn, and FrevelClouseMo, 0.7107 AMo,		2 se	1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	Ι	d I		d	Ι	
$101 \\ 200 \\ 211 \\ 112 \\ 220$	$\begin{array}{c} A \\ 4.81 \\ 3.64 \\ 2.91 \\ 2.71 \\ 2.58 \end{array}$	$\begin{array}{r} 6 \\ 100 \\ 15 \\ 75 \\ 15 \end{array}$	$\begin{array}{c} A \\ 4.\ 77 \\ 3.\ 60 \\ 2.\ 90 \\ 2.\ 68 \\ 2.\ 58 \end{array}$	$ \begin{array}{r} 10 \\ 100 \\ 30 \\ 80 \\ 30 \\ 30 \end{array} $	$\begin{array}{c} A\\ 4.\ 75\\ 3.\ 62\\ 2.\ 880\\ 2.\ 679\\ 2.\ 562\end{array}$	$10 \\ 100 \\ 15 \\ 54 \\ 11$	
$\begin{array}{c} 202 \\ 301 \\ 103 \\ 321 \\ 312 \end{array}$	2. 39 2. 27 1. 86	$20 \\ 8 \\ \\ -\overline{75}$	$2.382.272.025\overline{1.862}$	$50 \\ 20 \\ 10 \\ \bar{100}$	$\begin{array}{c} 2. \ 375 \\ 2. \ 254 \\ 2. \ 013 \\ 1. \ 913 \\ 1. \ 8510 \end{array}$	$ \begin{array}{r} 16 \\ 7 \\ 6 \\ 5 \\ 45 \end{array} $	
$\begin{array}{c} 400 \\ 411 \\ 420 \\ 004 \\ 332 \end{array}$	$ \begin{array}{r} 1. \ 81 \\ \hline 1. \ 62 \\ 1. \ 58 \\ 1. \ 50 \\ \end{array} $	$\begin{array}{c} 20\\ \overline{15}\\ 2\\ 23\end{array}$	$\begin{array}{c} 1. \ 818 \\ 1. \ 699 \\ 1. \ 619 \\ 1. \ 573 \\ 1. \ 500 \end{array}$	$50 \\ 10 \\ 40 \\ 20 \\ 60$	$\begin{array}{c} 1.\ 8100\\ 1.\ 6926\\ 1.\ 6195\\ 1.\ 5722\\ 1.\ 4999 \end{array}$	15 2 10 5 13	
$323 \\ 204 \\ 224 \\ 521 \\ 512$	$ \begin{array}{c} 1. \ 45 \\ \overline{1. \ 348} \\ \overline{1. \ 296} \end{array} $	$ 18 \overline{13} \overline{10} $	$ \begin{array}{r} 1. 446 \\ 1. \overline{3}\overline{4}\overline{1} \\ 1. \overline{2}\overline{9}\overline{7} \end{array} $	$\begin{array}{c} 60\\ \overline{80}\\ \overline{80}\\ \overline{80}\end{array}$	$\begin{array}{c} 1.\ 4499\\ 1.\ 4423\\ 1.\ 3397\\ 1.\ 3146\\ 1.\ 2946 \end{array}$	5 6 8 4 10	
$\begin{array}{c} 440 \\ 600 \\ 404 \\ 532 \\ 620 \end{array}$	1. 212 1. 190 1. 156	 5 8 	$ \begin{array}{r} 1. \ 207 \\ 1. \ 192 \\ 1. \ 1630 \\ \\ \end{array} $	$ \begin{array}{r} 30 \\ 40 \\ 60 \\ \end{array} $	$\begin{array}{c} 1.\ 2809\\ 1.\ 2069\\ 1.\ 1877\\ 1.\ 1554\\ 1.\ 1446 \end{array}$	$\begin{array}{c} 4\\ 4\\ 4\\ 6\\ 6\\ 6\end{array}$	
$\begin{array}{c} 424 \\ 116 \\ 640 \\ 534 \\ 712 \end{array}$	$ \begin{array}{c} 1.\ 132 \\ 1.\ 029 \\ 1.\ 002 \\ \end{array} \\ \left. \begin{array}{c} 0.\ 975 \end{array} \right. $	8 8 5 8	 		1. 1281 1. 0270 1. 0040 0. 9738	8 4 3 4	
$316 \\ 624 \\ 732 \\ 406 \\ 800$. 9533 . 9258 . 9100 . 9077 . 9051	$4 \\ 5 \\ 4 \\ 2 \\ 4$	

ASTM cards

Card number	Index lines	Radiation	Source
1-1215	2.192.294.39	Molybde- num.	Han awalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Vegard [2] 1922	Copper	1. 54 A

NBS sample. The sample of calcium nitrate was obtained from the Fisher Scientific Co. as the tetrahydrate. It was dehydrated at 700° C, and protected from the air by mixing with Dow Corning high vacuum grease. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of magnesium and silicon; 0.001 to 0.01 percent each of aluminum, barium, iron, sodium, and strontium; and 0.0001 to 0.001 percent each of silver, potassium, and manganese.

The sample is colorless. The index of refraction is 1.609.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units, and the d-values of the Vegard pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel Vegard National Bureau of Standards	$222 \\ 311 \\ 222$	$311 \\ 222 \\ 111$	$111 \\ 210 \\ 210$

Structural data. Jaeger and Melle [3] in 1928 determined that calcium nitrate has the space group T_h^e -Pa3 and 4[Ca(NO₃)₂] per unit cell. Calcium nitrate is used as a structure type. The unit-cell measurements reported by Vegard

The unit-cell measurements reported by Vegard and by Ringdal have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

192 193 193 195 195 195 1	Vegard [2]. Ringdal [4]. Menary [5]. National Bureau of Stand- ards.	A 7. 62 7. 615 7. 590 at 24° C 7.600 at 25° C

The density of calcium nitrate calculated from the NBS lattice constant is 2.482 at 25° C.

Calcium Nitrate, Ca(NO₃)₂ (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			19381922Hanawalt, Rinn, and FrevelVegardMo, 0.7107 ACu, 1.54 A				1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι	a	d	Ι	a `	d	Ι	a	
$ \begin{array}{c} 111\\ \overline{210}\\ 211\\ 220\\ 221\\ 311\\ 222\\ 321\\ 400\\ \end{array} $	$\begin{array}{c} A\\ 4, 40\\ \hline 3, 40\\ 3, 10\\ 2, 68\\ \hline 2, 53\\ 2, 29\\ 2, 19\\ 2, 01\\ 1, 89\\ \end{array}$	$ \begin{array}{r} 60 \\ -50 \\ 50 \\ 2 \\ 4 \\ 80 \\ 100 \\ 2 \\ 30 \\ \end{array} $	$\begin{array}{c} A\\ 7.\ 62\\ \hline 7.\ 60\\ 7.\ 59\\ 7.\ 58\\ \hline 7.\ 59\\ 7.\ 59\\ 7.\ 59\\ 7.\ 59\\ 7.\ 59\\ 7.\ 52\\ 7.\ 56\end{array}$	$\begin{array}{c} A \\ 4.45 \\ 3.92 \\ 3.46 \\ 3.14 \\ \hline \\ \hline \\ 2.31 \\ 2.20 \\ \hline \\ 1.91 \end{array}$	W W M M S S S M	$\begin{array}{c} A \\ 7.71 \\ \hline 7.769 \\ \hline 7.66 \\ 7.62 \\ \hline 7.64 \end{array}$	$\begin{array}{r} & A \\ 4.39 \\ \hline 3.40 \\ 3.10 \\ 2.69 \\ \hline 2.53 \\ 2.292 \\ 2.194 \\ 2.032 \\ 1.900 \end{array}$	$97 \\ -50 \\ 60 \\ 8 \\ 14 \\ 73 \\ 100 \\ 5 \\ 27 \\ 27$	$\begin{array}{c} A\\ 7.\ 60\\ \hline 7.\ 60\\ 7.\ 60\\ 7.\ 60\\ 7.\ 60\\ 7.\ 603\\ 7.\ 601\\ 7.\ 603\\ 7.\ 599\end{array}$	
$\begin{array}{c} 411\\ 331\\ 420\\ 421\\ 332\\ 422\\ 511\\ 432\\ 440\\ \end{array}$	$ \begin{array}{c} 1. 78 \\ 1. 73 \\ 1. 69 \\ 1. 65 \\ 1. 61 \\ 1. 54 \\ 1. 46 \\ 1. 408 \\ 1. 341 \end{array} $	$ \begin{array}{r} 12\\ 10\\ 2\\ 2\\ 4\\ 10\\ 4\\ 14\\ \end{array} $	$\begin{array}{c} 7.55\\ 7.54\\ 7.56\\ 7.56\\ 7.56\\ 7.55\\ 7.55\\ 7.55\\ 7.59\\ 7.58\\ 7.59\\ 7.59\end{array}$	 1. 46 	 w m	 7. 59 7. 59	$\begin{array}{c} 1.\ 791\\ 1.\ 743\\ 1.\ 699\\ 1.\ 658\\ 1.\ 620\\ \hline 1.\ 551\\ 1.\ 462\\ 1.\ 4110\\ 1.\ 3432\\ \end{array}$	$ \begin{array}{c} 10 \\ 8 \\ 8 \\ 1 \\ 1 \\ 2 \\ 6 \\ 3 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10$	7. 600 7. 599 7. 599 7. 600 7. 598 7. 598 7. 598 7. 598 7. 598 7. 598	

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1922 Vegard Cu, 1.54 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	I	a	d	Ι	a	d	Ι	a
$600 \\ 610 \\ 611 \\ 620 \\ 621$	A 		A 	A 		A 	$\begin{array}{c} A\\ 1.\ 2668\\ 1.\ 2497\\ 1.\ 2330\\ 1.\ 2019\\ 1.\ 1871 \end{array}$	2 < 1 < 1 < 1 < 1 < 1 < 1 < 1	$\begin{matrix} A \\ 7.\ 601 \\ 7.\ 602 \\ 7.\ 601 \\ 7.\ 602 \\ 7.\ 601 \end{matrix}$
$533 \\ 622 \\ 630 \\ 444 \\ 543$	1. 142	 	7.58	1. 146 1. 094	m 	7.60	$\begin{array}{c} 1.\ 1589\\ 1.\ 1459\\ 1.\ 1332\\ 1.\ 0969\\ 1.\ 0750 \end{array}$	${}^{4}_{{<1}}{{<1}\atop{<1}\atop{<1}}$	$\begin{array}{c} 7. \ 599 \\ 7. \ 601 \\ 7. \ 602 \\ 7. \ 600 \\ 7. \ 601 \end{array}$
$711 \\ 641 \\ 642 \\ 722 \\ 731$				1. 013 0. 9865	 	7. 58 7. 58	$\begin{array}{c} 1.\ 0642\\ 1.\ 0439\\ 1.\ 0156\\ 1.\ 0064\\ 0.\ 9894 \end{array}$	$< \begin{smallmatrix} 1 \\ 1 \\ 2 \\ 1 \\ 3 \end{smallmatrix}$	$\begin{array}{c} 7. \ 600 \\ 7. \ 600 \\ 7. \ 600 \\ 7. \ 598 \\ 7. \ 600 \end{array}$
$650 \\ 810 \\ 820 \\ 821 \\ 822$					 		$\begin{array}{c} . \ 9730 \\ . \ 9428 \\ . \ 9217 \\ . \ 9150 \\ . \ 8956 \end{array}$	$<1 \\ <1 \\ <1 \\ <1 \\ <1 \\ <1 \end{cases}$	$\begin{array}{c} 7.\ 599\\ 7.\ 601\\ 7.\ 600\\ 7.\ 601\\ 7.\ 599 \end{array}$
$831 \\ 751 \\ 662 \\ 840 \\ 911 \\ 0.42$. 8347		7. 60	$\begin{array}{c} 8835 \\ .8775 \\ .8718 \\ .8496 \\ .8342 \end{array}$	≤ 1 ≤ 1 1 2	7. 600 7. 599 7. 600 7. 599 7. 600
842 Average	of last five li		7. 59			7. 59	. 8293	1	7. 601

Calcium Nitrate, Ca(NO₃)₂ (cubic)-Continued

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Calcium Sulfide (oldhamite), CaS (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0980	$\begin{array}{c} 2.85\\ 2.00\\ 1.27\end{array}$	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Kustner [2] 1922	Copper	Ka
Holgersson [3] 1923	Copper	Ka
Oftedal [4] 1927	Copper	Ka

NBS sample. The sample of calcium sulfide

was obtained from the Fisher Scientific Co. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of silicon and strontium; 0.01 to 0.1 percent each of aluminum.

barium, iron, magnesium, titanium, and vanadium; 0.001 to 0.01 percent each of copper, manganese, nickel, and lead; and 0.0001 to 0.001 percent each of boron, chromium, potassium, and lithium.

The sample has a tan color. The refractive index is too high to be determined by the conventional liquid grain immersion method.

Interplanar spacings and intensity measure-ments. The *d*-values reported by Hanawalt, Rinn, and Frevel have been converted from kX to angstrom units. The d-values of the Kustner, Holgersson, and Oftedal patterns were calculated from reported Bragg angle data. The Kustner pattern did not include intensity measurements.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel Holgersson Oftedal National Bureau of Standards	$200 \\ 200 \\ 420 \\ 200$	$220 \\ 220 \\ 600 \\ 220$	$\begin{array}{r} 420 \\ 420 \\ 620 \\ 222 \end{array}$

Structural data. Kustner [2] in 1922 determined that calcium sulfide has sodium chloridetype structure, the space group O_h^5 -Fm3m, and 4(CaS) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units and the cell measurement reported by Davey [5] has been doubled for comparison with the NBS value.

Lattice constants

		······································
1922 1923 1923 1927 1927 1927 1948 1956	Kustner [2] Holgersson [3] Davey [5] Oftedal [4] Goldschmidt [6] Primak, Kaufman, and Ward [7]. Güntert and Faessler [8]	A 5.75 5.611 5.697 5.70 5.69 5.69 5.6951 5.6905 at 21.5°
1957	National Bureau of Stand- ard _S .	C. 5.6948 at 25° C.

The density of calcium sulfide calculated from the NBS lattice constant is 2.594 at 25° C.

Calcium Sulfide (old)	iamite), CaS ((cubic)
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hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1922 Kustner Cu, 1.5418 A		1923 Holgersson Cu, 1.5418 A		1927 Oftedal Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C						
	d	I	a	d	I	a	d	I	a	d	I	a	d	I	a
$ \begin{array}{c} 111\\200\\220\\311\\222\\400\\331\\420\\422\\\\440\\600\\620\\622\\444\\640\end{array} $	A 2. 85 2. 00 1. 63 1. 422 1. 271 1. 160 1. 006 0. 948 . 899 . 858 . 790 (*)	$ \begin{array}{r} 100 \\ 100 \\ 50 \\ 16 \\ \overline{60} \\ 32 \\ \\ 6 \\ 14 \\ 8 \\ 6 \\ \\ 5 \end{array} $	<i>A</i> 5. 70 5. 66 5. 65 5. 688 5. 684 5. 683 5. 691 5. 688 5. 686 5. 691 5. 697	<i>A</i> 2. 88 2. 03 1. 66 1. 43 1. 28 1. 17 1. 01 0. 956 . 908 . 867 		<i>A</i> 5. 76 5. 74 5. 75 5. 72 5. 72 5. 72 5. 72 5. 73 5. 71 5. 74 5. 74 5. 75 	A 2. 77 1. 98 1. 69 1. 63 1. 40 1. 26 1. 15 1. 09 0. 996 	vs vs vs vs vs m vs vs vs us m vs 	A 5. 54 5. 60 5. 65 5. 60 5. 63 5. 63 5. 63 5. 63 5. 63 	A 1. 28 1. 01 0. 950 . 900 		A 	$\begin{array}{c} A\\ 3.28\\ 2.846\\ 2.013\\ 1.717\\ 1.6439\\ 1.4238\\ 1.3065\\ 1.2737\\ 1.1627\\ 1.1627\\ 1.0068\\ 0.9491\\ .9005\\ .8585\\ .8220\\ .7897\\ \end{array}$	$ \begin{array}{c} <1 \\ 100 \\ 68 \\ <1 \\ 21 \\ 9 \\ <1 \\ 20 \\ 14 \\ \\ 4 \\ 8 \\ 7 \\ 7 \\ 1 \\ 7 \\ 7 \\ 1 \\ 7 \end{array} $	A 5. 70 5. 693 5. 694 5. 695 5. 695 5. 696 5. 696 5. 696 5. 696 5. 696 5. 6953 5. 6946 5. 6953 5. 6946 5. 6950 5. 6946
Avera	ge of last s	five	5. 691			5. 73			5. 62			5. 71			5. 6948

* Three additional lines are omitted.

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Cesium Sulfate, Cs_2SO_4 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0685	$3. 28 \\ 3. 14 \\ 2. 27$	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of cesium sulfate was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, potassium, magnesium, and rubidium; 0.001 to 0.01 percent each of aluminum, barium, germanium, sodium, silicon, and strontium; and 0.0001 to 0.001 percent each of iron and lithium.

The sample is colorless and optically negative with the indices of refraction $N\alpha = 1.561$, $N\beta =$ 1.570, N γ =1.572, and 2V \simeq 60°.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel.	022, 112	130, 200	042, 222
National Bureau of Standards.	022, 112	130	200

Structural data. Ogg [2] in 1928 determined that cesium sulfate has potassium sulfate-type structure, the space group D¹⁶_{2h}-Pmcn, and $4(Cs_2SO_4)$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	с
1916 1928 1930 1930 1957	Ogg and Hopwood [3]. Taylor and Boyer [4]. Ogg [5]. Tutton [6] National Bureau of Standards.	$\begin{matrix} A \\ 6. \ 231 \\ 6. \ 25 \\ 6. \ 261 \\ 6. \ 25 \\ 6. \ 264 \end{matrix}$	$\begin{array}{c} A \\ 10. \ 906 \\ 10. \ 94 \\ 10. \ 959 \\ 10. \ 95 \\ 10. \ 95 \\ 10. \ 95 \end{array}$	A 8. 215 8. 24 8. 254 8. 25 8. 242 at 25° C

The density of cesium sulfate calculated from the NBS lattice constants is 4.250 at 25° C.

References

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 [3] A. Ogg and F. L. Hopwood, A critical test of the super transmission of the super submerts like and the super transmission.
- crystallographic law of valency volumes; crystalline

hkl	1938 Hanawalt, and Frey Mo, 0.710	Rinn, vel 07 A	1957 National Bu of Standa Cu, 1.5405 A,	ireau rds 25° C
	d	Ι	d	Ι
$\begin{array}{c} 020 \\ 111 \\ 012 \\ 121 \\ 102 \end{array}$	$\begin{array}{c} A \\ \hline 4.56 \\ \hline 3.68 \\ \hline \end{array}$	$\begin{array}{c} \overline{10} \\ \overline{35} \\ \end{array}$	$\begin{array}{c} A \\ 5. 47 \\ 4. 54 \\ 3. 85 \\ 3. 684 \\ 3. 441 \end{array}$	$\begin{array}{c} 6 \\ 13 \\ 11 \\ 43 \\ 11 \end{array}$
$\begin{array}{c} 031 \\ 022 \\ 112 \\ 130 \\ 200 \end{array}$	$ \left. \begin{array}{c} 3.29 \\ 3.15 \end{array} \right. \right\} $	100 100	$\begin{cases} 3. \ 333 \\ 3. \ 290 \\ 3. \ 285 \\ \{ 3. \ 152 \\ 3. \ 129 \end{cases}$	
$131 \\ 122 \\ 040 \\ 220 \\ 013$	2. 91 2. 73 2. 66	$\begin{array}{c}5\\ 10\\\\ 20 \end{array}$	2. 949 2. 913 2. 736 2. 728 2. 665	$egin{array}{c} 4 \\ 9 \\ 12 \\ 10 \\ 27 \end{array}$
$\begin{array}{c} 041 \\ 221 \\ 212 \\ 141 \\ 042 \\ 222 \end{array}$	$ \left. \begin{array}{c} 2.59 \\ 2.42 \\ 2.28 \end{array} \right. $	20 10 45	$\left\{\begin{array}{ccc} 2.599\\ 2.580\\ 2.432\\ 2.400\\ 2.279\\ 2.279\\ 2.270\end{array}\right.$	$10 \\ 18 \\ 11 \\ 11 \\ 22 \\ 26$
$\begin{array}{c} 033 \\ 142 \\ 051 \\ 240 \\ 232 \\ 213 \end{array}$	$ \begin{array}{c} 2. 20 \\ -2. 11 \\ \\ 2. 04 \end{array} $	5 5 10	$ \begin{array}{c} 2. \ 194 \\ 2. \ 143 \\ 2. \ 115 \\ 2. \ 062 \\ \left\{ \begin{array}{c} 2. \ 057 \\ 2. \ 029 \end{array} \right. \end{array} $	$ \begin{array}{c} 11 \\ 8 \\ 11 \\ 4 \\ 7 \\ 12 \end{array} $
$151 \\ 104 \\ 052 \\ 024 \\ 321$	 1. 93	 5 	$\begin{array}{c} 2.\ 004 \\ 1.\ 957 \\ 1.\ 933 \\ 1.\ 929 \\ 1.\ 899 \end{array}$	$5 \\ 3 \\ 2 \\ 10 \\ 3$
$143 \\ 124 \\ 312 \\ 060 \\ 330$	} 1. 84 1. 80	15 5	$\left\{\begin{array}{c} 1.853\\ 1.842\\ 1.836\\ 1.824\\ 1.812\end{array}\right.$	$18 \\ 2 \\ 11 \\ 4 \\ 8$
$233 \\ 034 \\ 251 \\ 134 \\ 161$	1. 75 1. 71	 5 5	$\begin{array}{c} 1.\ 797\\ 1.\ 794\\ 1.\ 753\\ 1.\ 724\\ 1.\ 713 \end{array}$	$\begin{array}{c}4\\4\\9\\2\\2\end{array}$
$\begin{array}{c} 062 \\ 153 \\ 224 \\ 015 \\ 341 \end{array}$			$\begin{array}{c} 1.\ 668\\ 1.\ 652\\ 1.\ 642\\ 1.\ 630\\ 1.\ 627\end{array}$	ert ert ert ert ert ert ert ert
$\begin{array}{c} 162 \\ 260 \end{array}$	1. 57	-10^{-10}	$\begin{array}{c} 1.\ 612 \\ 1.\ 576 \end{array}$	1 4

structures of the alkali sulfates, Phil. Mag. 32. 518-525 (1916). [4] W. Taylor and T. Boyer, An investigation into the

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 [5] A. Ogg, The space group of the alkali sulfates, Phil. Mag. 9, 665-667 (1930).
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- (1930).

Gold Antimony (aurostibite), AuSb₂ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
5-0718	2. 003 3. 33 2. 98	Copper	Graham and Kai- man [1] 1952.

Additional published patterns

Source	Radiation
Oftedal [2] 1928	Copper, 1.539 A
Bottema and Jaeger [3] 1932	Copper, 1.539 A

NBS sample. The sample of gold antimony was prepared at NBS by D. E. Roberts. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of palladium; 0.001 to 0.01 percent each of copper, iron, mercury, lead, and silicon; and 0.0001 to 0.001 percent each of aluminum, magnesium, nickel, and tin.

The sample has a gray metallic luster and is opaque.

Interplanar spacings and intensity measurements. The *d*-values reported by Graham and Kaiman were converted from kX to angstrom units, and the values of the Oftedal and of the Bottema and Jaeger patterns were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Graham and Kaiman Oftedal Bottema and Jaeger National Bureau of Standards	$311 \\ 311 \\ 311 \\ 311 \\ 311$	$200 \\ 511 \\ 511 \\ 210$	$731 \\ 731 \\ 200 \\ 200$

Structural data. Oftedal [2] in 1928 determined that gold antimony has pyrite-type structure, the space group T_b^{\bullet} -Pa3, and 4(AuSb₂) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

anda

The density of gold antimony calculated from the NBS lattice constant is 9.907 at 25°C.

Gold Antimony (aurostibite), AuSb₂ (cubic)

hkl	1952 Graham and I Cu, 1.542		Kaiman A	C	1928 Oftedal Su, 1.542	A	Botter	1932 na and u, 1.542	Jaeger A	Natio S Cu, 1.	1957 nal Bur tandarc 5405 A,	reau of ls 25° C
	d	I	a	d	Ι	a	d	I	a	d	Ι	a
$ \begin{array}{r} 111 \\ 200 \\ 210 \\ 211 \\ 220 \\ \end{array} $	$\begin{matrix} A \\ 3.83 \\ 3.33 \\ 2.98 \\ 2.72 \\ 2.34 \end{matrix}$	$10 \\ 50 \\ 40 \\ 30 \\ 40$	$\begin{array}{c} A \\ 6.\ 63 \\ 6.\ 66 \\ 6.\ 66 \\ 6.\ 66 \\ 6.\ 62 \end{array}$	$ \begin{array}{r} A \\ \overline{3.32} \\ 2.97 \\ 2.71 \\ 2.35 \\ \end{array} $	m m m m	$\begin{array}{c} A \\ \hline 6. \ 64 \\ 6. \ 64 \\ 6. \ 65 \end{array}$	$\begin{matrix} A \\ 3.82 \\ 3.31 \\ 2.97 \\ 2.70 \\ 2.34 \end{matrix}$	$30 \\ 60 \\ 60 \\ 50 \\ 50 \\ 50$	$\begin{matrix} A \\ 6. \ 62 \\ 6. \ 62 \\ 6. \ 64 \\ 6. \ 61 \\ 6. \ 62 \end{matrix}$	$\begin{array}{r} A\\ 3.85\\ 3.33\\ 2.98\\ 2.719\\ 2.356\end{array}$	$32 \\ 69 \\ 74 \\ 55 \\ 54$	$\begin{array}{c} A \\ 6.\ 67 \\ 6.\ 67 \\ 6.\ 66 \\ 6.\ 66 \\ 6.\ 663 \end{array}$
	$ \begin{array}{r} \overline{2.003} \\ 1.918 \\ 1.840 \\ 1.777 \end{array} $	$100 \\ 10 \\ 10 \\ 10 \\ 20$	$ \begin{array}{r} 6. \ 64 \\ 6. \ 64 \\ 6. \ 63 \\ 6. \ 65 \end{array} $	$ \begin{array}{r} 1.97 \\ 1.92 \\ 1.84 \\ 1.77 \\ 1.77 $	vs vvw w w+	$\begin{array}{c} 6.53 \\ 6.65 \\ 6.63 \\ 6.62 \end{array}$	$\begin{array}{c} 2. \ 22 \\ 2. \ 00 \\ 1. \ 92 \\ 1. \ 84 \\ 1. \ 77 \end{array}$	$ \begin{array}{r} 40 \\ 100 \\ 30 \\ 40 \\ 50 \end{array} $	$ \begin{array}{r} \overline{6.} & \overline{64} \\ \overline{6.} & \overline{65} \\ \overline{6.} & \overline{63} \\ \overline{6.} & \overline{62} \end{array} $	$\begin{array}{c} 2.\ 009\\ 1.\ 922\\ 1.\ 848\\ 1.\ 779 \end{array}$	$100 \\ 17 \\ 16 \\ 30$	$\begin{array}{c} 6.\ 663\\ 6.\ 659\\ 6.\ 664\\ 6.\ 658\end{array}$
$\begin{array}{r} 400\\ 331\\ 420\\ 421\\ 332 \end{array}$	$ \begin{array}{r} 1.524\\ 1.485\\ 1.448\\ 1.417 \end{array} $	$ \begin{bmatrix} -\overline{5} \\ 10 \\ 10 \\ $	$ \begin{array}{r} 6. \ 64 \\ 6. \ 64 \\ 6. \ 64 \\ 6. \ 65 \end{array} $	$1. \ 64 \\ 1. \ 52 \\ 1. \ 48 \\ 1. \ 45 \\ 1. \ 41$	$\begin{array}{c} m+\\ vw\\ w-\\ m+\\ m \end{array}$	$\begin{array}{c} 6. \ 56 \\ 6. \ 62 \\ 6. \ 62 \\ 6. \ 64 \\ 6. \ 61 \end{array}$	$ \begin{array}{r} 1.52\\ 1.49\\ 1.45\\ 1.42 \end{array} $	$ar{10}\ 30\ 20\ 20\ 20$	$ \begin{array}{r} \hline 6. \ 62 \\ 6. \ 66 \\ 6. \ 64 \\ 6. \ 66 \\ \end{array} $	$\begin{array}{c} 1.\ 664\\ 1.\ 528\\ 1.\ 489\\ 1.\ 452\\ 1.\ 419 \end{array}$	$ \begin{array}{c} 6 \\ 11 \\ 12 \\ 7 \\ 6 \end{array} $	$\begin{array}{c} 6. \ 656 \\ 6. \ 660 \\ 6. \ 657 \\ 6. \ 655 \\ 6. \ 657 \end{array}$
$ \begin{array}{r} 422 \\ 511 \\ 432 \\ 521 \\ \end{array} $	$ \begin{array}{r} 1. 356 \\ \overline{1. 280} \\ 1. 233 \\ 1. 213 \end{array} $	$ 10 \\ \overline{30} \\ 10 \\ 5 5 $	$ \begin{array}{r} 6. \ 64 \\ \overline{6.} \ \overline{65} \\ 6. \ 64 \\ 6. \ 64 \end{array} $	$\begin{array}{c} 1. \ 35 \\ 1. \ 30 \\ 1. \ 28 \\ 1. \ 23 \\ 1. \ 21 \end{array}$	m+ w- vs m+ m-	$ \begin{array}{r} 6. \ 61 \\ \overline{6.} \ \overline{65} \\ 6. \ 62 \\ 6. \ 63 \end{array} $	$\begin{array}{c} 1. \ 36 \\ 1. \ 30 \\ 1. \ 28 \\ 1. \ 24 \\ 1. \ 21 \end{array}$	$20 \\ 10 \\ 80 \\ 20 \\ 20 \\ 20$	$ \begin{array}{r} 6. \ 66 \\ \overline{6.} \ \overline{65} \\ 6. \ 68 \\ 6. \ 63 \end{array} $	$ \begin{array}{r} 1.359\\ \overline{1.282}\\ 1.236\\ 1.215 \end{array} $	$10\\ \overline{25}\\ 10\\ 6$	$\begin{array}{c} 6. \ 657 \\ \hline 6. \ 659 \\ \hline 6. \ 657 \\ \hline 6. \ 656 \end{array}$
$\begin{array}{c} 440 \\ 531 \\ 600 \\ 610 \\ 611 \end{array}$	$\left. \begin{array}{c} 1. \ 177 \\ 1. \ 126 \\ 1. \ 109 \\ \end{array} \right\} \\ \left. \begin{array}{c} 1. \ 080 \end{array} \right. \right\}$	$20 \\ 5 \\ 10 \\ 10 \\ 10$	6. 66 6. 66 6. 65	$\begin{cases} 1. \ 17 \\ 1. \ 12 \\ 1. \ 11 \\ \{ 1. \ 09 \\ 1. \ 07 \end{cases}$	s+ w+ m s- m	6. 62 6. 63 6. 66 6. 63 6. 60	$\left. \begin{array}{c} 1. \ 18 \\ 1. \ 13 \\ 1. \ 11 \\ \end{array} \right\} \left. \begin{array}{c} 1. \ 08 \end{array} \right.$	50 20 20 20 20	6. 68 6. 69 6. 66	$\left\{\begin{array}{c}1.\ 1769\\1.\ 1254\\1.\ 1096\\1.\ 0945\\1.\ 0801\end{array}\right.$	$ \begin{array}{r} 16 \\ 2 \\ 2 \\ 1 \\ 2 \end{array} $	$\begin{array}{c} 6. \ 658 \\ 6. \ 658 \\ 6. \ 658 \\ 6. \ 568 \\ 6. \ 658 \\ 6. \ 658 \end{array}$

hkl	1952 Graham and Kaiman Cu, 1.542 A		1928 Oftedal Cu, 1.542 A		1932 Bottema and Jaeger Cu, 1.542 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C				
	d	Ι	a	d	Ι	a	d	Ι	a	d	Ι	a
$ \begin{array}{r} 620 \\ 533 \\ 622 \\ 630 \\ 631 \\ \hline 711 \\ 640 \\ \end{array} $	$\begin{array}{c} A \\ 1.\ 050 \\ 1.\ 013 \\ 1.\ 003 \\ 0.\ 991 \\ .\ 981 \\ \hline \\ \hline \\ .\ 934 \\ .\ 923 \end{array}$	$520 \\ 555 \\ 55 \\ 510 \\ 510 \\ 55 $	$\begin{array}{c} A \\ 6. \ 64 \\ 6. \ 65 \\ 6. \ 65 \\ 6. \ 65 \\ 6. \ 65 \\ \hline 6. \ 65 \\ \hline \\ 6. \ 67 \\ 6. \ 66 \end{array}$	$\begin{matrix} A \\ 1.\ 05 \\ 1.\ 01 \\ 1.\ 00 \\ 0.\ 989 \\ .\ 978 \\ .\ 956 \\ .\ 928 \\ .\ 919 \end{matrix}$	m s w w- w+ vw w	$\begin{array}{c} A \\ 6. 64 \\ 6. 62 \\ 6. 63 \\ 6. 63 \\ 6. 63 \\ \hline 6. 63 \\ \hline 6. 63 \\ 6. 63 \end{array}$	A 1. 05 1. 02 1. 00 0. 992 . 960	20 30 10 10 20 	A 6. 64 6. 69 6. 63 6. 65 	$\begin{array}{c} A \\ 1, 0526 \\ 1, 0153 \\ 1, 0039 \\ 0, 9925 \\ . 9816 \\ \hline \\ . 9324 \\ . 9233 \end{array}$	$1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ < 1 \\ $	$\begin{array}{c} A \\ 6.\ 657 \\ 6.\ 658 \\ 6.\ 659 \\ 6.\ 658 \\ 6.\ 657 \\ \hline 6.\ 659 \\ 6.\ 657 \\ \hline 6.\ 659 \\ 6.\ 658 \\ \hline \end{array}$
$\begin{array}{c} 641 \\ 721 \end{array}$. 914 . 906	$10\\10$	6. 65 6. 66	.912 .903	w m	$\begin{array}{c} 6. \ 64 \\ 6. \ 64 \end{array}$.9148 .9060	≥ 1 1	6. 660 6. 658
$642 \\ 731 \\ 650 \\ 732 \\ 800$. 890 . 867 . 853 . 846 . 833	$20 \\ 50 \\ 10 \\ 10 \\ 20$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$. 887 . 863 	s vs	6. 64 6. 63 	. 888 . 866 	30 60 	6. 64 6. 65 	. 8898 . 8669 . 8526 . 8459 . 8324	$\stackrel{1}{\stackrel{15}{<1}}_{\stackrel{1}{1}}$	$\begin{array}{c} 6. \ 659 \\ 6. \ 659 \\ 6. \ 659 \\ 6. \ 660 \\ 6. \ 6592 \end{array}$
$820 \\ 821 \\ 653 \\ 822$. 808 . 802 . 796 . 785	$\begin{array}{c} 20\\ 20\\ 5\\ 40 \end{array}$	$\begin{array}{c} 6. \ 66 \\ 6. \ 66 \\ 6. \ 66 \\ 6. \ 66 \\ \end{array}$					 		$\begin{array}{c} . \ 8076 \\ . \ 8016 \\ . \ 7959 \\ . \ 7847 \end{array}$	$<^2_1_2$	$\begin{array}{c} 6. \ 6593 \\ 6. \ 6588 \\ 6. \ 6588 \\ 6. \ 6586 \end{array}$
Avera line	ge of las	t five	6. 66			6. 64			6. 62			6. 6589

Gold Antimony (aurostibite), AuSB₂ (cubic)-Continued

References

- A. R. Graham and S. Kaiman, Aurostibite, AuSb₂; a new mineral in the pyrite group, Am. Mineralogist 37, 461-469 (1952).
 I. Oftedal, Über die Kristallstrukturen der Verbindungen
- [2] I. Oftedal, Über die Kristallstrukturen der Verbindungen RuS₂, OsS₂, MnTe₂ und AuSb₂, Z. physik. Chem. 135, 291-299 (1928).
- [3] J. A. Bottema and F. M. Jaeger, On the law of additive atomic heats in intermetallic compounds. IX. The compounds of tin and gold, and of gold and antimony, Proc. Acad. Amsterdam 35, 916–928 (1932).
- (1932).
 [4] O. Nail, A. Almin, and A. Westgren, Röntgenanalyse der Systeme Gold-Antimon und Silber-Zinn, Z. physik. Chem. 14, 81–90 (1931).

Gold Tin, AuSn (hexagonal)

ASTM cards. None.

Additional published patterns

Source	Radiation
Preston and Owen [1] 1927	Copper, 1.537
Bottema and Jaeger [2] 1932	Copper, K_{α}

NBS sample. The sample of gold tin was prepared at NBS by D. E. Roberts as a single crystal grown from a melt. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of palladium; 0.001 to 0.01 percent of copper; and 0.0001 to 0.001 percent each of silver, iron, and silicon. The sample is opaque and has a bright silver metallic luster.

Interplanar spacings and intensity measurements. The *d*-values of the Preston and Owen and of the Bottema and Jaeger patterns were calculated from reported Bragg angle data. The intensity measurements reported by Preston and Owen are numbered from 1 to 22 in order of decreasing intensity. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Preston and Owen Bottema and Jaeger National Bureau of Standards	$102 \\ 102 \\ 102 \\ 102$	$110 \\ 110 \\ 110 \\ 110$	$212 \\ 202 \\ 100$

Structural data. Preston and Owen [1] determined that gold tin has nickel arsenide-type structure, the space group D_{6h}^4 -P6₃/mmc, and 2(AuSn) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

	1	Jat	tice	constan	ts
--	---	-----	------	---------	----

-		a	с
1927 1931 1932 1957	Preston and Owen [1] Stenbeck and Westgren [3]. Bottema and Jaeger [2] National Bureau of Standards.	$\begin{matrix} A \\ 4.318 \\ 4.323 \\ 4.316 \\ 4.323 \end{matrix}$	A 5.508 5.523 5.507 5.517 at 25° C.

The density of gold tin calculated from the NBS lattice constants is 11.74 at 25° C.

References

- G. D. Preston and E. A. Owen, The atomic structure of AuSn, Phil. Mag. 4, 133-147 (1927).
 J. A. Bottema and F. M. Jeager, On the law of additive atomic heats in intermetallic compounds. IX. The compounds of tin and gold, and of gold and anti-mory. Proc. Acad. Sci. Amsterdam 25, 016 002. (1932).
 [3] S. Stenbeck and A. Westgren, Röntgenanalyse der Gold-Zinn, Z. physik. Chem. 14B, 91-96 (1931).

Gold Tin AuSn (hexagonal)

hkl	192 Prestor Owe Cu, 1.5	7 and en 42 A	193 Bottem Jaeg Cu, 1.5	2 a and er 42 A	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	I a	d	Ι	d	Ι	
$100 \\ 101 \\ 102 \\ 110 \\ 200$	$\begin{array}{c} A\\ 3.\ 76\\ 3.\ 09\\ 2.\ 22\\ 2.\ 16\\ 1.\ 86\end{array}$	$7\\6\\1\\2\\22$	$\begin{array}{c} A\\ 3.\ 75\\ 3.\ 09\\ 2.\ 21\\ 2.\ 15\\ 1.\ 87\end{array}$	$ \begin{array}{r} 40 \\ 40 \\ 100 \\ 80 \\ 20 \end{array} $	$\begin{array}{c} A\\ 3.\ 74\\ 3.\ 09\\ 2.\ 222\\ 2.\ 161\\ 1.\ 870 \end{array}$	$51 \\ 45 \\ 100 \\ 65 \\ 7$	
$201 \\ 112 \\ 103 \\ 202 \\ 210$	$ \begin{array}{c} 1. 77 \\ 1. 71 \\ 1. 65 \\ 1. 55 \\ \end{array} $	22 22 22 5	1.77 1.664 1.541 1.410	$ \begin{array}{c} 20 \\ -\overline{20} \\ 50 \\ 10 \end{array} $	$\begin{array}{c} 1.\ 772\\ 1.\ 702\\ 1.\ 652\\ 1.\ 549\\ 1.\ 415 \end{array}$	$ \begin{array}{r} 10 \\ 4 \\ 9 \\ 27 \\ 9 \end{array} $	
	$ \begin{array}{r} \overline{1.37} \\ \overline{1.28} \\ \overline{1.25} \end{array} $	$\frac{\overline{16}}{\overline{17}}$	$\begin{array}{c} 1.\ 376\\ 1.\ 363\\ 1.\ 310\\ 1.\ 290\\ 1.\ 261 \end{array}$	$20 \\ 10 \\ 10 \\ 20 \\ 50$	$\begin{array}{c} 1.\ 3705\\ 1.\ 3120\\ 1.\ 2950\\ 1.\ 2592 \end{array}$		
$300 \\ 114 \\ 302 \\ 214 \\ 204$	1. 16 	4 	$ \begin{array}{c} 1. \ 241 \\ 1. \ 159 \\ \overline{1. \ 17} \\ 1. \ 106 \end{array} $	$20 \\ 50 \\ -\overline{10} \\ 10 \\ 10$	$\begin{array}{c} 1.\ 2475\\ 1.\ 1637\\ 1.\ 1372\\ 1.\ 1220\\ 1.\ 1112 \end{array}$	$\overset{8}{\overset{14}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{$	
$220 \\ 105 \\ 221 \\ 310 \\ 311$	$\left. \begin{array}{c} 1.\ 07 \\ \\ \\ \\ \\ \hline \\ 1.\ 02 \end{array} \right $	18 19	$ \begin{array}{c} 1. \ 076 \\ 1. \ 056 \\ \overline{1. \ 018} \end{array} $	10 10 -10	1. 0808 1. 0594 1. 0382 1. 0204	$\begin{array}{c c} 4 \\ <1 \\ <1 \\ 2 \end{array}$	
$222 \\ 214 \\ 312 \\ 205 \\ 400$	0. 985 . 964	19 9 	0. 985 . 970	20 30 	$\begin{array}{c} 1.\ 0063\\ 0.\ 9882\\ .\ 9720\\ .\ 9509\\ .\ 9361 \end{array}$	$arprojlim 2 \\ 2 \\ 6 \\ \leqslant 1 \\ 1 \\ 1$	
$304 \\ 313 \\ 106 \\ 402 \\ 215$. 892 . 885 	 8 10 	. 923 . 892 . 884	40 	. 9258 . 9042 . 8938 . 8863 . 8706	$4 \\ 2 \\ 5 \\ 3 \\ 2$	
$320 \\ 224 \\ 321 \\ 403 \\ 314$. 848	$\overline{10}^{}$ $\overline{22}^{}$. 8587 . 8509 . 8486 . 8342 . 8298	$ \begin{array}{c} 1 \\ 7 \\ 3 \\ 1 \\ 2 \end{array} $	
$305 \\ 206 \\ 322 \\ 410$	} 	 10			. 8259 . 8200 . 8171	4 7 11	

* The intensities of the Preston and Owen pattern are in order of decreasing intensity.

Lanthanum Fluoride, LaF₃ (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
3-1013	2. 08 2. 04 1. 82	Copper	Oftedal [1] 1929.

Additional published patterns. None.

NBS sample. The sample of lanthanum fluoride was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of calcium and cerium; 0.01 to 0.1 percent each of aluminum, magnesium, praseodymium, strontium, terbium, and yttrium; 0.001 to 0.01 percent each of iron and silicon; and 0.0001 to 0.001 percent each of manganese and nickel.

The sample is colorless. The indices of refraction could not be determined as the particle size is too small.

Interplanar spacings and instensity measurements. The *d*-values of the Oftedal pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Oftedal National Bureau of Standards	$\begin{array}{c} 300 \\ 111 \end{array}$	$\begin{array}{c}113\\113\end{array}$	302 300

Structural data. The structure of lanthanum fluoride was redetermined by Oftedal [2] in 1931. The postulated structure is D_{6h}^3 -P6₃/mcm with 6(LaF₃) per unit cell.

The unit-cell measurements reported by Oftedal have been converted from kX to angstrom units for comparison with the NBS values.

		a	с
1929 1957	Oftedal [1] National Bureau of Standards.	<i>A</i> 7. 177 7. 184	A 7.344 7.351 at 25° C

The density of lanthanum fluoride calculated from the NBS lattice constants is 5.939 at 25° C.

- I. Oftedal, Über die Kristallstruktur von Tysonit und einigen künstlich dargestellten Lanthanidenfluoriden, Z. physik. Chem. B5, 272-291 (1929).
- [2] I. Oftedal, Zur Kristallstruktur von Tysonit (Ce, La, . . .)F₃, Z. physik. Chem. B13, 190-200 (1931).

hkl	192 Ofteo Cu, 1.53	929 1957 tedal National Bure of Standards .5392 A Cu, 1.5405 A 25° C		7 Bureau dards .05 A, C
	d	Ι	d	I
$002 \\ 110 \\ 111 \\ 112 \\ 300$	A 3. 699 3. 250 2. 588 2. 092	w w- s+	A 3. 67 3. 59 3. 229 2. 569 2. 075	$40 \\ 32 \\ 100 \\ 11 \\ 51$
$113 \\ 004 \\ 302 \\ 221 \\ 114$	$\begin{array}{c} 2.\ 039\\ 1.\ 848\\ 1.\ 817\\ 1.\ 755+\\ 1.\ 646 \end{array}$	s+w-s+s	$\begin{array}{c} 2. \ 025 \\ 1. \ 8377 \\ 1. \ 8064 \\ 1. \ 7451 \\ 1. \ 6364 \end{array}$	$54 \\ 5 \\ 33 \\ 20 \\ 4$
$222 \\ 223 \\ 304 \\ 115 \\ 411$	$\begin{array}{c} 1. \ 622 \\ 1. \ 457 \\ 1. \ 385 + \\ 1. \ 369 \\ 1. \ 344 \end{array}$	w-smmmode m+mmmode	$\begin{array}{c} 1.\ 6142\\ 1.\ 4487\\ 1.\ 3755\\ 1.\ 3604\\ 1.\ 3354 \end{array}$	$3 \\ 14 \\ 10 \\ 7 \\ 15$
$224 \\ 412 \\ 006 \\ 330 \\ 413$	1. 294 1. 281 1. 234 1. 204 1. 194	vw + vw + w - w - s	$\begin{array}{c} 1.\ 2849\\ 1.\ 2737\\ 1.\ 2254\\ 1.\ 1974\\ 1.\ 1877 \end{array}$	$egin{array}{c} 2 \\ 4 \\ 2 \\ 6 \\ 14 \end{array}$
$116 \\ 332 \\ 225 \\ 414 \\ 306$	$\left. \begin{array}{c} 1.\ 167 \\ 1.\ 145 - \\ 1.\ 099 \\ 1.\ 062 \end{array} \right.$	w s w s	1. 1601 1. 1384 1. 0921 1. 0549	2 10 3 8
$\begin{array}{c} 600\\ 226\\ 117\\ 334\\ 415 \end{array}$	1. 042 1. 007 1. 002	w- w s+	$\begin{array}{c} 1.\ 0370\\ 1.\ 0120\\ 1.\ 0078\\ 1.\ 0033\\ 0.\ 9978 \end{array}$	3 2 3 4 9
$521 \\ 522 \\ 523 \\ 416 \\ 227$	0. 9918	m+ 	9872 9616 9228 9094 9066	6 2 5 3 3
$604 \\ 441 \\ 700 \\ 515 \\ 524$	}		.9030 .8913 .8898 .8759	4 4 2 2
$336 \\ 614 \\ 443 \\ 622 \\ 308 \\ 435$	}		. 8564 . 8433 . 8402	6 4 6
$\begin{array}{c} 417 \\ 710 \\ 525 \\ 711 \\ 444 \\ 712 \end{array}$	}		. 8306 . 8249 . 8190 . 8069 . 8042	6 6 2 3

Lanthanum Oxychloride, LaOCl (tetragonal)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wavelength	
Sillén and Nylander [1] 1941.	Chro- mium.	K_{lpha}	

NBS sample. The sample of lanthanum oxychloride was prepared by heating lanthanum chloride heptahydrate at 100° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of praseodymium and silicon; 0.001 to 0.01 percent of calcium; and 0.0001 to 0.001 percent each of chromium and magnesium.

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

Interplanar spacings and intensity measurements. The *d*-values of the Sillén and Nylander pattern were calculated from reported Bragg angle data. The three strongest lines for each pattern are as follows:

Pattern	1	2	3
Sillén and Nylander National Bureau of Standards	$\begin{array}{c} 101 \\ 102 \end{array}$	$\begin{array}{c} 110\\ 101 \end{array}$	$\begin{array}{c} 102\\110\end{array}$

Structural data. Sillén and Nylander [1] in 1941 determined that lanthanum oxychloride has lead chloride-type structure, the space group D_{4h}^{r} -P4/nmm and 2(LaOCl) per unit cell. The unit-cell measurements reported by Sillén

The unit-cell measurements reported by Sillén and Nylander have been converted from kX to angstrom units for comparison with the NBS values.

		a	с
$1941 \\ 1957$	Sillén and Nylander [1] National Bureau of Standards.	<i>A</i> 4. 117 4. 120	A 6.879 6.882 at 25° C

The density of lanthanum oxychloride calculated from the NBS lattice constants is 5.411 at 25° C.

References

 L. G. Sillén and A. Nylander, The crystal structure of LaOCl, LaOBr and LaOI, Svensk. Kem. Tid. 53, 367 (1941).

hkl	1941 Sillén and Nylander Cr, 2.2909 A		195 National of Stand Cu, 1.54 25°	7 Bureau dards 405 A, C
	d	Ι	d	Ι
$\begin{array}{c} 001 \\ 101 \\ 002 \\ 110 \\ 111 \end{array}$	$\begin{array}{c} A \\ \hline 3.52 \\ 3.43 \\ 2.90 \\ \hline \end{array}$	s W S	$\begin{array}{c} A \\ 6.89 \\ 3.54 \\ 3.441 \\ 2.914 \\ 2.681 \end{array}$	$30 \\ 89 \\ 10 \\ 80 \\ 7$
$102 \\ 003 \\ 112 \\ 200 \\ 103$	2. 63 2. 29 2. 22 2. 06 2. 00	s W S S W	$\begin{array}{c} 2. \ 642 \\ 2. \ 294 \\ 2. \ 224 \\ 2. \ 060 \\ 2. \ 005 \end{array}$	$100 \\ 7 \\ 28 \\ 42 \\ 5$
$201 \\ 113 \\ 211 \\ 202 \\ 004$	$\begin{array}{c} 1.\ 971\\ 1.\ 799\\ 1.\ 778\\ 1.\ 765\\ 1.\ 719 \end{array}$	w m m w vw	$\begin{array}{c} 1.\ 975\\ 1.\ 803\\ 1.\ 780\\ 1.\ 768\\ 1.\ 720\\ \end{array}$	$6 \\ 26 \\ 29 \\ 7 \\ 2$
$212 \\ 104 \\ 203 \\ 114 \\ 220$	$\begin{array}{c} 1. \ 622 \\ 1. \ 586 \\ 1. \ 532 \\ 1. \ 481 \\ 1. \ 455 \end{array}$	s m w w m	$1. 624 \\ 1. 587 \\ 1. 533 \\ 1. 481 \\ 1. 457$	$39 \\ 15 \\ 8 \\ 4 \\ 11$
$213 \\ 221 \\ 005 \\ 301 \\ 222$	$\begin{array}{c} 1.\ 436\\ 1.\ 425\\ 1.\ 375\\ 1.\ 346\\ 1.\ 341 \end{array}$	vw vvw vw vw vw	$\begin{array}{c} 1.\ 436\\ 1.\ 425\\ 1.\ 376\\ 1.\ 347\\ 1.\ 342 \end{array}$	2 2 2 7 4
$204 \\ 105 \\ 310 \\ 311 \\ 302$	$ \begin{array}{r} 1. 320 \\ 1. 305 \\ 1. 302 \\ \hline 1. 275 \end{array} $	vw vvw m m	$\begin{array}{c} 1.\ 321\\ 1.\ 306\\ 1.\ 303\\ 1.\ 2805\\ 1.\ 2754 \end{array}$	$\begin{array}{c}2\\3\\10\\4\\8\end{array}$
$214 \\ 115 \\ 223 \\ 312 \\ 303$	$1.257 \\ 1.244 \\ 1.229 \\ 1.218 \\ 1.178$	m w vw m— vw	$\begin{array}{c} 1.\ 2573\\ 1.\ 2444\\ 1.\ 2295\\ 1.\ 2186\\ 1.\ 1778\\ \end{array}$	$\begin{array}{c}13\\3\\4\\6\\1\end{array}$
$205 \\ 313 \\ 321 \\ 215 \\ 322$			$\begin{array}{c} 1.\ 1446\\ 1.\ 1328\\ 1.\ 1275\\ 1.\ 1027\\ 1.\ 0845 \end{array}$	$ \begin{array}{c c} $
$304 \\ 116 \\ 314 \\ 400 \\ 323$			$\begin{array}{c} 1.\ 0733\\ 1.\ 0672\\ 1.\ 0388\\ 1.\ 0302\\ 1.\ 0231 \end{array}$	5 3 3 3 1
$206 \\ 225 \\ 411 \\ 402 \\ 330$			$\begin{array}{c} 1.\ 0019\\ 1.\ 0003\\ 0.\ 9888\\ .\ 9868\\ .\ 9713 \end{array}$	3 5 5 4 3
$\begin{array}{c} 412 \\ 107 \\ 324 \\ 315 \\ 403 \end{array}$			$\begin{array}{c} .9596\\ .9568\\ .9519\\ .9463\\ .9399\end{array}$	8 7 3 2
332 420 226			$ \begin{array}{r} .9346 \\ .9212 \\ .9010 \end{array} $	$1\\5\\4$

Lead Molybdate (wulfenite), PbMoO₄ (tetragonal)

ASTM cards

Card number	Card Index Radiation		Source
2-0544	$\begin{array}{c} 3. \ 17 \\ 2. \ 00 \\ 1. \ 77 \end{array}$	Copper	G. A. Harcourt [1] 1942.

Additional published patterns

Source	Radiation	Wavelength
Zambonini and Levi [2] 1925.	Copper	K _α

NBS sample. The sample of lead molybdate was precipitated from solutions of lead chloride and sodium molybdate. The sample was annealed at 400° C for 2 hours to sharpen the diffraction pattern. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of silicon; 0.01 to 0.1 percent each of aluminum and calcium; 0.001 to 0.01 percent each of silver, barium, magnesium, and strontium; and 0.0001 to 0.001 percent each of chromium, copper, iron, manganese, and tin.

The sample has a pale-yellow color. The indices of refraction could not be determined because the particle size is too small.

Interplanar spacings and intensity measurements. The *d*-values reported by Zambonini and Levi were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Harcourt Zambonini and Levi National Bureau of Standards.	$112 \\ 112 \\ 112 \\ 112$	$303, 312 \\ 303, 312 \\ 204$	$204 \\ 204 \\ 303, 312$

Structural data. Vegard and Refsum [3] in 1925 determined that lead molybdate has calcium tungstate-type structure, the space group C_{4b}^6 -I4₁/a, and 4(PbMoO₄) per unit cell.

The "a" measurement reported by Zambonini and Levi (3.81 A) was multiplied by $2/\sqrt{2}$, the "a" measurements reported by Vegard and Refsum (7.672 A) and by Aanerud (7.679 A) were multiplied by $\sqrt{2}/2$, and the "c" measurement reported by Zambonini and Levi was doubled for comparison with the NBS values. All of the measurements were converted from kX to angstrom units.

425326°-57-4

Lattice constants

		a	с
1925	Zambonini and Levi [4]	$A_{5,501}$	A 12 04
$1928 \\ 1931$	Vegard and Refsum [3] Append [5]	5.425 5.430	12.01 12.10 12.15
$1943 \\ 1057$	Sillén and Nylander [6]	5. 435	12. 10 12. 10 12. 11 of
1907	Standards.	0. 400	25° C

The density of lead molybdate calculated from the NBS lattice constants is 6.815 at 25° C.

hkl	194 Harco Cu, 1.54	2 ourt 418 A	1925 Zambonini and Levi Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	Ι	d	Ι	d	Ι
$ 101 \\ 112 \\ 004 \\ 200 \\ $	A 3. 17 3. 00 2. 67	$100 \\ 10 \\ 20 \\ -$	$ \begin{array}{c} A \\ 3. \overline{09} \\ 2. 91 \\ 2. \overline{61} \end{array} $	vs m mw	A 4. 96 3. 244 3. 028 2. 718	$ \begin{array}{c} 11 \\ 100 \\ 22 \\ 24 \\ - \end{array} $
$211 \\ \bar{105} \\ 213 \\ 204$	$2. 35 2. 20 \overline{2.00}$	$5 - 2 - \overline{40}$	2. 30 1. 97	- - - - -	$\begin{array}{c} 2. \ 383 \\ \hline 2. \ 212 \\ 2. \ 082 \\ 2. \ 021 \end{array}$	$8\\ \overline{5}\\ 7\\ 31$
$220 \\ 116 \\ 303 \\ 312 \\ 224$	$1.96 \\ 1.77 \\ 1.64 \\$	20 40 50 -	1. 88 1. 75 1. 62 1. 59	m s vs ms	$ \begin{array}{c} 1. 920 \\ 1. 787 \\ 1. 653 \\ 1. 622 \end{array} $	$ \begin{array}{r} 14 \\ 18 \\ 25 \\ 12 \end{array} $
$\begin{array}{c} 008 \\ 321 \\ 314 \\ 323 \\ 217 \end{array}$	$\left. \begin{array}{c} 1.\ 50 \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	2 - -	1. 48	- w -	1. 515 1. 496 1. 411	3 2 2
$\begin{array}{c} 400 \\ 208 \\ 316 \\ 325 \\ 332 \\ 413 \end{array}$	1. 35 1. 30 }	2 -40 -	1. 30 1. 29 1. 26	m s w -	1. 359 1. 3229 1. 3085 1. 2802 1. 2535	$ \begin{array}{c} 3 \\ 7 \\ 12 \\ 2 \\ 5 \end{array} $
$ \begin{array}{r} 404 \\ \bar{420} \\ 228 \\ 415 \end{array} $	1. 24 1. 21 1. 182	$10 \\ 10 \\ 10 \\ -$	1. 23 1. 22 1. 20 1. 17	m w m m	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$5 \\ \bar{5} \\ < 1 $
$1 \cdot 1 \cdot 10 \\ 327 \\ 318 \\ 424 \\ 406$	$ \begin{cases} 1.\ 150 \\ \\ 1.\ 120 \end{cases} $	10 - 20	 1. 11	- - ms	1. 1550 1. 1354 1. 1277	$\begin{vmatrix} 3\\<1\\6 \end{vmatrix}$
$336 \\ 512 \\ 503 \\ 408 \\ 2 \cdot 1 \cdot 11$	$1.\ 075\\ \Big\}1.\ 045\\ \Big\}1.\ 005$	10 20 10	1. 07 1. 04 1. 00	mw s mw	$1. 0814 \\ 1. 0497 \\ \{1. 0110 \\ 1. 0030 \end{cases}$	3 5 2 <1

hkl	1942 Harco Cu, 1.54	2 ourt +18 A	192 Zambo and I Cu, 1.54	5 onini zevi 418 A	1957 Nation Bureau Standa Cu, 1.54 25° 0	7 nal 1 of .rds 05 A, C
	d ,	Ι	d	Ι	d	Ι
$\begin{array}{c} 3.1.10\\ 525\\ 440\\ 428\\ 516\\ 532\\ 444\\ 600\\ 2.2.12\\ 3.3.10\\ 604\\ 446\\ 620\\ 536\\ 541\\ 2.21\\ \end{array}$	$\begin{array}{c} A \\ 0. 986 \\ \\ . 945 \\ \\ . 918 \\ \\ . 890 \\ . 880 \\ . 857 \\ . 845 \\ . 845 \\ \end{array}$	$20 \\ - \\ 30 \\ - \\ 10 \\ - \\ 5 \\ 5 \\ 5 \\ 30$	$\begin{array}{c} A \\ 0.981 \\ \hline \\ \\ .941 \\ \hline \\ .915 \\ \hline \\ .887 \\ .875 \\ .867 \\ .857 \\ .844 \\ \end{array}$	ms - - - - - - - - - - - - - - - - - - -	$\begin{array}{c} A\\ 0.9900\\ .9795\\ .9609\\ .9475\\ .9426\\ .9212\\ .9156\\ .9057\\ .8935\\ .8800\\ .8678\\ .8593\\ .8462\\ \end{array}$	$\begin{array}{c} 4\\ <1\\ <1\\ 4\\ 4\\ 3\\ 3\\ 1\\ 2\\ 2\\ 1\\ 1\\ 3\\ \end{array}$
$\begin{array}{r} 624 \\ 606 \\ 448 \\ 4 \cdot 0 \cdot 12 \\ 5 \cdot 1 \cdot 10 \end{array}$	$\left. \begin{array}{c} . 825 \\ . 811 \\ . \overline{800} \end{array} \right.$	30 30 30	. 817 . 802	vw - ms	. 8267 . 8112 . 8102 . 8002	3 2 2 3

Lead Molybdate (wulfenite), PbMoO₄ (tetragonal) —Continued

References

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- gist 27, 63-113 (1942).
 [2] F. Zambonini and G. R. Levi, Richerche sull'isomorfismo dei molibdati dei metalli delle terre rare con quelli del calcio, dello stronzio, del bario e del piombo. II. Struttura dei molibdati di Ca, Sr, Ba, Pb, Rend. accad. Lincei 2, 225-230 (1925).
- quein del calcio, dello stronzio, del bario e del piombo. II. Struttura dei molibdati di Ca, Sr, Ba, Pb, Rend. accad. Lincei 2, 225–230 (1925).
 [3] L. Vegard and A. Refsum, Further investigations on the structure of crystals belonging to the scheelite group, Neues Jahrbuch Mineral. 1, 207–208 (1928).
 [4] F. Zambonini and G. R. Levi, Richerche sull'isomorphic della targe mathematical della targe accession.
- [4] F. Zambonini and G. R. Levi, Richerche sull'isomorfismo dei molibdati dei metalli delle terre rare con quelli del calcio, dello stronzio, del bario e del piombo. III. De duzioni dall'analisi rontgenografica dei molbdati di Ca, Sr, Ba, Pb, Rend. accad. Lincei 2, 303–305 (1925).
- [5] K. Aanerud, Mischkristallbildung der scheelitgruppe durch Fällung von Lösungen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. 1931, No. 13, (1931).
 [6] L. Sillén and A. Nylander, On the oxygen positions in
- [6] L. Sillén and A. Nylander, On the oxygen positions in tungstates and molybdates with the scheelite structure, Arkiv Kemi. Mineral. Geol. A17 No. 4 (1943).

Lead Tungstate (stolzite), PbWO₄ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
2-0527	$\begin{array}{c} 3.\ 21 \\ 2.\ 01 \\ 1.\ 65 \end{array}$	Copper	British Museum.

Additional published patterns. A pattern reported by Aanerud [3] was not included because of the poor agreement with other work. NBS sample. The sample of lead tungstate

NBS sample. The sample of lead tungstate was precipitated from solutions of lead nitrate and sodium tungstate. The sample was annealed at 500° C for 2 hours. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of arsenic, barium, sodium, silicon, and strontium; and 0.001 to 0.01 percent each of aluminum, bismuth, calcium, magnesium, molybdenum, titanium, and zinc.

The sample has a pale-yellow color. The indices of refraction could not be determined as the particle size is too small. Interplanar spacings and intensity measurements. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
British Museum National Bureau of Standards	$\frac{112}{112}$	$\frac{204}{204}$	$\begin{array}{c} 312\\ 312\end{array}$

Structural data. Vegard and Refsum [1] in 1928 determined that lead tungstate, stolzite, has calcium tungstate-type structure, the space group C_{4h}^6 -I4₁/a, and 4(PbWO₄) per unit cell. Shaw and Claringbull [2] have reported that the monoclinic form of PbWO₄, raspite, transforms irreversibly to the tetragonal form, stolzite, at about 400° C.

The "a" measurements reported by Vegard and Refsum (7.712 A) and by Aanerud (7.727 A) have been multiplied by $\sqrt{2}/2$ for comparison with the NBS values. All of the measurements have been converted from kX to angstrom units.

Lead Tungstate (storzite), $PDWO_4$ (tetragona	Lead	Tungstate	(stolzite),	PbWO ₄	(tetragonal	I)
--	------	-----------	-------------	-------------------	-------------	----

hkl	British M Cu, 1.5	Iuseum 41 A	195 National of Stanc Cu, 1.5405	7 Bureau dards A, 25° C
	d	Ι	d	Ι
	A		A	
$ \begin{array}{r} 112 \\ 004 \\ 200 \\ 211 \end{array} $	$\begin{array}{c} 3. \ 57 \\ 3. \ 21 \\ 2. \ 99 \\ 2. \ 71 \\ 2. \ 21 \end{array}$	$egin{array}{c} 40 \\ 100 \\ 40 \\ 60 \\ 20 \end{array}$	$\begin{array}{c} 3.\ 252\\ 3.\ 014\\ 2.\ 732\\ 2.\ 394 \end{array}$	$\begin{array}{r} \overline{100}\\ 22\\ 32\\ 1\end{array}$
204	2.01 1.95	$\frac{80}{20}$	2. 024	35
$220 \\ 222 \\ 116$	$ \begin{array}{c} 1. \ 91 \\ 1. \ 82 \\ 1. \ 76 \end{array} $	$50\\40\\70$	$\begin{array}{c} 1.\ 9309\\ 1.\ 8377\\ 1.\ 7817 \end{array}$	$\begin{array}{c} 16 \\ < 1 \\ 21 \end{array}$
$312 \\ 224 \\ 008 \\ \\ 400$	$ \begin{array}{c} 1. \ 65 \\ 1. \ 61 \\ 1. \ 50 \\ 1. \ 44 \\ 1. \ 36 \end{array} $		$ \begin{array}{c} 1. \ 6603 \\ 1. \ 6255 \\ 1. \ 5056 \\ \hline 1. \ 3653 \end{array} $	$33 \\ 16 \\ 3 \\ \\ 4$
$208 \\ 316 \\ 332 \\ 404 \\ 420$	$\begin{array}{c} 1. \ 30 \\ 1. \ 25 \\ 1. \ 23 \\ 1. \ 22 \end{array}$		$\begin{array}{c} 1.\ 3184\\ 1.\ 3092\\ 1.\ 2590\\ 1.\ 2436\\ 1.\ 2213 \end{array}$	7 8 6 5 5
$\begin{array}{c} 228\\\hline1\cdot1\cdot10\\424\\336\end{array}$	$\begin{array}{c} 1. \ 18 \\ 1. \ 16 \\ 1. \ 15 \\ 1. \ 13 \\ 1. \ 08 \end{array}$	$60 \\ 20 \\ 40 \\ 60 \\ 40$	$ \begin{array}{r} 1. \ 1872 \\ \hline 1. \ 1498 \\ 1. \ 1317 \\ 1. \ 0836 \\ \end{array} $	5 $\frac{4}{7}$ 4
$512 \\ 408 \\ 0.0.12 \\ 3.1.10 \\ 440$	1. 05 1. 01	70 40 	$\begin{array}{c} 1.\ 0546\\ 1.\ 0114\\ 1.\ 0040\\ 0.\ 9882\\ .\ 9656 \end{array}$	6 3 1 6 1
$\begin{array}{r} 428 \\ 516 \\ 2 \cdot 0 \cdot 12 \\ 532 \\ 444 \end{array}$			$\begin{array}{c} . \ 9486\\ . \ 9451\\ . \ 9423\\ . \ 9256\\ . \ 9193\end{array}$	3 5 2 4 2
$\begin{array}{c} 600\\ \underline{2\cdot2\cdot12}\\ 3\cdot3\cdot10\\ 604\\ 620 \end{array}$			$\begin{array}{c} . \ 9104 \\ . \ 8906 \\ . \ 8796 \\ . \ 8713 \\ . \ 8635 \end{array}$	1 3 3 3 3
$536 \\ 1 \cdot 1 \cdot 14 \\ 624 \\ 448 \\ 4 \cdot 0 \cdot 12$. 8488 . 8398 . 8301 . 8127 . 8088	5 3 5 2 3
$5 \cdot 1 \cdot 10$. 8004	5

Lattice constants					
		a	с		
		A	A		
$1928 \\1931 \\1943 \\1957$	Vegard and Refsum [1] Aanerud [3] Sillén and Nylander [4] National Bureau of Standards.	$\begin{array}{c} 5. \ 453 \\ 5. \ 464 \\ 5. \ 459 \\ 5. \ 4616 \end{array}$	12.034 12.055 12.040 12.046 at 25° C		

The density of lead tungstate, stolzite, calculated from the NBS lattice constants is 8.410 at 25° C.

- L. Vegard and A. Refsum, Further investigations on the structure of crystals belonging to the scheelite group, Neues. Jahrb. Mineral. 1, 207-208 (1928).
- [2] R. Shaw and G. F. Claringbull, X-ray study of raspite (monoclinic PbWO₄), American Mineral. 40, Nos. 9 and 10, 933 (1955).
- [3] K. Aanerud, Mishkristallbildung der scheelitgruppe durch Fällung von Lösungen, Skrifter Norske Videnskaps Akad. Olso I. Mat.-Naturv. Kl. 1931, No. 13 (1931).
- [4] L. Sillén and Nylander, On the oxygen positions in tungstates and molybdates with the scheelite structure, Arkiv for Kemi, Mineral. Geol., 17A No. 4 (1943).

Lithium Iodate, LiIO₃ (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
3-0369	3. 49 2. 74 4. 75	Molyb- denum	Zachariasen and Barta [1] 1931.

Additional published patterns. None. NBS sample. The sample of lithium iodate was obtained from the City Chemical Corp., New York, N. Y. The sample was recrystallized and heated to 100°C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium and sodium; 0.001 to 0.01 percent each of aluminum, barium, magnesium, nickel, silicon, and strontium; and 0.0001 to 0.001 percent each of silver, chromium, copper, iron, potassium, manganese, and lead.

The sample is colorless. The indices of refraction could not be determined by the usual liquid grain immersion method because the sample reacted with the higher index liquids.

Interplanar spacings and intensity measure-ments. The d-values reported by Zachariasen and Barta were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Zachariasen and Barta National Bureau of Standards	$\begin{array}{c} 101 \\ 101 \end{array}$	$\begin{array}{c}112\\110\end{array}$	$\begin{array}{c} 211 \\ 100 \end{array}$

Structural data. Zachariasen and Barta [1] in 1931 determined that lithium iodate has the space group D_6^6 -P6₃22 and 2(LiIO₃) per unit cell. Lithium iodate is used as a structure-type.

The unit-cell measurements reported by Zachariasen and Barta have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	с
1931 1957	Zachariasen and Barta [1]- National Bureau of Standards.	A 5. 480 5. 481	A 5. 165 5. 172 at 25° C

The density of lithium iodate calculated from the NBS lattice constants is 4.487 at 25° C.

References

1] W. H. Zachariasen and F. A. Barta, Crystal structure of lithium iodate, Phys. Rev. 37, 1626-1630 (1931).

hkl	193 Zacharias Bart	1 en and ta	1957 National Bureau o Standards	
	Mo, 0.7	107 A	Cu, 1.5405	A, 25° C
	d	Ι	d	Ι
$100 \\ 101 \\ 110 \\ 002 \\ 111 \\ 200 \\ 102 \\ 201 \\ 112 \\ 112 \\ 00 \\ 102 \\ 201 \\ 112 \\ 00 \\ 102 \\ $	A 4. 74 3. 50 2. 74 2. 58 2. 419 2. 369 2. 267 2. 155 1. 889 1. 889	w+ vs ms vw w w w ms s	$\begin{array}{c} A\\ 4.\ 75\\ 3.\ 50\\ 2.\ 741\\ 2.\ 587\\ 2.\ 422\\ 2.\ 374\\ 2.\ 272\\ 2.\ 158\\ 1.\ 882\\ 1.\ $	$23 \\ 100 \\ 27 \\ 8 \\ 2 \\ 8 \\ 10 \\ 18 \\ 23 \\ 2 \\ 3 \\ 2 \\ 3 \\ 2 \\ 3 \\ 2 \\ 3 \\ 3$
$ \begin{array}{c} 210 \\ 202 \\ 211 \\ 103 \\ 300 \\ 212 \\ \end{array} $	$ \begin{array}{c} 1. 794 \\ 1. 747 \\ 1. 695 \\ 1. 618 \\ 1. 580 \\ 1. 4721 \\ 1. 4577 \end{array} $	vw vw s m m	$ \begin{array}{c} 1. 795 \\ 1. 750 \\ 1. 696 \\ 1. 621 \\ 1. 583 \\ 1. 473 \\ \end{array} $	$ \begin{array}{c} 3 \\ 3 \\ 19 \\ 7 \\ 6 \\ 3 \end{array} $
203 220 302	$ \begin{array}{c} 1. 3929 \\ 1. 3693 \\ 1. 3491 \\ 1. 3237 \end{array} $		$ \begin{array}{c} 1.395\\ 1.370\\ 1.349 \end{array} $	5 3 5
$\begin{array}{c} 310\\ 311\\ 104\\ 213\\ 222 \end{array}$	$\begin{array}{c} 1. \ 3163\\ 1. \ 2749\\ 1. \ 2457\\ 1. \ 2413\\ 1. \ 2095 \end{array}$		$\begin{array}{c} 1. \ 3162 \\ 1. \ 2755 \\ 1. \ 2472 \\ 1. \ 2430 \\ 1. \ 2109 \end{array}$	
$ \begin{array}{c c} 400 \\ 312 \\ \overline{114} \end{array} $	$\begin{array}{c} 1. \ 1852 \\ 1. \ 1728 \\ 1. \ 1715 \\ 1. \ 1645 \end{array}$		$ \begin{array}{c} 1. 1865 \\ 1. 1732 \\ \hline 1. 1696 \end{array} $	< 1 4 2
$ \begin{array}{c c} 401 \\ 204 \\ 320 \\ 402 \end{array} $	1. 1557 		$ \begin{array}{c} 1. 1567 \\ 1. 1354 \\ 1. 0891 \\ 1. 0785 \end{array} $	$ 1 \\ < 1 \\ < 1 \\ 1 \\ 1$
321 214 313			$ \begin{array}{c} 1.0657\\ 1.0489\\ 1.0464\\ 1.0464 \end{array} $	3 1 2
$ \begin{array}{c} 410 \\ 105 \\ 322 \\ 304 \end{array} $			$ \begin{array}{c} 1.0339\\ 1.0109\\ 1.0034\\ 1.0012 \end{array} $	$\begin{vmatrix} 1\\2\\1\\1\end{vmatrix}$
$ \begin{array}{r} 403 \\ 412 \\ 500 \\ 205 \end{array} $			$\begin{array}{c c} 0. \ 9775 \\ . \ 9617 \\ . \ 9495 \\ . \ 9484 \end{array}$	$\begin{vmatrix} 2\\ 2\\ 2\\ <1 \end{vmatrix}$
$ \begin{array}{c c} 224 \\ 501 \\ 314 \\ 323 \end{array} $			$\begin{array}{c c} . 9404 \\ . 93^{2}8 \\ . 9224 \\ . 9208 \end{array}$	$\begin{vmatrix} 1\\ 1\\ 1\\ 2 \end{vmatrix}$
330 215 502			$\begin{array}{c} .9134 \\ .8959 \\ .8911 \\ \end{array}$	$ $ $< \frac{1}{2}$ < 1
$ \begin{array}{r} 421 \\ 404 \\ 332 \\ 510 \end{array} $			$\begin{array}{c c} . 8838 \\ . 8742 \\ . 8614 \\ . 8525 \end{array}$	$\begin{vmatrix} 2\\ <1\\ <1\\ <1 \end{vmatrix}$
$422 \\ 511 \\ 324 \\ 502$			$\begin{array}{c} . 8477 \\ . 8413 \\ . 8328 \\ . 8328 \\ . 8316 \end{array}$	$ $ $ $ $ $ $ $ $ $ $ $ $ $ $ $ $ $
$503 \\ 116 \\ 315 \\ 512$. 8316 . 8222 . 8133 . 8097	$\begin{pmatrix} 2\\ <1\\ \\ <1 \end{pmatrix}$
414 423 600			. 8083 . 7957 . 7911	

ASTM cards

Card number	Index lines	Radiation	Source
1-1225	2. 13 3. 59 2. 79	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [2] 1928	Copper	

NBS sample. The sample of lithium nitrate was obtained as the hydrate from Johnson, Matthey & Co., Ltd., London. It was heated to 150° C to remove the water of hydration and mixed with silicone grease to prevent deliquescence. Their spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of calcium; and 0.0001 to 0.001 percent each of sodium, magnesium, and copper.

The sample is colorless and optically negative with the indices of refraction $N_0 = 1.729$ and $N_e =$ 1.429.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units, and the *d*-values of the Zachariasen pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel Zachariasen National Bureau of Standards	$113 \\ 113 \\ 012$	$012 \\ 012 \\ 113$	104 104 104

Structural data. Zachariasen [2] in 1928 determined that lithium nitrate has calcite-type structure, the space group D_{3d}^6 -R3c, and 2(LiNO₃) per unit rhombohedral cell or 6(LiNO₃) per unit hexagonal cell.

The unit-cell measurements reported by Zachariasen have been converted to hexagonal cell values and from kX to angstrom units for comparison with the NBS values.

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
 W. H. Zachariasen, Untersuchungen über die Kristall-struktur von Sesquioxyden und Verbindungen ABO₃, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. 1928, No. 4, (1928).

Lattice constants

1928 Zachariasen [2] 1957 National Bureau of Standards.	$\begin{array}{c} a \\ \hline A \\ 4.70 \\ 4.692 \end{array}$	<i>c</i> 15. 3 15.22 at 25° C.
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The density of lithium nitrate calculated from the NBS lattice constants is 2.367 at 25° C.

ī							
hkl	193 Hanav Rinn, Frey Mo, 0.7	8 valt, and vel 107 A	1928 Zachari Cu, 1.54	3 asen 418 A	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι	d	Ι	d	Ι	
$ \begin{array}{c} 012 \\ 104 \\ 006 \\ \overline{113} \end{array} $	$ \begin{array}{c} A\\ 3.59\\ 2.79\\ 2.54\\ 2.13 \end{array} $	$\begin{array}{r} 67\\53\\20\\1\overline{0}0\end{array}$	$\begin{array}{c} A\\ 3.\ 60\\ 2.\ 75\\ 2.\ 54\\ 2.\ 36\\ 2.\ 12 \end{array}$		$ \begin{array}{r} A \\ 3. 60 \\ 2. 79 \\ 2. 54 \\ \hline 2. 134 \end{array} $	$100 \\ 83 \\ 74 \\ 8\overline{6}$	
$\begin{array}{c} 202 \\ 018 \\ 116 \\ 211 \\ 1.0.10 \\ 214 \end{array}$	$1.95 \\ 1.72 \\ 1.53 \\ 1.423$	1 11 27 1	1. 965 1. 714 1. 523 1. 423	5 25 25 5	1. 968 1. 725 1. 528 1. 425	2 14 9 2	
$119 \\ 125 \\ 300 \\ 0.0.12 \\ 217$	$ \left. \begin{array}{c} 1. \ 374 \\ 1. \ 358 \\ 1. \ \overline{258} \end{array} \right. $	20 13 -4	$\begin{array}{c} 1.\ 365\\ 1.\ 355\\ 1.\ 274\\ 1.\ 255 \end{array}$	$40 \\ 10 \\ 5 \\ 15$	$\begin{array}{c} 1. \ 373 \\ 1. \ 355 \\ 1. \ 269 \\ 1. \ 255 \end{array}$	$\begin{array}{c}14\\7\\3\\4\end{array}$	
$ \begin{array}{r} 128 \\ 306 \\ 223 \\ 1 \cdot 1 \cdot 12 \\ 312 \end{array} $	$ \begin{cases} 1. \ 196 \\ 1. \ 142 \\ 1. \ 119 \end{cases} $	4 1 3	1. 192 1. 143 1. 113	20 5 10	1. 195 1. 144 1. 116	3 < 1 1	
$\begin{array}{c} 2 \cdot 1 \cdot 10 \\ 134 \\ 315 \\ 0 \cdot 1 \cdot 14 \\ 1 \cdot 2 \cdot 11 \end{array}$	$ \left. \begin{array}{c} 1.\ 084 \\ \\ 1.\ 0\overline{2}7 \end{array} \right. $	4 - - 1	1. 080 1. 028	20 - 10	$\begin{array}{c} 1.\ 0812\\ 1.\ 0587\\ 1.\ 0511\\ 1.\ 0279 \end{array}$	$2 \\ \stackrel{1}{\stackrel{1}{\stackrel{1}{\stackrel{1}{\stackrel{1}{\stackrel{1}{\stackrel{1}{\stackrel{1}$	
$\begin{array}{c} 042 \\ 404 \\ 318 \\ 229 \\ 045 \end{array}$	1. 010 0. 984 }	3 3 - -	1. 007 0. 9832 . 9703	15 15 10 -	$\begin{array}{c} 1.\ 0073\\ 0.\ 9817\\ .\ 9698\\ .\ 9641 \end{array}$	$\stackrel{1}{\stackrel{2}{\stackrel{1}{\scriptstyle 1}}}_{<1}$	
$\begin{array}{c} 1 \cdot 1 \cdot 15 \\ 321 \\ 3 \cdot 0 \cdot 12 \\ 1 \cdot 3 \cdot 10 \\ 048 \end{array}$	$\left. \begin{array}{c} . \ 935 \\ . \ 929 \\ \overline{. \ 897} \end{array} \right.$	1 1 - 1			.9311 .9260 .9058 .8961	$3 \\ < 1 \\ 1 \\ 1$	
$235 \\ 140 \\ 327$. 892 	1 		- - -	. 8915 . 8867 . 8569	$\stackrel{\leq 1}{\stackrel{>}{\stackrel{>}{\stackrel{>}{\stackrel{>}{\sim}}}}_1$	

Magnesium Carbonate (magnesite), MgCO₃ (trigonal)

ASTM cards

Card numbe r s	Index lines	Radiation	Source
3-0773	$\begin{array}{c} 2.75\\ 2.10\\ 1.70\end{array}$	Molybde- num	Dow Chemical Co.
2-0871	$\begin{array}{c} 2. \ 74 \\ 2. \ 10 \\ 1. \ 70 \end{array}$	Copper	Michigan Alkali Co.
2-0905	$\begin{array}{c} 2.\ 70\\ 2.\ 10\\ 1.\ 70 \end{array}$	Copper	British Museum.
3–0788	$\begin{array}{c} 2.\ 73\\ 2.\ 10\\ 1.\ 70 \end{array}$	Molybde- num	New Jersey Zinc Co.
2–0875	2. 74 1. 70 2. 10	Molybde- num	United Steel Com- panies and A. K. Boldyrev et al. [1] 1938.

Additional published patterns. None.

NBS sample. The sample of magnesium carbonate was obtained from the Baker Chemical Co., Phillipsburg, N. J. It was heated in a hydrothermal bomb at 120,000 psi and 280 °C for 4 days. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium and sodium; 0.001 to 0.01 percent each of aluminum, iron, manganese, molybdenum, lead, silicon, and strontium; and 0.0001 to 0.001 percent each of barium, chromium, copper, and nickel.

The sample is colorless and optically negative. The indices of refraction are $N_e=1.510$ and $N_o=1.700$. Interplanar spacings and intensity measurements. The *d*-values of all of the patterns were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Dow Chemical Co Michigan Alkali Co British Museum New Jersey Zinc Co United Steel Companies Boldyrev et al National Bureau of Standards	$104 \\ 104 \\ 104 \\ 104 \\ 104 \\ 104 \\ 104 \\ 104$	$113 \\ 113 \\ 113 \\ 113 \\ 116 \\ 116 \\ 113$	116 116 116 116 113 113 113 116 116 116 113 116

Structural data. Wyckoff [2] in 1920 determined that magnesium carbonate has calcite-type structure, the space group D_{3d}^{6} -R $\overline{3}c$, and 2(MgCO₃) per unit rhombohedral cell or 6(MgCO₃) per unit hexagonal cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values. Cell measurements reported by Brentano and Adamson [5] and Ferrari and Colla [6] are not included because they were given as large pseudocubic cell values.

	Danice constan		
		<i>a</i>	с
$1935 \\ 1937 \\ 1957$	Schoklitsch [3] Bragg [4] National Bureau of Standards.	$\begin{matrix} A \\ 4.596 \\ 4.58 \\ 4.6332 \end{matrix}$	A 14. 91 14. 84 15. 015 at 25°C

The density of magnesium carbonate calculated from the NBS lattice constants is 3.009 at 25°C.

Magnesium Carbonate (magnesite), MgCO₃ (trigonal)

hkl	Dow C ical (Mo,	hem- Co.	Michi Alkali Cu,	igan Co.	Brit Muse Cu,	ish eum	New J Zinc Mo,	ersey Co.	United Compa Mo,		193 Boldy et a Fe,	8 /rev al.	195 Natio Burea Stand Cu, 1.5 25°	57 onal ou of ards 5405, C
	d	Ι	d	Ι	d	Ι	d	Ι	d	1	d	Ι	d	I
$ \begin{array}{r} 104 \\ 006 \\ \hline 110 \end{array} $	$ \begin{array}{c} A \\ \hline 2.76 \\ 2.52 \\ \hline 2.32 \end{array} $	100 17 	<i>A</i> 2. 75 2. 51		$ \begin{array}{c} A\\ 3. 03\\ 2. 71\\ 2. 51\\ \hline 2. 32 \end{array} $	$ \begin{array}{r} 60 \\ 100 \\ 60 \\ -\overline{60} \\ \overline{60} \end{array} $	$ \begin{array}{c} A \\ \hline 2.74 \\ 2.51 \\ 2.42 \\ 2.32 \end{array} $	$ \begin{array}{r} \overline{100} \\ 5 \\ 1 \\ 3 \end{array} $	$ \begin{array}{r} A\\ 3.54\\ 2.75\\ 2.51\\ \hline 2.31\\ \end{array} $	$ \begin{array}{r} 20 \\ 100 \\ 60 \\ -\overline{40} \end{array} $	A 2. 742 2. 505		A 2. 742 2. 503 2. 318	$ \begin{array}{c} \overline{100}\\ 17\\ -\overline{4} \end{array} $
113 022 024 116	2. 10 2. 00 1. 93 1. 84 1. 77 1. 70	- 65 5 20 3 5 65 	$\begin{array}{c} 2. \ 14 \\ 2. \ 10 \\ \hline 1. \ 93 \\ \hline \\ 1. \ 77 \\ 1. \ 70 \\ 1. \ 67 \\ 1. \ 64 \\ 1. \ 56 \end{array}$	$ \begin{array}{c c} 10 \\ 80 \\ -\overline{40} \\ \\ 10 \\ 80 \\ 5 \\ 5 \\ 10 \end{array} $	$ \begin{array}{r} 2.10\\ 1.95\\ 1.88\\ 1.76\\ 1.70\\ 1.65\\ 1.55\\ \end{array} $	$ \begin{bmatrix} \overline{80} \\ \overline{60} \\ 40 \\ 40 \\ $	2. 10 1. 94 1. 78 1. 70 	-67 -16 3 60 	2. 10 1. 93 1. 77 1. 70 	- 8 0 - 6 0 40 90 	2. 105 1. 939 1. 770 1. 700 	- <u>90</u> - <u>60</u> 20 100 	2. 102 1. 939 1. 769 1. 700 	$ \begin{array}{c} 43 \\ 12 \\ \\ 3 \\ $

Magnesium Carbonate (magnesite), MgCO₃ (trigonal)—Continued

hkl	Dow C ical (Mo,	hem- Co.	Miehi Alkali Cu,	igan Co.	Briti Muse Cu,	sh sum	New Ja Zinc (Mo,	ersey Co.	United Compa Mo,	- Steel anies	193 Boldy et a Fe,	8 rev I.	195 Nation Bureau Stand Cu, 1.5 25°	57 al of ards 5405, C
	d	Ι	d	Ι	d	Ι	d	Ι	d	Ι	d	Ι	d	Ι
$211 \\ 122 \\ 1 \cdot 0 \cdot 10 \\ 214$	$\begin{array}{c} A \\ 1.51 \\ 1.49 \\ 1.41 \end{array}$	9 11 13	$ \begin{array}{c} A \\ 1.51 \\ 1.49 \\ 1.40 \\ 1.38 \\ \end{array} $	$ \begin{array}{c} 10 \\ 30 \\ 20 \\ 5 \end{array} $	$ \begin{array}{r} A \\ 1.51 \\ 1.48 \\ 1.40 \end{array} $	40 60 50	A 1. 51 1. 49 1. 41	7 8 8	$ \begin{array}{c} $	40 50 60	$\begin{array}{c} A \\ 1.506 \\ 1.488 \\ 1.407 \end{array}$	30 50 50	A 1. 510 1. 488 1. 426	4 5 4
$208 \\ 119 \\ 300$	$ 1.35 \\ 1.34 $	$\frac{1}{17}$	$ \begin{array}{c} 1.37 \\ 1.35 \\ 1.34 \end{array} $	5 20 40	$ 1.36 \\ 1.33 \\ 1.51 $	 40 60	$ \begin{array}{c} 1. 37 \\ 1. 35 \\ 1. 34 \\ 1. 30 \end{array} $	$\begin{array}{c}1\\5\\13\\1\end{array}$	$ 1. 37 \\ 1. 35 \\ 1. 34 $	20 60 60	$ \begin{array}{r} 1.370\\ 1.355\\ +1.339 \end{array} $	5 60 70	$ 1. 371 \\ 1. 354 \\ 1. 338 $	3 7 8
$\begin{array}{c} 0.0.12\\ 217\\ 0.2.10\\ 128\\ 306\end{array}$	$ \begin{array}{c} 1. 25 \\ \overline{1. 20} \\ 1. 18 \end{array} $	8 <u>-</u> 7	1. 25 1. 24 1. 18	10 5 20	1. 25 1. 24 1. 20 1. 18	40 40 20 40	1. 25 1. 23 1. 20 1. 18	$\frac{2}{1}$ $\frac{1}{3}$	1. 25 1. 24 1. 20 1. 18	50 20 40 50	1. 252 1. 239 1. 202 1. 191	30 20 50 5	1. 252 1. 2386 1. 2022 1. 1798	$\begin{array}{c} 3\\ \leqslant 1\\ <1\\ <1 \end{array}$
$ \begin{array}{r} 220 \\ 2.0.11 \\ \hline 1.1.12 \\ 2.1.10 \\ 134 \end{array} $	$ \begin{array}{c} 1. 16 \\ 1. 13 \\ 1. 11 \\ 1. 10 \\ 1. 07 \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 3 \\ 13 \end{array} $	 1. 07	 20	$ \begin{array}{c} 1. \ 16 \\ 1. \ 13 \\ \hline 1. \ 10 \\ 1. \ 06 \end{array} $	20 20 $-\bar{20}$ 60	1. 16 1. 07	1 11	1. 16 1. 13 1. 10 1. 07	20 20 $-\bar{40}$ 70	1. 158 1. 102 1. 067	5 - 80 50	$1.\ 1583$ $1.\ 1297$ $\overline{1.\ 1011}$ $1.\ 0669$	$ \begin{array}{c} <1 \\ <1 \\ \hline <1 \\ \hline <1 \\ 4 \end{array} $
$ \begin{array}{r} 226 \\ 1 \cdot 2 \cdot 11 \\ - 404 \\ 318 \end{array} $	0. 973 . 963	 7 5	$ \begin{array}{r} 1. \ 05 \\ 1. \ 01 \\ \overline{0. \ 970} \\ 959 \end{array} $	$\begin{array}{r} 5\\10\\-\overline{20}\\20\end{array}$	1. 05 1. 01 	40 40 	1. 05	1	$ 1. 05 1. 01 \overline{0.969} \\ . 957 $	$50 \\ 40 \\ -\bar{70} \\ 70 \\ 70$	1. 014 1. 007	20 20	$ \begin{array}{r} 1.\ 0510\\ 1.\ 0145\\ \hline 0.\ 9692\\ .\ 9573 \end{array} $	$\begin{array}{c}1\\<1\\-\frac{2}{1}\\1\end{array}$
$ \begin{array}{r} 2 \cdot 0 \cdot 14 \\ 2 \cdot 1 \cdot 13 \\ 1 \cdot 1 \cdot 15 \\ 2 \cdot 21 \\ 2 \cdot 1 \cdot 15 \\ 2 \cdot 2 \cdot 1 \\ \end{array} $. 919	 13							. 951 . 946 . 919	10 50 60			. 9455 . 9188	$\overline{<1}$
$\begin{array}{r} 321\\ 3.0.12\\ 1.0.16\\ 324\\ 0.48\\ 140\end{array}$) } 		. 915 . 884 . 875	$40 \\ -10 \\ 10 \\ 10$. 914	100			. 9134 . 8941 . 8837 . 8758	
$\begin{array}{c} 418\\ 3\cdot 1\cdot 11\\ 327\\ 0\cdot 0\cdot 18\\ 4\cdot 0\cdot 10\end{array}$	} }												. 8626 . 8460 . 8346	<1 <1 <1
$\begin{array}{r} 416 \\ 238 \\ 2.1,16 \\ 502 \end{array}$	}												. 8265 . 7981	<1 1

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- [5] J. Brentano and J. Adamson, Precision measurements of X-ray reflections from erystal powders. The lattice constants of zine carbonate, manganese earbonate and cadmium oxide, Phil. Mag. 7, 507–517 (1929).
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Magnesium Sulfate Heptahydrate (epsomite), MgSO₄·7H₂O (orthorhombic) **ASTM** cards

Card number	Index lines	Radiation	Source
1-0399	4. 22 2. 66 5. 9	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

ASTM card 1–0354 reports powder data for the hexahydrate, $MgSO_4 \cdot 6H_2O$, although the crystal data reported is that of the heptahydrate, epsomite. Additional published patterns. None.

NBS sample. The sample of magnesium sulfate heptahydrate was obtained from the Johnson Matthey Co., Ltd., London. Their spectrographic analysis showed the following impurities: 0.001 to 0.01 percent of calcium; and 0.0001 to 0.001 percent each of copper and silicon.

The sample is colorless and optically negative with the refractive indices $N\alpha = 1.430$, $N\beta = 1.453$, $N\gamma = 1.459$, and $2V \simeq 40^{\circ}$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel- National Bureau of Stand- ards.	$\begin{array}{c} 121\\121\end{array}$	$240, 420 \\ 120$	$\begin{array}{c} 020\\ 240 \end{array}$

Structural data. Westenbrink [2] in 1926 determined that magnesium sulfate heptahydrate has the space group D_2^4 -P2₁2₁2₁, and $4(MgSO_4 \cdot 7H_2O)$ per unit cell. Magnesium sulfate heptahydrate is used as a structure-type.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	с
1000		A	A	A
$1926 \\ 1930$	Cardoso [3]	11.91 11.93	12.03 12.04	6.87 6.88
1932	Barnes and Hunter [4]_	11.96	12.05	6.879
1957	National Bureau of Standards.	11. 86	11. 99	6. 858 at 25° C.

The density of magnesium sulfate heptahydrate calculated from the NBS lattice constants is 1.678 at 25° C.

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 H. G. K. Westenbrink, The space groups of the rhombic and moneclinic hentabydrates of the sulfates of
- and monoclinic heptahydrates of the sulfates of bivalent metals, Proc. Accad. Sci. Amsterdam 29, 1223-1232 (1926).
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- space groups of epsomite, Nature 130, 96 (1932).

hkl	193 Hanawalt and Fi Mo, 0.7	8 5, Rinn, revel 107 A	195 National of Stan Cu, 1.5405	7 Bureau dards A, 25° C
 	d	Ι	d	Ι
$\begin{array}{c} 020\\ 011\\ 120\\ 201\\ 121 \end{array}$	$ \begin{array}{c} A \\ 5.9 \\ \hline 5.3 \\ 4.51 \\ 4.23 \\ \end{array} $	$\begin{array}{c} 20\\ \hline 20\\ 8\\ 100 \end{array}$	$\begin{array}{c} A \\ 5.99 \\ 5.95 \\ 5.35 \\ 4.48 \\ 4.21 \end{array}$	$22 \\ 6 \\ 26 \\ 14 \\ 100$
$130 \\ 310 \\ 031 \\ 301 \\ 320$	<pre>3.77 3.42</pre>	10 12 	$\left\{\begin{array}{rrrr} & 3.\ 79 \\ & 3.\ 76 \\ & 3.\ 453 \\ & 3.\ 424 \\ & 3.\ 304 \end{array}\right.$	$ \begin{array}{c} 13 \\ 7 \\ 16 \\ 2 \\ 3 \end{array} $
$112 \\ 040 \\ 022 \\ 410 \\ 212$	$ \begin{array}{c} 3.18\\ 2.97\\ 2.88 \end{array} $	2 18 20	$\begin{cases} 3.178 \\ 3.000 \\ 2.977 \\ 2.880 \end{cases}$	${6 \\ 13 \\ 14 \\ 20 }$
$330 \\ 041 \\ 240 \\ 420 \\ 241$	$ \begin{array}{c} 2.75\\ 2.67\\ 2.49 \end{array} $	$\frac{1}{8}$ 40 2	$\begin{cases} 2.812 \\ 2.748 \\ 2.677 \\ 2.659 \\ 2.493 \end{cases}$	$1 \\ 14 \\ 24 \\ 22 \\ 2 \\ 2$
$\begin{array}{c} 421 \\ 340 \\ 150 \\ 042 \\ 431 \end{array}$	2. 38 2. 27	$\frac{5}{2}$	2. 482 2. 389 2. 352 2. 258 2. 253	$<^{1}_{5}_{1}_{57}$
$\begin{array}{c} 250 \\ 151 \end{array}$	}		2. 229	4
$\begin{array}{c} 113 \\ 412 \end{array}$	2. 21	7	2. 206	· 11
$\frac{251}{440}$	2. 10	6	2. 115	7
$\begin{array}{c} 242 \\ 530 \end{array}$	}		$\begin{array}{c} 2.110\\ 2 040 \end{array}$	4
$\begin{array}{c} 441 \\ 052 \end{array}$	2.03	2	2. 017	3
351	} 1.96	ð	1. 964	4
432 531 601	}		1. 955	3
260	}		1.900 1.894	$\frac{1}{2}$
$233 \\ 611 \\ 540 \\ 261 \\ 451$	1. 88 1. 80	4 4	$\begin{array}{c} 1. \ 882 \\ 1. \ 877 \\ 1. \ 861 \\ 1. \ 826 \\ 1. \ 799 \end{array}$	$\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}$
$541 \\ 361$			1. 795	2
062 601	} 1.72	4	1.726 1.712	3
162			1. 710	2
$170 \\ 114 \\ 710 $	}		1.695 1.679	$\frac{2}{<1}$
710 071 262	J		1. 661	3
433			1. 650	3
$\begin{array}{c} 503 \\ 270 \end{array}$	}		1. 646	1
$\begin{array}{c} 171 \\ 124 \end{array}$			1. 632	4

Magnesium Sulfide, MgS (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1-1096	$\begin{array}{c} 2. \ 60 \\ 1. \ 83 \\ 1. \ 50 \end{array}$	Molybde- num	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Holgersson [2] 1923	Iron	Kα

NBS sample. The sample of magnesium sulfide was prepared at NBS by direct combination of the elements in a sealed, fused silica tube at 620° C. The cell size remained constant when it was prepared either with a deficient or an excess of 5 percent of sulfur. Spectrographic analysis of the magnesium showed the following impurities: 0.001 to 0.01 percent of calcium; and 0.0001 to 0.001 percent each of aluminum, copper, iron, and silicon. Spectrographic analysis of the sulfur showed the following impurities: 0.01 to 0.1 percent of sodium; 0.001 to 0.01 percent each of barium, magnesium, and silicon; and 0.0001 to 0.001 percent of calcium.

The sample is colorless. The index of refraction could not be determined by the usual liquid grain immersion method because the sample is too fine-grained.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel have been converted from kX to angstrom units. The *d*-values of the Holgersson pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel Holgersson National Bureau of Standards	$200 \\ 200 \\ 200 \\ 200$	$220 \\ 220 \\ 220 \\ 220$	$222 \\ 222 \\ 222 \\ 222$

Structural data. Holgersson [2] in 1923 determined that magnesium sulfide has sodium chloride-type structure, the space group O_h^5 -Fm3m, and 4(MgS) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1923 Holgersson Fe, 1.9373 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C			
	d	Ι	a	d	Ι	a	d	Ι	a
$ \begin{array}{c} 111\\200\\220\\222\\400\\420\\422\\440\\600\\620\\622\\\end{array} $	$\begin{array}{c} A\\ 3.\ 00\\ 2.\ 60\\ 1.\ 83\\ 1.\ 499\\ 1.\ 299\\ 1.\ 299\\ 1.\ 160\\ 1.\ 060\\ 0.\ 920\\ .\ 867\\ .\ 823\\ .\ 784\\ (a) \end{array}$	$5 \\ 100 \\ 83 \\ 40 \\ 20 \\ 40 \\ 33 \\ 8 \\ 13 \\ 8 \\ 8 \\ 8 \\ 8 \\ 8 \\ 8 \\ 8 \\ 8 \\ 8 \\ $	$\begin{array}{c} A\\ 5.\ 20\\ 5.\ 20\\ 5.\ 18\\ 5.\ 19\\ 5.\ 196\\ 5.\ 188\\ 5.\ 193\\ 5.\ 204\\ 5.\ 202\\ 5.\ 205\\ 5.\ 200\\ \end{array}$	A 2.53 1.79 1.47 1.27 1.14 1.05	s s m s s	A 5. 06 5. 09 5. 08 5. 10 5. 14 	$\begin{array}{c} A\\ 3.\ 004\\ 2.\ 601\\ 1.\ 8388\\ 1.\ 5010\\ 1.\ 3001\\ 1.\ 1630\\ 1.\ 0617\\ 0.\ 9194\\ .\ 8667\\ .\ 8222\\ .\ 7840 \end{array}$	$ \begin{array}{c} 8 \\ 100 \\ 60 \\ 15 \\ 7 \\ 13 \\ 10 \\ <1 \\ 6 \\ 6 \\ 5 \\ \end{array} $	$\begin{array}{c} A\\ 5,\ 203\\ 5,\ 202\\ 5,\ 201\\ 5,\ 200\\ 5,\ 200\\ 5,\ 200\\ 5,\ 201\\ 5,\ 201\\ 5,\ 201\\ 5,\ 200\\ 5,\ 200\\ 5,\ 200\\ 5,\ 200\\ \end{array}$
Average of last five lines		5. 200			5. 09			5. 200	

Magnesium Sulfide, MgS (cubic)

* Four additional lines are omitted.

Lattice constants

1927 Goldschmidt [3] 5.20 1948 Primak, Kaufman, and Ward [4]. 5.20 1956 Güntert and Faessler [5] 5.2034 at 21° (5.2034 at 21° (5.200 at 25° (ards.	1923 1927 1948 1956 1957	Holgersson [2] Goldschmidt [3] Primak, Kaufman, and Ward [4]. Güntert and Faessler [5] National Bureau of Stand- ards.	A 5.08 5.20 5.20 5.2034 at 21° C 5.200 at 25° C
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The density of magnesium sulfide calculated from the NBS lattice constant is 2.663 at 25° C.

References

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Manganese(II) Carbonate (rhodochrosite), MnCO₃ (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-0785	$\begin{array}{c} 2. 85 \\ 1. 76 \\ 1. 99 \end{array}$	Molybde- num.	Krieger [1] 1930.
1-0981	$\begin{array}{c} 2. \ 84 \\ 1. \ 76 \\ 3. \ 65 \end{array}$	Molybde- num.	Hanawalt, Rinn, and and Frevel [2] 1938.
2-0798	$\begin{array}{c} 2.84 \\ 1.78 \\ 2.18 \end{array}$	Iron	British Museum.
3-1280	(a)	(a)	Brentano and Adam- son [3] 1929.

* No powder data.

Additional published patterns. None.

NBS sample. The sample of manganous carbonate was precipitated from solutions of manganous sulfate and sodium bicarbonate. It was heated in a CO_2 atmosphere for 3 days at 400° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium; 0.001 to 0.01 percent caeh of aluminum, calcium, magnesium, and silicon; and 0.0001 to 0.001 percent each of silver, barium, chromium, copper, and iron.

The sample is pale pink. The indices of refraction could not be determined as the sample is too finc-grained.

Interplanar spacings and intensity measurements. The *d*-values reported by Krieger, by Hanawalt, Rinn, and Frevel, and by the British Museum were eonverted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Krieger Hanawalt, Rinn, and Fre- vel. British Museum National Bureau of Stand- ards.	104 104 104 104	018, 116 018, 116 018, 116 018, 116 012	$202 \\ 012 \\ 113 \\ 116$

Structural data. Wyckoff [4] in 1920 determined that manganous earbonate has ealcite-type structure, the space group D_{3d}^6 -R3c, and 2(MnCO₃) per unit rhombohedral cell or $6(MnCO_3)$ per unit hexagonal eell.

The unit-cell measurements reported by Wyckoff have been converted from kX to angstrom units. The values reported by Oftedahl were assumed to be in angstrom units. Cell measurements were reported by Brentano and Adamson [3] and Ferrari and Colla [6], but because they were given as large pseudocubie ccll values, they were not included in the lattice constants table.

Lattice constants



The density of manganous carbonate ealeulated from the NBS lattice constants is 3.697 at 25° C.
hkl	1930 Krieger Mo,		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		British Museum Fe,		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	Ι	d	Ι	d	Ι	d	Ι
$\begin{array}{c} 012 \\ \hline 104 \\ \hline 110 \\ 113 \\ 202 \\ 024 \\ 018 \\ 116 \\ 211 \\ 122 \\ 214 \\ \hline 208 \\ \hline 030 \\ 0.0.12 \\ 0.2.10 \\ 128 \\ \hline 1.1.12 \end{array}$	$\begin{array}{c} A\\ \hline 2.856\\ \hline 2.394\\ 2.184\\ 1.994\\ 1.813\\ 1.766\\ \hline 1.543\\ 1.460\\ \hline 1.543\\ 1.460\\ \hline 1.312\\ 1.261\\ 1.224\\ 1.199\\ 1.130\\ \end{array}$	$ \begin{array}{c} \hline \hline 100 \\ 40 \\ 40 \\ 50 \\ 30 \\ 80 \\ \hline 40 \\ 40 \\ 40 \\ \hline 5 \\ 10 \\ 20 \\ 5 \\ 20 \\ \end{array} $	<i>A</i> 3. 66 2. 85 2. 36 2. 16 2. 00 1. 82 1. 76 1. 53 1. 455 1. 368 1. 301 	$ \begin{array}{r} 30 \\ \overline{100} \\ 12 \\ 12 \\ 2 \\ 50 \\ \overline{6} \\ 4 \\ \overline{4} \\ 2 \\ \overline{12} \\ 2 \\ 50 \\ \overline{6} \\ 4 \\ \overline{12} \\ 2 \\ \overline{50} \\ \overline{6} \\ 4 \\ \overline{12} \\ \overline{12} \\ 2 \\ \overline{50} \\ \overline{6} \\ 4 \\ \overline{12} \\ \overline{12} \\ 2 \\ \overline{50} \\ \overline{6} \\ 4 \\ \overline{12} \\ \overline{12} \\ \overline{2} \\ \overline{50} \\ \overline{6} \\ 4 \\ \overline{12} \\ \overline{12} \\ \overline{12} \\ \overline{50} \\ \overline{6} \\ 4 \\ \overline{12} \\ \overline{12} \\ \overline{12} \\ \overline{12} \\ \overline{50} \\ \overline{6} \\ \overline{4} \\ \overline{12} \\ \overline{12} \\ \overline{12} \\ \overline{12} \\ \overline{50} \\ \overline{6} \\ \overline{4} \\ \overline{12} \\ $	$\begin{array}{c} A\\ 3.\ 66\\ 3.\ 14\\ 2.\ 85\\ 2.\ 64\\ 2.\ 41\\ 2.\ 18\\ 2.\ 01\\ 1.\ 84\\ 1.\ 78\\ 1.\ 56\\ 1.\ 54\\ 1.\ 46\\ 1.\ 44\\ 1.\ 42\\ 1.\ 41\\ 1.\ 39\\ 1.\ 32\\ 1.\ 23\\ 1.\ 22\\ 1.\ 20\\ \end{array}$	$\begin{array}{c} 60\\ 40\\ 100\\ 20\\ 60\\ 70\\ 60\\ 40\\ 80\\ 80\\ 40\\ 50\\ 50\\ 20\\ 20\\ 20\\ 20\\ 20\\ 20\\ 20\\ 20\\ 20\\ 2$	$\begin{array}{c c} & A \\ 3.\ 66 \\ \hline 2.\ 84 \\ \hline 2.\ 39 \\ \hline 2.\ 39 \\ \hline 2.\ 000 \\ 1.\ 829 \\ 1.\ 770 \\ 1.\ 763 \\ \hline 1.\ 763 \\ 1.\ 556 \\ 1.\ 533 \\ 1.\ 452 \\ \hline 1.\ 423 \\ \hline 1.\ 423 \\ \hline 1.\ 379 \\ 1.\ 306 \\ 1.\ 248 \\ 1.\ 221 \\ \hline 1.\ 146 \\ \hline \end{array}$	$\begin{array}{c} 35\\ \hline 100\\ \hline 20\\ 27\\ 23\\ 12\\ 30\\ 33\\ 1\\ 13\\ 1\\ \hline \\ \hline 1\\ \hline 10\\ <1\\ 3\\ \\ \\ 1\\ \hline 1\\ \hline 10\\ <1\\ 3\\ \\ \\ 1\\ \hline 1\\ \hline 1\\ \hline 1\\ \hline 1\\ \hline 1\\ \hline $

Manganese(II) Carbonate (rhodochrosite), MnCO₃ (trigonal)

^a Seven additional lines are omitted.

References

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Mercury(I) Bromide, Hg₂Br₂ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0675	$\begin{array}{c} 3. \ 29 \\ 4. \ 30 \\ 2. \ 12 \end{array}$	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength	
Havighurst [2] 1925 Hylleraas [3] 1925	Molyb- denum. Iron.	0.710 A K _α	

NBS sample. The sample of mercurous bromide was obtained from the City Chemical Corp., New York, N. Y. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of iron, magnesium, and silicon; and 0.0001 to 0.001 percent each of barium, calcium, chromium, copper, and manganese. The sample is colorless and optically positive.

The sample is colorless and optically positive. The indices of refraction were not determined as the particle size of the sample is too small.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel and by Havighurst were converted from kX to angstrom units, and the *d*-values of the Hylleraas pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel_ Havighurst Hylleraas National Bureau of Stand- ards.	$110 \\ 110 \\ 110 \\ 110 \\ 110$	$101 \\ 114 \\ 219, 228 \\ 101$	$114\\101\\114\\114$

Mercury(I) Bromide, Hg₂Br₂ (tetragonal)

hkl	193 Hanawalt and Fi Mo, 0.7	8 t, Rinn, revel 107 A	192 Havigi Mo, 0.7	25 hurst 107 A	192 Hyller Fe, 1.93	5 raas 323 A	1957 National Bureau of Standards Cu, 1.5405 A, 25° C			
	d	I	d	Ι	d	I	d	I		
$101 \\ 110 \\ 103 \\ 004 \\ 200$	$ \begin{array}{c} A \\ 4.31 \\ 3.30 \\ \hline 2.78 \\ 2.32 \\ \end{array} $	$50 \\ 100 \\ -20 \\ 24 \\ 24$	$\begin{array}{c} A \\ 4.31 \\ 3.287 \\ \hline 2.776 \\ 2.340 \end{array}$	$ \begin{array}{c c} 40 \\ 100 \\ -\overline{40} \\ 30 \end{array} $	$ \begin{array}{c} A \\ 4.32 \\ 3.316 \\ \hline 2.794 \\ 2.347 \end{array} $	$40 \\ 100 \\ -30 \\ 70$	$\begin{array}{c} A \\ 4.30 \\ 3.30 \\ 2.906 \\ 2.785 \\ 2.3339 \end{array}$	$ \begin{array}{r} 48 \\ 100 \\ 1 \\ 30 \\ 24 \end{array} $		
$114 \\ 211 \\ 105 \\ 204 \\ 220$	$\begin{array}{c} 2. \ 12 \\ 2. \ 05 \\ 2. \ 00 \\ 1. \ 78 \\ 1. \ 64 \end{array}$	$40 \\ 4 \\ 16 \\ 12 \\ 4$	$\begin{array}{c} 2. \ 123 \\ 2. \ 054 \\ 2. \ 008 \\ 1. \ 793 \\ 1. \ 647 \end{array}$	$\begin{array}{c} 60 \\ 15 \\ 35 \\ 25 \\ 15 \end{array}$	$\begin{array}{c} 2. \ 138 \\ 2. \ 062 \\ 2. \ 016 \\ 1. \ 796 \\ 1. \ 655 \end{array}$		$\begin{array}{c} 2. \ 1281 \\ 2. \ 0512 \\ 2. \ 0106 \\ 1. \ 7885 \\ 1. \ 6496 \end{array}$	$ \begin{array}{r} 44 \\ 10 \\ 24 \\ 17 \\ 8 \end{array} $		
$215 \\ 310 \\ 224 \\ 008 \\ 314$	$ \begin{array}{r} 1.52\\ 1.473\\ 1.423\\ \hline 1.307 \end{array} $	8 4 8 $$ 4	$\begin{array}{c} 1. \ 521 \\ 1. \ 474 \\ 1. \ 421 \\ 1. \ 391 \\ 1. \ 305 \end{array}$	$25 \\ 10 \\ 20 \\ 4 \\ 20$	$ \begin{array}{r} 1.529\\ 1.480\\ 1.423\\ \hline 1.310 \end{array} $	$50\\40\\40$	$\begin{array}{c} 1.\ 5228\\ 1.\ 4752\\ 1.\ 4192\\ 1.\ 3919\\ 1.\ 3039 \end{array}$	$\begin{array}{c} 12\\7\\8\\1\\6\end{array}$		
$118 \\ 305 \\ 109 \\ 208 \\ 400$	$ \left. \begin{array}{c} 1.\ 277 \\ 1.\ 200 \\ \end{array} \right. \right\} $	4 4 	1. 281 1. 201	15 20 	1. 288 1. 199 1. 169	w 70 10	$\left\{\begin{array}{l} 1.\ 2828\\ 1.\ 2750\\ 1.\ 1961\\ 1.\ 1668\end{array}\right.$	$4 \\ 2 \\ 6 \\ 1$		
$325 \\ 330 \\ 404 \\ 219 \\ 228$	 } 1.066	 4	1. 121 1. 066	5 15	1. 121 1. 102 1. 079 1. 066	$30 \\ 15 \\ 15 \\ 100$	1. 1193 1. 1000 1. 0761 1. 0644	$\leq 1 \\ 1 \\ 6$		
$\begin{array}{c} 420 \\ 334 \\ 318 \\ 415 \\ 424 \end{array}$			$ \overline{1.016} 0.972 $	 4 			$\begin{array}{c} 1.\ 0440\\ 1.\ 0233\\ 1.\ 0131\\ 1.\ 0095\\ 0.\ 9767\end{array}$	$\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{2}{\overset{1}{\overset{1}{\overset{1}{$		
$309 \\ 329 \\ 408 \\ 435 \\ 1 \ 0.13$	}					 	. 9687 . 8945 . 8609 . 8427	$\begin{array}{c}1\\2\\\leqslant^1_1\end{array}$		
$\begin{array}{c} 419 \\ 428 \\ 532 \end{array}$	}						. 8352 . 7925	<1 <1		

Structural data. Hylleraas [3] in 1925 determined that mercurous bromide has mercurous chloride-type structure, the space group $D_{4b}^{17}-I4/$ mmm, and 2(Hg₂Br₂) per unit cell.

The "a" measurements reported by Hylleraas (6.62 A) and by Vegard (6.595 A) have been multiplied by $\sqrt{2}/2$ for comparison with the NBS values. All of the measurements have been converted from kX to angstrom units.

Lattice constants

		<i>a</i>	c
$ \begin{array}{r} 1925 \\ 1925 \\ 1927 \\ 1957 \end{array} $	Havighurst [2] Hylleraas [3] Vegard [4] National Bureau of Standards.	$\begin{array}{c} 4. \ 66 \\ 4. \ 68 \\ 4. \ 666 \\ 4. \ 667 \end{array}$	$ \begin{array}{c} 11.12 \\ 11.18 \\ 11.142 \\ 11.138 \text{ at} \\ 25^{\circ} \text{ C.} \end{array} $

Mercury(II) Selenide (tiemannite), HgSe (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-0402	$\begin{array}{c} 3. \ 48 \\ 2. \ 13 \\ 1. \ 82 \end{array}$	Copper	DeJong [1] 1926. Harcourt [2] 1942.
3-0408	$\begin{array}{c} 3.\ 38\\ 2.\ 10\\ 1.\ 79 \end{array}$	Copper	Harcourt [2] 1942.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [3] 1926 Earley [4] 1950	Copper Copper	$egin{array}{c} { m K}_{lpha} \\ { m K}_{lpha 1} \end{array}$

NBS sample. The sample of mercuric selenide was obtained from the City Chemical Corp., New York, N.Y. It was annealed at 300° C in a sealed glass tube. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of magnesium and silicon; and 0.0001 to 0.001 percent each of silver, copper, and iron.

The sample is lead-gray and opaque.

Interplanar spacings and intensity measurements. The *d*-values reported by DeJong, Harcourt, and Earley were converted from kX to angstrom units, and the d-values of the Zachariasen pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
DeJong Harcourt Zachariasen Earley National Bureau of Standards	$220 \\ 111 \\ 111 \\ 111 \\ 111 \\ 111$	$311 \\ 220 \\ 20 $	$111 \\ 311 \\ 311 \\ 311 \\ 311 \\ 311$

The density of mercurous bromide calculated from the NBS lattice constants is 7.678 at 25° C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
- [2] R. J. Havighurst, Crystal structure of the mercurous halides, Am. J. Sci. 10, 15–28 (1925).
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- [4] L. Vegard, Gitterschwankungen bei Mischkristallbildung durch Fällung von Lösungen, Z. Physik 43, 299 (1927).

Structural data. DeJong [1] in 1926 determined that mercuric selenide has sphalerite-type structure, the space group T_d^2 -F43m, and 4 (HgSe) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants



The density of mercuric selenide calculated from the NBS lattice constant is 8.239 at 25° C.

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 [4] J. W. Earley, Description and synthesis of the selenide
- minerals, Am. Mineralogist 35, 338-364 (1950).
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hkl	D Cu,	1926 DeJon 1.541	g 8 A	Ha Cu,	1942 arcou 1.541	rt 8 A	1926 t Zachariasen 3 A Cu, 1.5418 A		1950 Earley Cu, 1.5405 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C			
	d	I	a	d	I	a	d	Ι	a	d	Ι	a	d	Ι	a
$ \begin{array}{r} 111\\ 200\\ 220\\ 311\\ 222 \end{array} $	$\begin{array}{c} A\\ 3.\ 4\\ 3.\ 0\\ 2.\ 13\\ 1.\ 82\\ 1.\ 74 \end{array}$		$\begin{array}{c} A \\ 5.9 \\ 6.0 \\ 6.02 \\ 6.04 \\ 6.03 \end{array}$	$\begin{array}{c} A \\ 3. 39 \\ 2. 96 \\ 2. 10 \\ 1. 79 \\ 1. 72 \end{array}$	$100 \\ 20 \\ 80 \\ 80 \\ 10$	$\begin{array}{c} A \\ 5.87 \\ 5.92 \\ 5.94 \\ 5.94 \\ 5.96 \end{array}$	$\begin{array}{c} A\\ 3.\ 51\\ 3.\ 04\\ 2.\ 15\\ 1.\ 833\\ 1.\ 755 \end{array}$	$ \begin{array}{r} 100 \\ 20 \\ 100 \\ 80 \\ 10 \end{array} $	$\begin{array}{c} A \\ 6.\ 08 \\ 6.\ 08 \\ 6.\ 08 \\ 6.\ 08 \\ 6.\ 08 \\ 6.\ 08 \end{array}$	$\begin{array}{c} A\\ 3.51\\ 3.05\\ 2.14\\ 1.833\\ 1.758\end{array}$	$100 \\ 20 \\ 80 \\ 80 \\ 5$	$\begin{array}{c} A \\ 6. \ 08 \\ 6. \ 10 \\ 6. \ 05 \\ 6. \ 08 \\ 6. \ 09 \end{array}$	$\begin{array}{c} A\\ 3.51\\ 3.041\\ 2.151\\ 1.835\\ 1.757\end{array}$	$ \begin{array}{r} 100 \\ 15 \\ 51 \\ 32 \\ 3 \end{array} $	$\begin{array}{c} A \\ 6.\ 08 \\ 6.\ 082 \\ 6.\ 084 \\ 6.\ 086 \\ 6.\ 086 \end{array}$
$\begin{array}{r} 400\\ 331\\ 420\\ 422\\ 511\end{array}$	$\begin{array}{c} 1.\ 51\\ 1.\ 39\\ 1.\ 36\\ 1.\ 23\\ 1.\ 16 \end{array}$	$ \begin{array}{r} 40 \\ 60 \\ 10 \\ 80 \\ 60 \end{array} $	$\begin{array}{c} 6. \ 04 \\ 6. \ 06 \\ 6. \ 08 \\ . \ 6. \ 03 \\ 6. \ 03 \end{array}$	$ \begin{array}{r} 1. 49 \\ 1. 36 \\ \overline{1. 22} \\ 1. 15 \end{array} $	$ \begin{array}{r} 20 \\ 40 \\ \overline{40} \\ 30 \end{array} $	$5.965.96\overline{5.98}5.985.98$	$\begin{array}{c} 1.\ 522\\ 1.\ 396\\ 1.\ 355\\ 1.\ 241\\ 1.\ 170 \end{array}$	$20 \\ 40 \\ 10 \\ 50 \\ 30$	$\begin{array}{c} 6. & 09 \\ 6. & 08 \\ 6. & 06 \\ 6. & 08 \\ 6. & 08 \\ 6. & 08 \end{array}$	$\begin{array}{c} 1.\ 518\\ 1.\ 397\\ 1.\ 358\\ 1.\ 241\\ 1.\ 171 \end{array}$	$10 \\ 20 \\ 5 \\ 20 \\ 10$	$\begin{array}{c} 6. \ 07 \\ 6. \ 09 \\ 6. \ 07 \\ 6. \ 080 \\ 6. \ 085 \end{array}$	$\begin{array}{c} 1. \ 521 \\ 1. \ 396 \\ 1. \ 361 \\ 1. \ 2424 \\ 1. \ 1707 \end{array}$	$ \begin{array}{c} 6 \\ 9 \\ 2 \\ 8 \\ 4 \end{array} $	$\begin{array}{c} 6.\ 084\\ 6.\ 085\\ 6.\ 087\\ 6.\ 086\\ 6.\ 083 \end{array}$
$\begin{array}{c} 440 \\ 531 \\ 600 \\ 620 \\ 533 \end{array}$	$ \begin{array}{c} 1. \ 07 \\ 1. \ 02 \\ 0. \ 955 \\ \\ \end{array} $	10 20 10 	$\begin{array}{c} 6. \ 05 \\ 6. \ 03 \\ \hline 6. \ 04 \\ \hline \end{array}$	$\begin{array}{r} 1.\ 06\\ 1.\ 017\\ 0.\ 952\\ .\ 919 \end{array}$	$ \begin{array}{c} 20 \\ 20 \\ \bar{30} \\ 20 \end{array} $	$ \begin{array}{c} 6. \ 00 \\ 6. \ 02 \\ \hline 6. \ 02 \\ 6. \ 03 \\ \end{array} $	$ \begin{array}{c} 1. \ 074 \\ 1. \ 028 \\ \hline 0. \ 961 \\ . \ 927 \\ \end{array} $	$ \begin{array}{c c} 20 \\ 40 \\ \bar{3}0 \\ 20 \end{array} $	$ \begin{array}{c} 6. 08 \\ 6. 08 \\ \hline 6. 08 \\ 6. 08 \\ 6. 08 \end{array} $	$ \begin{array}{r} 1.\ 076\\ 1.\ 027\\ \hline 0.\ 961\\ .\ 928\\ \end{array} $	$ \begin{array}{c} 10 \\ 20 \\ - 5 \\ 5 \end{array} $	6.087 6.076 6.078 6.085	$\begin{array}{c} 1.\ 0757\\ 1.\ 0286\\ 1.\ 0141\\ 0.\ 9622\\ .\ 9282 \end{array}$	2^{3}_{12}	$\begin{array}{c} 6. \ 085 \\ 6. \ 085 \\ 6. \ 085 \\ 6. \ 086 \\ 6. \ 087 \end{array}$
$\begin{array}{c} 444 \\ 711 \\ 642 \\ 731 \end{array}$.844 .806 .787	$\begin{array}{c} \overline{20}\\ 30\\ 20\end{array}$	$\begin{array}{c} & - & - & - \\ & 6 & 0 & 3 \\ & 6 & 0 & 4 \end{array}$		- - - -		. 877 . 851 . 813 . 792	$5 \\ 5 \\ 10 \\ 10 \\ 10$	$\begin{array}{c} 6.\ 076\\ 6.\ 077\\ 6.\ 084\\ 6.\ 083 \end{array}$. 8784 . 8519 . 8130 . 7921	$2 \\ 1 \\ 2 \\ 1$	$\begin{array}{c} 6. \ 086 \\ 6. \ 084 \\ 6. \ 084 \\ 6. \ 084 \end{array}$
Aver fiv	age of e lines	last	6. 04			6. 03		-	6. 08		-	6. 081		-	6. 085

Mercury(II) Selenide (tiemannite), HgSe (cubic)

Nickel Sulfate Hexahydrate (retgersite), NiSO₄ · 6H₂O (tetragonal)

ASTM cards

Card Inde numbers lines		Radiation	Source		
1-0388	$\begin{array}{c} 4. \ 26 \\ 4. \ 6 \\ 2. \ 72 \end{array}$	Molybde- num	Hanawalt, Rinn, and Frevel [1] 1938.		
1-0389			This is a continua- tion of the previ- ous card.		

Additional published patterns

Source	Radiation	Wavelength
Borghijs [2] 1937	Copper	Κα

NBS sample. The sample of nickel sulfate hexahydrate was obtained from the Johnson Matthey Co., Ltd., London, in the form of the heptahydrate. The sample was heated in an oven for 15 minutes at about 90°C and cooled at room temperature. The Johnson Matthey spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of calcium, silicon, and magnesium; and 0.0001 to 0.001 percent each of copper and sodium. The sample has a pale blue-green color and is

The sample has a pale blue-green color and is optically negative with the indices of refraction $N_0=1.513$ and $N_e=1.487$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units and the *d*-values of the Borghijs pattern were calculated from reported Bragg angle data. The Borghijs pattern did not include intensity measurements. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel_ National Bureau of Stand- ards.	$\begin{array}{c}112\\112\end{array}$	$004, 111 \\ 004$	$\begin{array}{c} 204\\ 203 \end{array}$

Structural data. Beevers and Lipson [3] in 1932 determined that nickel sulfate hexalydrate has the space group $D_4^4-P4_12_12$ (or its enantiomorph $D_4^8-P4_32_1$) with 4(NiSO₄·6H₂O) per unit eell. Nickel sulfate hexalydrate is used as a structure-type.

Several unit-eell measurements have been converted from kX to angstrom units for comparison with the NBS values. The "a" value reported by Beevers and Lipson for the larger tetragonal cell has been converted to the smaller cell value.

Lattice constants

1932	Beevers and Lipson [3]	a A 6, 80 6, 790	c A 18. 3 18. 240
1937 1949 1957	Borghijs [2] Frondel and Palache [4] National Bureau of Stand- ards.	6. 790 6. 779 6. 782	18. 249 18. 24 18.28 at 25°C

The density of nickel sulfate hexahydrate calculated from the NBS lattice constants is 2.075 at 25° C.

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- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemieal analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457–512 (1938).
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- [3] C. A. Beevers and H. Lipson, The crystal structure of nickel sulphate hexahydrate, NiSO₄-6H₂O, Z. Krist. 83, 123-135 (1932).
- [4] C. Frondel and C. Palache, Retgersite, NiSO₄·6H₂O, a new mineral, Am. Mineralogist 34, 188–194 (1949).

Nickel Sulfate Hexahydrate (retgersite), NiSO₄·6H₂O (tetragonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1937 Borghijs Cu, 1.5418 A		195 Natic Burea Standa Cu, 1.5- 25°	7 onal u of ards 405 A, C
	d	1	đ	Ι	d	Ι
$101 \\ 111 \\ 004 \\ 112 \\ 104$	$ \begin{array}{c} A \\ 6. \ 4 \\ 1. \ 6 \\ 4. \ 27 \\ 3. \ 97 \end{array} $	$4 \\ 25 \\ 100 \\ 2$	A 4. 86 4. 24 4. 11		$\begin{matrix} A \\ 6.36 \\ \{4.64 \\ \{4.57 \\ 4.25 \\ 3.789 \end{matrix}$	
$113 \\ 200 \\ 201 \\ 202 \\ 210$	3. 78 3. 39 3. 23 3. 19 	$\begin{array}{c} 2\\12\\2\\2\\\end{array}$	3. 60		3. 768 3. 392 3. 336 3. 179 3. 033	$5\\11\\7\\4\\3$
$203 \\ 115 \\ 212 \\ 106 \\ 204$	2. 97 2. 73	18 - - 20	2.962.902.72		$\begin{array}{c} 2.\ 964\\ 2.\ 908\\ 2.\ 880\\ 2.\ 778\\ 2.\ 721 \end{array}$	$ \begin{array}{r} 19 \\ 6 \\ 3 \\ 2 \\ 18 \\ \end{array} $
$116 \\ 214 \\ 215 \\ 224 \\ 312$	$2.58 \\ \overline{2.35} \\ 2.13 \\ 2.07 $	$\begin{array}{c} 20\\ \bar{1}6\\ 20\\ 2\end{array}$	$\begin{array}{c} 2.52\\ 2.33\\ 2.12\\ 2.088\end{array}$		$\begin{array}{c} 2.\ 571\\ 2.\ 526\\ 2.\ 334\\ 2.\ 125\\ 2.\ 088 \end{array}$	$13 \\ 8 \\ 12 \\ 11 \\ 4$
$118 \\ 313 \\ 225 \\ 217 \\ 314$	2.02 1.98	-4 -2 -	$2.022 \\ 1.984 \\ 1.942$		$\begin{array}{c} 2.\ 062\\ 2.\ 023\\ 2.\ 006\\ 1.\ 978\\ 1.\ 941 \end{array}$	$< 1 \\ < 1 \\ < 1 \\ 4 \\ 2$
$208 \\ 320 \\ 315 \\ 218 \\ 323$	$ \begin{array}{c} 1.89\\ \overline{1.85}\\ 1.83\\ 1.80\\ \end{array} $	$\begin{array}{c}10\\-\\4\\2\\2\end{array}$	$ \begin{array}{r} 1. 895 \\ 1. 850 \\ 1. 824 \\ \end{array} $		$\begin{array}{c} 1.\ 895\\ 1.\ 880\\ 1.\ 849\\ 1.\ 825\\ 1.\ 799 \end{array}$	${6 \atop {3 \atop {5 \atop {3} \atop {1} \atop {1} }}}$
$\begin{array}{c} 227 \\ 1 \cdot 0 \cdot 10 \\ 316 \\ 324 \\ 1 \cdot 1 \cdot 10 \end{array}$	$ \Big\} \frac{1.75}{1.75} \\ 1.70$	- 10 - 8	$1.751 \\ 1.721 $	-	$\begin{array}{c} 1.\ 766\\ 1.\ 755\\ 1.\ 740\\ 1.\ 708 \end{array}$	$\begin{array}{c} 1 \\ 6 \\ 1 \\ 5 \end{array}$
$\begin{array}{c} 401 \\ 219 \\ 317 \\ 228 \\ 411 \end{array}$	1. $\overline{65}$	- - 8 -	1. 687 1. $\overline{653}$		$\begin{array}{c} 1.\ 688\\ 1.\ 6559\\ 1.\ 6535\\ 1.\ 6372 \end{array}$	$\begin{array}{c} 4\\ 2\\ 2\\ 3\end{array}$
$\begin{array}{c} 403 \\ 404 \\ 413 \\ 229 \end{array}$]] 1. 59 (^a)	- 4 -	1. 616 1. 614 1. 540 (^b)	-	1. 6329 1. 5888 1. 5496	$\begin{vmatrix} 2\\<1\\1 \end{vmatrix}$

^a Sixteen additional lines are omitted.

^b Eight additional lines are omitted.

Potassium Bromate, KBrO₃ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
10743	$\begin{array}{c} 3. \ 21 \\ 3. \ 01 \\ 4. \ 39 \end{array}$	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [2] 1928	Copper	K

NBS sample. The sample of potassium bromate was obtained from the J. T. Baker Chemical Co., Phillipsburgh, N. J. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of rubidium; 0.001 to 0.01 percent of barium; and 0.0001 to 0.001 percent each of aluminum, calcium, magnesium, and silicon.

The sample is colorless and optically negative with the indices of refraction $N_0=1.678$ and $N_e=1.599$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units and the *d*-values of the Zachariasen pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel Zachariasen National Bureau of Standards	$012 \\ 012 \\ 012 \\ 012$	$110 \\ 202 \\ 110$	$101 \\ 104 \\ 101$

Structural data. Zachariasen [2] in 1928 determined that potassium bromate has the space group C_{3v}^5 -R3m with 1(KBrO₃) per unit rhombohedral cell or 3(KBrO₃) per unit hexagonal cell. Potassiom bromate is used as a structure-type.

The unit-cell measurements of Zachariasen have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	с
$1928 \\ 1957$	Zachariasen [2] National Bureau of Standards.	$\begin{matrix} A \\ 6. \ 018 \\ 6. \ 014 \end{matrix}$	$\begin{array}{c} A \\ 8.157 \\ 8.156 \\ \mathrm{at}\ 25^{\circ}\ \mathrm{C} \end{array}$

The density of potassium bromate calculated from the NBS lattice constants is 3.256 at 25° C.

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457–512 (1938).
- [2] W. H. Zachairasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO₃, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1928**, No. 4 (1928).

hkl	193 Hanaw Rinn, Frev	8 valt, and el	1928 Zachariasen		195 Natio Burea Stand	57 onal ou of ards
	0.7107	Ϋ́Α	Cu, 1.5	Cu, 1.5418 A		405 A, C
	d	Ι	d	Ι	d	I
$101 \\ 012 \\ 110 \\ 003 \\ 021$	A 4. 39 3. 21 3. 01 2. 73	$50 \\ 100 \\ 63 \\ 5 \\$	$\begin{array}{c} A \\ 4. \ 42 \\ 3. \ 23 \\ 3. \ 03 \\ 2. \ 75 \\ 2. \ 46 \end{array}$	$35 \\ 100 \\ 50 \\ 10 \\ 15 $	$\begin{array}{c} A \\ 4. 39 \\ 3. 21 \\ 3. 008 \\ 2. 718 \\ 2. 482 \end{array}$	$60 \\ 100 \\ 70 \\ 10 \\ 2$
$202 \\ 113 \\ 211 \\ 104 \\ 122$	$ \begin{array}{c} 2.18\\ 2.01\\ 1.89\\ 1.77 \end{array} $	50 8 25 25	$\begin{cases} 2. 20 \\ 2. 02 \\ 1. 93 \\ 1. 91 \\ 1. 78 \end{cases}$	$ \begin{array}{r} 70 \\ 10 \\ 50 \\ 60 \\ 20 \end{array} $	$\begin{array}{c} 2. \ 196 \\ 2. \ 017 \\ 1. \ 914 \\ 1. \ 899 \\ 1. \ 773 \end{array}$	$49 \\ 7 \\ 10 \\ 16 \\ 21$
$300 \\ 024 \\ 220 \\ 303 \\ 131$	1. 73 1. 60 1. 50 1. 463	10 10 10 8 	$\begin{array}{c} 1.\ 74\\ 1.\ 61\\ 1.\ 51\\ 1.\ 47\\ 1.\ 42 \end{array}$	$5 \\ 10 \\ 40 \\ 5 \\ 50$	$\begin{array}{c} 1.\ 737\\ 1.\ 606\\ 1.\ 504\\ 1.\ 463\\ 1.\ 422 \end{array}$	$11 \\ 7 \\ 11 \\ 2 \\ 3$
$214 \\ 205 \\ 312 \\ 223 \\ 125$	1. 415 1. 383 1. 361 1. 238	$25 \\ 5 \\ 15 \\ 15 \\$	$ \begin{array}{c} 1. 39 \\ 1. 37 \\ 1. 32 \\ 1. 26 \end{array} $	5 40 10 10	${ \begin{array}{c} 1.\ 416 \\ \{1.\ 383 \\ 1.\ 362 \\ 1.\ 3158 \\ 1.\ 2561 \end{array} } }$	$11 \\ 2 \\ 10 \\ 3 \\ 1$
$116 \\ 321 \\ 134 \\ 232 \\ 140$		 10 10 5	$ \begin{array}{c} 1. 24 \\ 1. 18 \\ \left\{\begin{array}{c} 1. 15 \\ 1. 14 \end{array}\right. $	50 40 25 25	$ \begin{array}{c} 1.\ 2393 \\ \{1.\ 1822 \\ 1.\ 1788 \\ 1.\ 1467 \\ 1.\ 1367 \end{array} $	$\begin{array}{c} 6\\ 3\\ 4\\ 4\\ 4\\ 4\end{array}$
$\begin{array}{c} 404 \\ 306 \\ 027 \\ 413 \\ 324 \end{array}$	$ \begin{array}{c} 1. \ 102 \\ 1. \ 076 \\ \hline 1. \ 027 \end{array} $	5 -5	$\begin{array}{c} 1. \ 10 \\ 1. \ 09 \\ 1. \ 06 \\ 1. \ 05 \\ 1. \ 03 \end{array}$	$ \begin{array}{r} 10 \\ 5 \\ 25 \\ 10 \\ 20 \end{array} $	$\begin{array}{c} 1.\ 0973\\ 1.\ 0701\\ 1.\ 0635\\ 1.\ 0488\\ 1.\ 0310 \end{array}$	$egin{array}{c} 1 \\ 2 \\ 1 \\ 2 \\ 3 \end{array}$
$\begin{array}{c} 045 \\ 226 \\ 330 \\ 018 \\ 241 \end{array}$	1. 006		1. 02 1. 01 1. 00 	2.5 25 25 	$\begin{array}{c} 1.\ 0174\\ 1.\ 0086\\ 1.\ 0022\\ 1.\ 0006\\ 0.\ 9774 \end{array}$	$<^{1}_{3}_{4}_{<1}$
$235 \\ 422 \\ 208 \\ 333 \\ 511$			 	 	$\begin{array}{c} . \ 9638 \\ . \ 9568 \\ . \ 9494 \\ . \ 9405 \\ . \ 9298 \end{array}$	$\overset{1}{\underset{{\scriptstyle \leftarrow}1}{\overset{1}{\underset{{\scriptstyle \leftarrow}1}}}}$
$054 \\ 152 \\ 137$)		 		.9276 .9119	$\frac{2}{3}$
009	}				. 9068 8865	2
505					. 8780	<1
$\begin{array}{c} 416 \\ 600 \end{array}$	ן ו				. 8720	4
$\frac{119}{514}$	<u>۲</u>				. 8503	о З
$342 \\ 250 \\ 318 \\ 063 \\ 155$. 8380 . 8341 . 8329 . 8270 . 8115	3 3 2 <1 <1
$336 \\ 1 \cdot 0 \cdot 10 \\ 048 \\ 253 \\ 434$. 8067 . 8058 . 8030 . 7975 . 7895	$\overset{1}{\overset{1}{\underset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{$

ASTM cards

Card number	Index lines	Radiation	Source
1-1035	2. 73 3. 04 2. 53	Molyb- denum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of potassium cyanate was obtained from the City Chemical Corp., New York, N. Y. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of sodium and rubidium; and 0.0001 to 0.001 percent each of aluminum, barium, calcium, copper, magnesium, and silicon.

The sample is colorless and optically negative with the refractive indices $N_o=1.575$ and $N_e=1.412$.

Interplanar spacings and intensity measurements. The d-values reported by Hanawalt, Rinn, and Frevel have been converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel National Bureau of Standards	$\begin{array}{c} 112\\112\end{array}$	$\begin{array}{c} 200\\ 200 \end{array}$	$\begin{array}{c} 211\\ 211\end{array}$

Structural data. Hendricks and Pauling [2] in 1925 determined that potassium cyanate has potassium trinitride-type structure, the space group D_{4h}^{4s} -I4/mcm and 4(KCNO) per unit cell.

The unit-cell measurements reported by Hendricks and Pauling have been converted from kX to angstrom units for comparison with the NBS values.

Lattice	constants

1925 1957	Hendricks and Pauling [2] National Bureau of	$\begin{array}{c} a \\ \hline \\ 6.082 \\ 6.084 \end{array}$	<i>c</i> <i>A</i> 7. 044 7. 034 at
1957	National Bureau of Standards.	6. 084	7. 034 at 25° C

The density of potassium cyanate calculated from the NBS lattice constants is 2.069 at 25° C.

Potassium	Cyanate,	KCNO	(tetragonal)
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hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25°C	
	d	Ι	d	Ι
$110 \\ 002 \\ 200 \\ 112 \\ 211$	$\begin{array}{c} A \\ 4.30 \\ \hline 3.05 \\ 2.74 \\ 2.54 \end{array}$	$ 14 \overline{50} 100 30 $	$\begin{array}{c} A \\ 4. 31 \\ 3. 52 \\ 3. 05 \\ 2. 724 \\ 2. 538 \end{array}$	$16 \\ 1 \\ 43 \\ 100 \\ 26$
$202 \\ 220 \\ 310 \\ 222 \\ 213$	$\begin{array}{c} 2. \ 30 \\ 2. \ 14 \\ 1. \ 92 \\ 1. \ 84 \\ 1. \ 77 \end{array}$	$30 \\ 20 \\ 25 \\ 12 \\ 10$	$\begin{array}{c} 2.\ 302\\ 2.\ 152\\ 1.\ 925\\ 1.\ 835\\ 1.\ 777 \end{array}$	$23 \\ 16 \\ 16 \\ 6 \\ 5$
$\begin{array}{c} 004\\ 312\\ 321\\ 114\\ 204 \end{array}$	$ \begin{array}{c} 1. 75 \\ 1. 68 \\ \\ 1. 63 \\ 1. 52 \end{array} $	$\begin{array}{c}10\\20\\\\4\\12\end{array}$	$\begin{array}{c} 1.\ 759\\ 1.\ 6885\\ 1.\ 6414\\ 1.\ 6284\\ 1.\ 5232 \end{array}$	$\begin{array}{c}9\\11\\2\\2\\7\end{array}$
$\begin{array}{c} 402 \\ 224 \\ 332 \\ 314 \\ 422 \end{array}$	$\begin{array}{c} 1. \ 39 \\ 1. \ 36 \\ 1. \ 33 \\ 1. \ 30 \\ 1. \ 27 \end{array}$	$12 \\ 20 \\ 12 \\ 8 \\ 2$	$\begin{array}{c} 1.\ 3968\\ 1.\ 3616\\ 1.\ 3279\\ 1.\ 2983\\ 1.\ 2690 \end{array}$	5874
$215 \\ 510 \\ 404 \\ 116 \\ 206$	$ \begin{array}{c} 1. 19 \\ 1. 15 \\ 1. 13 \\$	$\begin{array}{c} - & - & - \\ & 2 \\ & 2 \\ & 8 \\ - & - & - \end{array}$	$\begin{array}{c} 1.\ 2499\\ 1.\ 1931\\ 1.\ 1503\\ 1.\ 1311\\ 1.\ 0939 \end{array}$	$\overset{1}{\underset{4}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset$
$\begin{array}{c} 424 \\ 226 \\ 600 \\ 316 \\ 514 \end{array}$	1. 07 1. 00	6 4 	$\begin{array}{c} 1.\ 0761\\ 1.\ 0294\\ 1.\ 0140\\ 1.\ 0010\\ 0.\ 9876 \end{array}$	$\overset{4}{\overset{1}{\overset{1}{\overset{3}{\overset{3}{\overset{1}{\overset{3}{\overset{1}{\overset{3}{\overset{1}{\overset{3}{\overset{1}{\overset{3}{\overset{1}{\overset{3}{\overset{1}{\overset{3}{\overset{1}{\overset{3}{\overset{1}{\overset{3}{\overset{1}{\overset{3}{3$
$\begin{array}{c} 620 \\ 217 \\ 406 \\ 444 \end{array}$.9622 .9427 .9288 .9178	$\overset{\leq 1}{\underset{< 1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset$

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
- [2] S. B. Hendricks and L. Pauling, The crystal structures of sodium and potassium trinitrides and potassium cyanate and the nature of the trinitride group, J. Am. Chem. Soc. 47, 2904–2920 (1925).

Potassium Fluotitanate, K₂TiF₆ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-1218	$\begin{array}{c} 2. \ 18 \\ 3. \ 39 \\ 2. \ 85 \end{array}$	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Card number 1-1218 is listed as $K_2 TiF_6 H_2O$. The *d*-values of the pattern can be indexed according to the structure data given for anhydrous $K_2 TiF_6$.

Additional published patterns. None.

NBS sample. The sample of potassium fluotitanate was obtained from the Baker Chemical Co., Phillipsburg, N. J. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of rubidium; 0.001 to 0.01 percent each of aluminum, calcium, sodium, lead, silicon, and strontium; and 0.0001 to 0.001 percent each of iron and magnesium.

The sample is colorless and optically negative. The indices of refraction are N_0 =1.476 and N_e = 1.456.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel National Bureau of Standards	$\begin{array}{c} 201\\ 101 \end{array}$	$\begin{array}{c} 101\\ 201\end{array}$	110 110

Structural data. Siegel [2] in 1952 determined that potassium fluotitanate has potassium fluogermanate-type structure, the space group $D_{3a}^3 - P\overline{3}ml$, and $1(K_2TiF_6)$ per unit cell.

Lattice	constants
	00100001000

		<i>a</i>	с
$1952 \\ 1957$	Siegel [2] National Bureau of Standards.	$\begin{array}{c} A \\ 5.\ 715 \\ 5.\ 7271 \end{array}$	$\begin{array}{c} A \\ 4.656 \\ 4.6619 \text{ at} \\ 25^{\circ} \text{ C.} \end{array}$

The density of potassium fluotitanate calculated from the NBS lattice constants is 3.010 at 25° C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	Ι	d	I
	A		A	
$100 \\ 001 \\ 101 \\ 110 \\ 200$	4. 96 4. 66 3. 40 2. 86 2. 47	$19 \\ 9 \\ 59 \\ 26 \\ 8$	4. 96 4. 66 3. 397 2. 866 2. 481	$30 \\ 20 \\ 100 \\ 41 \\ 10$
$111\\002\\201\\102\\112$	2. 34 2. 18 2. 10	$15 \\ 100 \\ 14 \\$	2. 440 2. 331 2. 190 2. 109 1. 8077	$4 \\ 24 \\ 100 \\ 24 \\ 2$
$211 \\ 202 \\ 300 \\ 003 \\ 212$	$ \begin{array}{r} 1. 73 \\ 1. 69 \\ 1. 65 \\ \hline 1. 463 \end{array} $	$ \begin{array}{c} 10 \\ 19 \\ 5 \\ $	$\begin{array}{c} 1.\ 7394\\ 1.\ 6986\\ 1.\ 6526\\ 1.\ 5541\\ 1.\ 4613 \end{array}$	$14 \\ 21 \\ 7 \\ 3 \\ 10$
$220 \\ 113 \\ 311 \\ 203 \\ 222$	1. 433 1. 365 1. 321 	12 8 8	$\begin{array}{c} 1.\ 4320\\ 1.\ 3660\\ 1.\ 3187\\ 1.\ 3164\\ 1.\ 2194 \end{array}$	$14 \\ 10 \\ 9 \\ 9 \\ 2$
$\begin{array}{c} 401 \\ 312 \\ 004 \\ 104 \\ 303 \end{array}$	1. 198 1. 137 	3 5 	$\begin{array}{c} 1. \ 1982 \\ 1. \ 1844 \\ 1. \ 1653 \\ 1. \ 1345 \\ 1. \ 1325 \end{array}$	$\begin{array}{c} 4\\ 3\\ 1\\ 4\\ 4\end{array}$
$321 \\ 402 \\ 410 \\ 114 \\ 204 \\ 411$	 }	 	1. 1055 1. 0947 1. 0820 1. 0793 1. 0546	3 3 3 1 1
$223 \\ 322 \\ 214 \\ 412 \\ 403$			$\begin{array}{c} 1.\ 0531\\ 1.\ 0225\\ 0.\ 9897\\ .\ 9815\\ .\ 9696 \end{array}$	$2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ $
$330 \\ 304 \\ 005 \\ 421 \\ 105$			$\begin{array}{c} . \ 9546 \\ . \ 9524 \\ . \ 9324 \\ . \ 9190 \\ . \ 9164 \end{array}$	$ \begin{array}{c} 1 \\ 1 \\ 3 \\ 3 \end{array} $
$224 \\ 413 \\ 511 \\ 205 \\ 422 \\ 215$	 		$\begin{array}{c} . \ 9041 \\ . \ 8884 \\ . \ 8750 \\ . \ 8728 \\ . \ 8697 \\ . \ 8349 \end{array}$	1 5 2 2 3 2

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
- [2] S. Siegel, The crystal structure of K₂TiF₆, Acta Cryst. 5, 683-684 (1952).

Potassium Metaperiodate, KIO₄ (tetragonal)

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1000

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ASTM cards

Card number	Index lines	Radiation	Source
1-0618	$ \begin{array}{c} 3. \ 41 \\ 5. \ 2 \\ 2. \ 11 \end{array} $	Molyb- denum	Hanawalt, Rinn, aud Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Hylleraas [2] 1926	Iron	K_{α}

NBS sample. The sample of potassium metaperiodate was obtained from the City Chemical Corp., New York, N. Y. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of calcium; 0.001 to 0.01 percent of rubidium; and 0.0001 to 0.001 percent each of aluminum barium, calcium, iron, lithium, magnesium, silicon, and strontium.

The sample is colorless and optically positive. The indices of refraction are $N_0=1.619$ and $N_e=1.648$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt Rinn, and Frevel were converted from kX to angstrom units and the *d*-values of the Hylleraas pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel- Hylleraas National Bureau of Stand- ards.	$112 \\ 112 \\ 112 \\ 112$	$101 \\ 312 \\ 101$	$204 \\ 411, 208 \\ 204$

Structural data. Hylleraas [2] in 1926 determined that potassium metaperiodate has calcium tungstate-type structure, the space group $C_{4h}^6-I4_1/a$, and $4(KIO_4)$ per unit cell. The unit-cell measurement reported by Hyl-

The unit-cell measurement reported by Hylleraas has been converted from kX to angstrom units for comparison with the NBS value.

		a	c
1926 1957	Hylleraas [2] National Bureau of Standards.	<i>A</i> 5. 76 5. 7304	A 12. 65 12.604 at 25° C.

The density of the potassium metaperiodate calculated from the NBS lattice constant is 3.690 at 25° C.

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
- [2] E. Hylleraas, The atomic arrangement in the tetragonal crystals of $K_2I_2O_8$ potassium metaperiodate, Z. Physik. **39**, 308–321 (1926).

	Hana Rinn,	walt, and	Hyller:	aas	Natic Burea Stand	i onal u of orda
hkl	Mo, 0.7	7107 A	Fe, 1.93	60 A	Cu, 1.54 25°	105 A, C
	d	Ι	d	Ι	d	I
$101 \\ 112 \\ 004 \\ 200 \\ 202$	$\begin{array}{c} A \\ 5. \ 2 \\ 3. \ 40 \\ 3. \ 14 \\ 2. \ 86 \\ \end{array}$	$40 \\ 100 \\ 16 \\ 16 \\$	$\begin{array}{c} A \\ 5.\ 21 \\ 3.\ 42 \\ 3.\ 17 \\ 2.\ 88 \end{array}$	$20 \\ 100 \\ 20 \\ 30 \\$	$\begin{array}{c} A \\ 5.\ 22 \\ 3.\ 41 \\ 3.\ 15 \\ 2.\ 867 \\ 2.\ 608 \end{array}$	$59 \\ 100 \\ 15 \\ 20 \\ 2$
$211 \\ 114 \\ 105 \\ 213 \\ 204$	$2.51 \\ \overline{2.31} \\ 2.17 \\ 2.11 \\ $	$ \begin{array}{c} 10\\ \overline{}\\ \overline{}\\ \overline{}\\ 3\\ 24 \end{array} $	2. 52 2. 19 2. 13	25 10 50	$\begin{array}{c} 2.\ 512\\ 2.\ 487\\ 2.\ 306\\ 2.\ 187\\ 2.\ 121 \end{array}$	$10 \\ 4 \\ 3 \\ 6 \\ 25$
$220 \\ 301 \\ 116 \\ 215 \\ 312$	2. 02 1. 86 1. 79 1. 74	$8\\-\bar{16}\\6\\24$	$2.04 \\ 1.871 \\ 1.806 \\ 1.750$	$\begin{array}{c}25\\35\\\hline1\\60\end{array}$	$\begin{array}{c} 2.\ 027\\ 1.\ 890\\ 1.\ 8660\\ 1.\ 7977\\ 1.\ 7409 \end{array}$	$9 \\ 14 \\ 10 \\ 7 \\ 24$
$224 \\ 321 \\ 008 \\ 305$	1.70 1.57 1.52	8 5 1	1. 713 1. 580	$\frac{35}{15}$	1. 7042 1. 5783	18 6 2
323	1. 02		1. 493		1. 4869	4
$217 \\ 400 \\ 411 \\ 208$	$\left. \begin{array}{c} 1.470\\ 1.427\\ \end{array} \right\}_{}$	1	1. 468 1. 439 1. 381	10 10 60	$ \begin{array}{c} 1. 4733 \\ 1. 4328 \\ 1. 3812 \end{array} $	$\frac{3}{5}$
316	1. 371	16			1. 3720	11
$413 \\ 332 \\ 404$	$\Big\} 1.317$	3	1. 328	25	1. 3209	7
$\begin{array}{c} 404\\ 420\\ 228\end{array}$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		$\begin{array}{c} 1. \ 3096 \\ 1. \ 2871 \\ 1. \ 2480 \end{array}$	$\begin{array}{c} 20\\ 25\\ 15\end{array}$	$\begin{array}{c} 1. \ 3044 \\ 1. \ 2816 \\ 1. \ 2433 \end{array}$	
$\begin{array}{c} 415 \\ 1 \cdot 1 \cdot 10 \\ 424 \\ 501 \\ 336 \end{array}$		 	1. 2075 1. 1918	-15 35 	$\begin{array}{c} 1.\ 2174\\ 1.\ 2030\\ 1.\ 1875\\ 1.\ 1416\\ 1.\ 1361 \end{array}$	$\begin{smallmatrix}1\\4\\22\\2\\2\\2\end{smallmatrix}$
$\begin{array}{c} 512 \\ 503 \end{array}$	}				1. 1065	3
$521 \\ 408 \\ 0.0.12$	}			 	1. 0604 1. 0506	<1 1
$505 \\ 3 \cdot 1 \cdot 10 \\ 440 \\ 428 \\ 516$		 		 	$\begin{array}{c} 1.\ 0430\\ 1.\ 0348\\ 1.\ 0132\\ 0.\ 9944\\ .\ 9908 \end{array}$	$2 \\ 2 \\ 1 \\ 2 \\ 1$
$532 \\ 507 \\ 444 \\ 600 \\ 3 \cdot 3 \cdot 10$		 		 	$\begin{array}{c} . \ 9711 \\ . \ 9670 \\ . \ 9643 \\ . \ 9551 \\ . \ 9214 \end{array}$	$3 \\ < 1 \\ 1 \\ 1 \\ 1 \\ 1$
$\begin{array}{c} 613 \\ 604 \\ 620 \\ 536 \\ 615 \end{array}$					$\begin{array}{c} . \ 9192 \\ . \ 9138 \\ . \ 9062 \\ . \ 8898 \\ . \ 8826 \end{array}$	$\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{3}{}}}}}}_{1}$
$\begin{array}{c} 624 \\ 448 \end{array}$	2				. 8705	2
631	J				. 0020	-

Potassium Permanganate, KMnO₄ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0725	$\begin{array}{c} 3.\ 22\\ 2.\ 95\\ 3.\ 57\end{array}$	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
McCrone [2] 1950		

NBS sample. The sample of potassium permanganate was obtained from the Baker Chemical Co., Phillipsburg, N. J. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, magnesium, rubidium, and silicon; and 0.0001 to 0.001 percent each of copper and iron.

The sample has a dark brown-purple color. The indices of refraction could not be determined by the usual liquid grain immersion method because the sample is very dark, nearly opaque.

Interplanar spacings and intensity measure-ents. The *d*-values reported by Hanawalt, ments. Rinn, and Frevel and by McCrone were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel McCrone National Bureau of Standards	$211 \\ 211 \\ 211 \\ 211$	$\begin{array}{c}112\\210\\210\end{array}$	$210 \\ 112 \\ 112 \\ 112$

Structural data. Basche and Mark [3] in 1926 determined that potassium permanganate has barium sulfate-type structure, the space group D_{2b}^{16} -Pnma, and 4(KMnO₄) per unit cell.

References

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
- W. C. McCrone, Potassium permanganate, KMnO₄, Anal. Chem. 22, 1459 (1950).
 W. Basche and H. Mark, Über die Struktur von Ver-bindungen des Typus MeXO₄, Z. Krist. 64, 1–70 (1992) (1926).
- [1920].
 [4] R. C. L. Mooney, The crystal structure of potassium permanganate, Phys. Rev. 37, 1306–1310 (1931).
 [5] A. L. Greenberg and G. H. Walden, Studies of equilibrium solid solutions of ionic lattices. Systems: KMnO₄-KClO₄-H₂O and NH₄Cl-MnCl-H₂O, J. Chem. Phys. 8, 645 (1940).

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

		stants		
		a	ь	с
$1926 \\ 1931 \\ 1940$	Basche and Mark [3]_ Mooney [4] Greenberg and Wal-	$egin{array}{c} A \\ 8.\ 86 \\ 9.\ 11 \\ 9.\ 117 \end{array}$	$\begin{array}{c} & A \\ 5. \ 66 \\ 5. \ 73 \\ 5. \ 7191 \end{array}$	A 7. 24 7. 42 7. 426 at
1950 1957	den [5]. McCrone [2] National Bureau of Standards.	9. 098 9. 122	5. 730 5. 715	23 to 29° C. 7. 394 7. 430 at 25° C.

The density of potassium permanganate calculated from the NBS lattice constants is 2.709 at 25° C.

hkl	19 Hana Rinn Fre Mo, 0.	1938 Hanawalt, Rinn, and Frevel Io, 0.7107 A		1950 McCrone		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	Ι	d	Ι	d	Ι	
$ \begin{array}{r} 101 \\ 200 \\ 011 \\ 201 \\ 002 \end{array} $	$ \begin{array}{c} A \\ 5.7 \\ 4.56 \\ 3.90 \\ 3.72 \end{array} $	8 50 8 30	$\begin{matrix} A \\ 5.\ 72 \\ 4.\ 54 \\ 3.\ 85 \\ 3.\ 70 \end{matrix}$	21 50 21 35	$\begin{matrix} A \\ 5.79 \\ \{4.57 \\ 4.53 \\ 3.89 \\ 3.718 \end{matrix}$	$ 13 \\ 11 \\ 47 \\ 22 \\ 44 $	
$\begin{array}{c} 210 \\ 102 \\ 211 \\ 112 \\ 202 \end{array}$	$\begin{array}{c} 3.58\\ 3.44\\ 3.23\\ 2.96\\ 2.87 \end{array}$		$\begin{array}{c} 3. \ 54 \\ 3. \ 42 \\ 3. \ 21 \\ 2. \ 94 \\ 2. \ 87 \end{array}$	$90 \\ 35 \\ 100 \\ 82 \\ 54$	$\begin{array}{c} 3.\ 567\\ 3.\ 437\\ 3.\ 217\\ 2.\ 948\\ 2.\ 879 \end{array}$	$93 \\ 21 \\ 100 \\ 73 \\ 34$	
$ \begin{array}{c} 020 \\ 212 \\ \overline{302} \\ 221 \end{array} $	2.57	30 	2.562.432.342.28	37 vw vw 9	2.8612.574 $2.3532.305$	$ \begin{array}{r} 36 \\ 28 \\ 1 \\ 1 \\ 1 \end{array} $	
$113 \\ 203 \\ 213 \\ 303 \\ 004 \\ 412$	$ \left. \begin{array}{c} 2. \ 19 \\ 2. \ 03 \\ 1. \ 93 \\ 1. \ 84 \end{array} \right\} $	$\begin{array}{c} 60\\ 2\\ 4\\ 20\end{array}$	2. 18 1. 98 1. 91 1. 84	65 vw 12 22	$\begin{cases} 2. \ 202 \\ 2. \ 177 \\ 2. \ 034 \\ 1. \ 920 \\ \{1. \ 857 \\ 1. \ 839 \end{cases}$	$31\\44\\1\\10\\14\\14$	
$123 \\ 104 \\ 230 \\ 223 \\ 511$	1.74 	 10 	$ 1. \overline{81} \\ 1. 75 \\ 1. 73 \\ 1. 71 $		$\begin{array}{c} 1.\ 835\\ 1.\ 820\\ 1.\ 755\\ 1.\ 731\\ 1.\ 693 \end{array}$	$12 \\ 20 \\ 7 \\ 21 \\ 1$	
403 323 124	$ \begin{array}{r} 1.68\\ 1.60\\ 1.54 \end{array} $	$\frac{8}{\overline{6}}$	$\begin{array}{c} 1.\ 66\\ 1.\ 63\\ 1.\ 59\\ 1.\ 53\end{array}$	15 vw 12 vw	$ \begin{array}{r} 1. \ 676 \\ 1. \ 595 \\ 1. \ 535 \end{array} $	9 $-\overline{7}$ 2	

ASTM cards

Card numbers	Index lines	Radiation	Source
1-0616	3. 412. 411. 97		Davey [1] 1923.
1–0609	$\begin{array}{c} 3. \ 43 \\ 2. \ 42 \\ 1. \ 53 \end{array}$	Molyb- denum	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns. None.

NBS sample. The sample of rubidium bromide was obtained from the City Chemical Co., New York, N. Y. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of potassium; 0.01 to 0.1 percent of calcium; 0.001 to 0.1 percent each of silver, aluminum, and silicon; and 0.0001 to 0.001 percent each of barium, chromium, iron, magnesium, and sodium.

The sample is colorless and the index of refraction is 1.553.

Interplanar spacings and intensity measurements. The *d*-values reported by Davey and by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Davey Hanawalt, Rinn, and Frevel National Bureau of Standards	$200 \\ 200 \\ 200 \\ 200$	$220 \\ 220 \\ 220 \\ 220$	$222 \\ 420 \\ 222$

Structural data. Davey [3] in 1921 determined that rubidium bromide has sodium chloride-type structure, the space group O_h^5 -Fm3m, and 4(RbBr) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value. The value reported by Davey has been doubled.

Lattice constants

1921	Davey [3]	A 6, 944
1922	Posnjak and Wyckoff [4]	6.94
1923	Davey [1]	6.840
1924	Havighurst, Mack, and	6.882
	and Blake [5].	
1926	Ott [6]	6.868
1948	Mehmel [7]	6.86
1957	National Bureau of Stand-	6. 889 at 25° C
	ards.	

The density of rubidium bromide calculated from the NBS lattice constant is 3.359 at 25°C.

Rubidium Bromide, RbBr (cubic)

hkl	1923 Davey Mo, 0.7107 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι	a	' d	Ι	a	d	Ι	a
$\begin{array}{c} 200\\ 220\\ 222\\ 400\\ 420\\ \end{array}\\ \begin{array}{c} 422\\ 440\\ 600\\ 620\\ 622\\ \end{array}$	$\begin{array}{c} A\\ 3, 42\\ 2, 41\\ 1, 974\\ 1, 706\\ 1, 530\\ 1, 399\\ 1, 213\\ 1, 142\\ 1, 085\\ 1, 032\\ \end{array}$	$ \begin{array}{r} 100 \\ 67 \\ 20 \\ 7 \\ 20 \\ 13 \\ 3 \\ 7 \\ 3 \\ 3 \\ 3 \\ 3 \\ 3 \\ 3 \\ 3 \\ 3 \end{array} $	$\begin{array}{c} A\\ 6,84\\ 6,82\\ 6,838\\ 6,824\\ 6,887\\ 6,887\\ 6,854\\ 6,862\\ 6,852\\ 6,862\\ 6,862\\ 6,846\\ \end{array}$	$\begin{array}{c} A \\ 3, 44 \\ 2, 42 \\ 1, 97 \\ 1, 71 \\ 1, 53 \\ 1, 40 \\ \hline 1, 14 \\ \\ \end{array}$	$ \begin{array}{r} 100 \\ 57 \\ 17 \\ 11 \\ 34 \\ 23 \\ \hline 11 \\$	$\begin{array}{c} A \\ 6.88 \\ 6.84 \\ 6.82 \\ 6.84 \\ 6.84 \\ 6.84 \\ \hline 6.86 \\ \hline 6.84 \\ \hline \\ \end{array}$	$\begin{array}{c} A\\ 3, 44\\ 2, 436\\ 1, 989\\ 1, 722\\ 1, 541\\ 1, 406\\ 1, 218\\ 1, 148\\ 1, 0892\\ 1, 0384\\ \end{array}$	$ \begin{array}{r} 100 \\ 73 \\ 25 \\ 11 \\ 23 \\ 15 \\ 4 \\ 7 \\ 5 \\ 4 \end{array} $	$\begin{array}{c} A\\ 6,88\\ 6,891\\ 6,890\\ 6,887\\ 6,892\\ 6,892\\ 6,888\\ 6,889\\ 6,889\\ 6,889\\ 6,888\\ 6,889\\ 6,888\\ \end{array}$
$ \begin{array}{r} 444 \\ 640 \\ 642 \\ 800 \\ 820 \\ 822 \\ 662 \\ \end{array} $			 	 			$\begin{array}{c} 0. \ 9946 \\ . \ 9554 \\ . \ 9207 \\ . \ 8611 \\ . \ 8353 \\ . \ 8111 \\ . \ 7902 \end{array}$	$2 \\ 3 \\ 4 \\ 1 \\ 2 \\ \leqslant 1 \\ 1$	6, 891 6, 889 6, 890 6, 889 6, 888 6, 888 6, 888
Average	of last five l	ines	6. 855			6. 84			6. 889

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Silver Chlorate, AgClO₃ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
2-0764	2.89 1.71 1.27	Chromium	Harang [1] 1928.

Additional published patterns. None.

NBS sample. The sample of silver chlorate was obtained from the City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of silicon and titanium; and 0.0001 to 0.001 percent each of aluminum, chromium, iron, and magnesium.

The sample is colorless, and it is optically positive. The indices of refraction were not determined because the sample reacts with the liquid grain immersion oils.

Interplanar spacings and intensity measurements. The *d*-values of the Harang pattern were calculated from Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Harang National Bureau of Standards	$\begin{array}{c} 202 \\ 202 \end{array}$	$\begin{array}{c} 422\\ 220 \end{array}$	$\begin{array}{c} 622\\ 200 \end{array}$

Structural data. Náray-Szabó and Pócza [2] in 1942 determined that silver chlorate has the space group C_{4h}^5 -I4/m with 8(AgClO₃) per unit cell. Silver chlorate is used as a structure-type.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

hkl	1927 Harar <i>hkl</i> Cr, 2.29		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	Ι	d	Ι
$ \begin{array}{r} 101 \\ 200 \\ 002 \\ 211 \\ 220 \end{array} $	$\begin{array}{c} A \\ \hline 4.\ 27 \\ 3.\ 95 \\ 3.\ 44 \\ 3.\ 01 \end{array}$	m w m s	$\begin{array}{c} A \\ 5.81 \\ 4.25 \\ 3.973 \\ 3.429 \\ 3.006 \end{array}$	$ \begin{array}{r} 6 \\ 38 \\ 15 \\ 31 \\ 46 \end{array} $
$202 \\ 310 \\ 301 \\ 103 \\ 222$	$\begin{array}{c} 2.90 \\ 2.70 \\ 2.65 \\ \hline 2.39 \end{array}$	vs vw vw	$\begin{array}{c} 2.900\\ 2.688\\ 2.668\\ 2.527\\ 2.395 \end{array}$	$\begin{array}{c}100\\5\\4\\4\\22\end{array}$

hkl	1927 Harang Cr, 2.2909 A		1957 National Bu of Standar Cu, 1.5405 A,	reau ds 25° C
	d	Ι	d	Ι
	A		A	
$321 \\ 213 \\ 400 \\ 004 \\ 420$	$\begin{array}{c} 2. \ 25 \\ 2. \ 17 \\ 2. \ 12 \\ \hline 1. \ 90 \end{array}$	w m s 	$\begin{array}{c} 2.\ 260\\ 2.\ 171\\ 2.\ 124\\ 1.\ 9844\\ 1.\ 9012 \end{array}$	$\begin{array}{c} 6 \\ 15 \\ 25 \\ 4 \\ 20 \end{array}$
402	1. 87	m	1. 8739	10
$204 \\ 323 \\ 422 \\ 510$	1. 76 1. 71	w vs	$\begin{array}{c} 1.\ 7984\\ 1.\ 7593\\ 1.\ 7146\\ 1.\ 6665 \end{array}$	$3 \\ 7 \\ 22 \\ 2$
$501 \\ 224 \\ 413 \\ 314 \\ 105$	1. 66	m 	$\begin{array}{c} 1.\ 6620\\ 1.\ 6556\\ 1.\ 6263\\ 1.\ 5973\\ 1.\ 5603 \end{array}$	$5 \\ 9 \\ 2 \\ 1 \\ 3$
$521 \\ 440 \\ 215 \\ 404 \\ 503$	$ \begin{array}{r} 1.50\\ 1.45\\ 1.43\\ \end{array} $	w w w	$\begin{array}{c} 1. \ 5485 \\ 1. \ 5027 \\ 1. \ 4646 \\ 1. \ 4505 \\ 1. \ 4302 \end{array}$	2 3 3 3 3
$600 \\ 442 \\ 305 \\ 611 \\ 424$	1. 40	W 	$\begin{array}{c} 1.\ 4165\\ 1.\ 4054\\ 1.\ 3844\\ 1.\ 3759\\ 1.\ 3727 \end{array}$	$\begin{array}{c}1\\4\\1\\2\\1\end{array}$
$532 \\ 620 \\ 602 \\ 325 \\ 622$	1. 34 1. 33 1. 27	s s vs	$\begin{array}{c} 1.\ 3686\\ 1.\ 3438\\ 1.\ 3338\\ 1.\ 3170\\ 1.\ 2728 \end{array}$	$\begin{array}{c}1\\3\\4\\2\\4\end{array}$
$206 \\ 415 \\ 613 \\ 444 \\ 316 \\ 543$	}		$\begin{array}{c} 1.\ 2635\\ 1.\ 2576\\ 1.\ 2353\\ 1.\ 1983\\ 1.\ 1870 \end{array}$	$\begin{array}{c}1\\1\\2\\2\\2\\2\end{array}$
$640 \\ 505 \\ 604 \\ 633 \\ 642$			$\begin{array}{c} 1. \ 1787 \\ 1. \ 1599 \\ 1. \ 1528 \\ 1. \ 1423 \\ 1. \ 1298 \end{array}$	$2 \\ 1 \\ < 1 \\ 2 \\ 2$
$525 \\ 624 \\ 336 \\ 703$	}		$\begin{array}{c} 1. \ 1194 \\ 1. \ 1125 \\ 1. \ 1038 \end{array}$	$1 \\ 1 < 1$

Lattice constants

1927 1928	Ferrari and Fontana [3] Zachariasen [4] Mineu: Sachi and Pácco	a A 8. 50 8. 492 8. 50 ²	c A 7. 93 7.92 7.91
1097	Forrari and Fontana [2]	8 50	7 02
1947	reman and romana [5]	0, 00	1. 95
1928	Zachariasen [4]	8.492	7.92
1942	Náray-Szabó and Pócza	8.503	7.91
	[2].		
1957	National Bureau of	8.498	7.938 at
	Standards.		$25^{\circ} C$

The density of silver chlorate calculated from the NBS lattice constants is 4.433 at 25° C.

References

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Silver Molybdate, Ag₂MoO₄ (cubic)

ASTM cards

Card number	s Index lines	Radiation	Source
1-1002	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Molybde- num.	Hanawalt, Rinn, and Frevel [1]
3-1317	7 1. 64 (^a)	(a)	1938. Wyckoff [2] 1922.

^a No powder data.

Additional published patterns. None.

NBS sample. The sample of silver molybdate was precipitated from solutions of silver sulfate and sodium molybdate. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of aluminum, cobalt, magnesium, and silicon.

The sample has a pale-yellow color. The indices of refraction could not be determined because the particle size is too small.

Interplanar spacings and intensity measurements. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel National Bureau of Standards	$\begin{array}{c} 311\\ 311\end{array}$	$\begin{array}{c} 511\\ 440\end{array}$	$\begin{array}{c} 440\\511\end{array}$

Structural data. Wyckoff [2] in 1922 determined that silver molybdate has magnesium aluminate-type structure, the space group O_h^{7-} Fd3m, and 8(Ag₂MoO₄) per unit cell.

The unit-cell measurements reported by Wyckoff have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

1922Wyckoff [2]1957National Bureau of Stand- ards.	A 9.28 9.3127 at 25° C
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The density of silver molybdate calculated from the NBS lattice constant is 6.178 at 25° C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι	a	d	Ι	a
$111 \\ 220 \\ 311 \\ 222 \\ 400$	$\begin{array}{c} A \\ 5. \ 3 \\ 3. \ 29 \\ 2. \ 81 \\ 2. \ 69 \\ 2. \ 32 \end{array}$	$6 \\ 17 \\ 100 \\ 17 \\ 14$	$\begin{array}{c} A\\ 9.\ 18\\ 9.\ 31\\ 9.\ 32\\ 9.\ 28\\ 9.\ 28\end{array}$	$\begin{matrix} A \\ 5. 38 \\ 3. 292 \\ 2. 808 \\ 2. 689 \\ 2. 329 \end{matrix}$	$7 \\ 28 \\ 100 \\ 26 \\ 17$	$\begin{array}{c} A\\ 9.\ 31\\ 9.\ 31\\ 9.\ 31\\ 9.\ 32\\ 9.\ 32\\ 9.\ 32 \end{array}$
$331 \\ 422 \\ 511 \\ 440 \\ 531$	2. 12 1. 89 1. 78 1. 64	5 6 42 43 	9. 24 9. 26 9. 25 9. 28	$\begin{array}{c} 2. \ 138 \\ 1. \ 900 \\ 1. \ 792 \\ 1. \ 6461 \\ 1. \ 5754 \end{array}$	$5 \\ 9 \\ 30 \\ 32 \\ 2$	$\begin{array}{c} 9. \ 32 \\ 9. \ 31 \\ 9. \ 312 \\ 9. \ 313 \\ 9. \ 320 \end{array}$
$\begin{array}{c} 620 \\ 533 \\ 622 \\ 444 \\ 642 \end{array}$	$\begin{array}{c} 1.\ 478\\ 1.\ 425\\ 1.\ 409\\ 1.\ 358\\ 1.\ 248 \end{array}$	$\begin{array}{c}1\\11\\11\\11\\5\end{array}$	$\begin{array}{c} 9. \ 35 \\ 9. \ 34 \\ 9. \ 35 \\ 9. \ 41 \\ 9. \ 34 \end{array}$	$\begin{array}{c} 1.\ 4725\\ 1.\ 4201\\ 1.\ 4037\\ 1.\ 3444\\ 1.\ 2444 \end{array}$	$ \begin{array}{c} 3 \\ 8 \\ 8 \\ 3 \\ 4 \end{array} $	$\begin{array}{c} 9. \ 313 \\ 9. \ 312 \\ 9. \ 311 \\ 9. \ 313 \\ 9. \ 312 \\ 9. \ 312 \end{array}$
$731 \\ 800 \\ 822 \\ 751 \\ 662$	1. 213 1. 166 1. 099 1. 077	$ \begin{array}{c} 17 \\ 3 \\ 1 \\ 9 \\ \end{array} $	9. 32 9. 33 9. 33 9. 33 9. 33	$\begin{array}{c} 1.\ 2125\\ 1.\ 1638\\ 1.\ 0975\\ 1.\ 0753\\ 1.\ 0683 \end{array}$	$\begin{array}{c}14\\3\\6\\2\end{array}$	$\begin{array}{c} 9. \ 313 \\ 9. \ 310 \\ 9. \ 313 \\ 9. \ 312 \\ 9. \ 313 \end{array}$
$\begin{array}{c} 840 \\ 664 \\ 931 \\ 844 \\ 10 \cdot 2 \cdot 0 \end{array}$	$1. 045 \\ 0. 980 \\ . 953 \\ . 917$	$\begin{array}{c}1\\\\2\\5\\1\end{array}$	9. 35 9. 35 9. 34 9. 35	$\begin{array}{c} 1.\ 0412\\ 0.\ 9928\\ .\ 9761\\ .\ 9503\\ .\ 9134 \end{array}$	$ \begin{array}{c} 1 \\ 1 \\ 3 \\ 5 \\ 2 \end{array} $	$\begin{array}{c} 9.\ 313\\ 9.\ 314\\ 9.\ 312\\ 9.\ 311\\ 9.\ 311\\ 9.\ 3147\end{array}$
$951 \\ 10.2.2 \\ 10.4.2 \\ 11.1.1 \\ 880$. 9003 . 8961 . 8501 . 8397 . 8231	5 3 2 2 2	$\begin{array}{c} 9.\ 3128\\ 9.\ 3127\\ 9.\ 3125\\ 9.\ 3129\\ 9.\ 3127\end{array}$
$\begin{array}{c} 10{\cdot}6{\cdot}0\\ 11{\cdot}3{\cdot}3\\ 10{\cdot}6{\cdot}2 \end{array}$. 7985 . 7899 . 7871	$\begin{array}{c} 2\\ 4\\ 4\end{array}$	$\begin{array}{c} 9.\ 3121 \\ 9.\ 3129 \\ 9.\ 3130 \end{array}$
Averag lines	ge of last	five	9. 34			9. 3127

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
 R. W. G. Wyckoff, The crystal structure of silver
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ASTM cards

Card number	Index lines	Radiation	Source
1-0961	$\begin{array}{c} 2.86\\ 3.17\\ 2.64 \end{array}$	Molybde- num.	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns. None.

NBS sample. The sample of silver sulfate was obtained from J. T. Baker Chemical Co. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, iron, magnesium, and silicon; and 0.0001 to 0.001 percent each of calcium and lead.

The sample is colorless and optically negative. The indices of refraction are $N\alpha = 1.756$, $N\beta = 1.775$, and $N\gamma = 1.782$. The value of 2V could not be determined.

Interplanar spacings and intensity measure-ments. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel.	$\frac{113}{113}$	040	220
National Bureau of Standards		220	040

Structural data. Herrmann and Ilge [1] in 1931 determined that silver sulfate has sodium sulfatetype structure, the space group D_{2h}^{24} -Fddd, and $8(Ag_2SO_4)$ per unit cell.

The unit-cell measurements reported by Herrmann and Ilge have been converted from kX to angstrom units for comparison with the NBS values.

Lattice	constants
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		<i>a</i>	<i>b</i>	с
1931 Herrm [1]. 1957 Nation	aann and Ilge 5. nal Bureau of 5.	$egin{array}{c} A \\ 859 \\ 8167 \end{array}$	$A \\ 12.684 \\ 12.704$	A 10. 271 10. 269 at

The density of the silver sulfate calculated from the NBS lattice constants is 5.457 at 25° C.

hkl	193 Hanawalt and Fr Mo, 0.7	8 5, Rinn, revel 107 A	195 National of Stan Cu, 1.5 25°	7 Bureau dards 405A, C
	d	Ι	d	Ι
$ \begin{array}{c} 111\\022\\040\\113\\220\\\end{array} $	$\begin{matrix} A \\ 4.\ 71 \\ 3.\ 98 \\ 3.\ 17 \\ 2.\ 86 \\ 2.\ 64 \end{matrix}$	7 27 53 100 53	$\begin{matrix} A \\ 4.\ 71 \\ 3.\ 994 \\ 3.\ 173 \\ 2.\ 873 \\ 2.\ 644 \end{matrix}$	$ \begin{array}{r} 12 \\ 27 \\ 73 \\ 100 \\ 86 \end{array} $
$202 \\ 133 \\ 222 \\ 151 \\ 242$	$\begin{array}{c} 2.52\\ 2.41\\ 2.35\\ 2.27\\ 1.97\end{array}$	$11 \\ 33 \\ 1 \\ 8 \\ 11$	$\begin{array}{c} 2.529\\ 2.420\\ 2.350\\ 2.271\\ 1.979 \end{array}$	$20 \\ 34 \\ 4 \\ 9 \\ 11$
$\begin{array}{c} 062 \\ 153 \\ 311 \\ 135 \\ 331 \end{array}$	1. 91 1. 75	-40 	$\begin{array}{c} 1. \ 957 \\ 1. \ 925 \\ 1. \ 883 \\ 1. \ 761 \\ 1. \ 7375 \end{array}$	
$ \begin{array}{r} 260 \\ 313 \\ 026 \\ \hline 333 \end{array} $	$\begin{array}{c} 1.\ 70\\ 1.\ 66\\ 1.\ 64\\ 1.\ 58\\ 1.\ 56\end{array}$	$13 \\ 9 \\ 7 \\ 1 \\ 9$	$ \begin{array}{c} 1.\ 7113\\ 1.\ 6726\\ 1.\ 6513\\ \hline 1.\ 5666\\ \end{array} $	$ \begin{array}{r} 19 \\ 11 \\ 6 \\ \\ 11 \end{array} $
$173 \\ 206 \\ 400 \\ 353 \\ 422$	$\begin{array}{c} 1.\ 53\\ 1.\ 465\\ 1.\ 447\\ 1.\ 400\\ 1.\ 361 \end{array}$	9 5 1 7 1	$\begin{array}{c} 1. \ 5459 \\ 1. \ 4746 \\ 1. \ 4545 \\ 1. \ 4059 \\ 1. \ 3665 \end{array}$	$\begin{vmatrix} 10 \\ 4 \\ 4 \\ 7 \\ 4 \end{vmatrix}$
$335 \\ 246 \\ 066 \\ 440 \\ 193$	} 1. 330 1. 270	11 4	$\begin{array}{c} 1.\ 3372\\ 1.\ 3310\\ 1.\ 3224\\ 1.\ 2736 \end{array}$	$\begin{array}{c} 6\\ 1\\ 7\\ 6\end{array}$
$373 \\ 048 \\ 444 \\ 317 \\ 228$	1. 230 1. 187 1. 161	5 1 4 	$\begin{array}{c} 1.\ 2362\\ 1.\ 1883\\ 1.\ 1775\\ 1.\ 1651\\ 1.\ 1557\end{array}$	
$513 \\ 426 \\ 139 \\ 393$	1. 112 1. 091 }	3 4 	$ \begin{array}{r} 1.0979 \\ 1.0925 \\ 1.0825 \end{array} $	$\frac{2}{2}$
$286 \\ 480 \\ 533 \\ 553 \\ 484$	1.075		$\begin{array}{c} 1.\ 0807\\ 1.\ 0724\\ 1.\ 0661\\ 1.\ 0101\\ 0.\ 9895 \end{array}$	3 4 4 3 2
$\begin{array}{r} 466 \\ 620 \\ 3{\cdot}11{\cdot}3 \\ 179 \\ 622 \end{array}$	}		. 9817 . 9583 . 9531 . 9416	3 2 2 3

- K. Herrmann and W. Ilge, The structure of silver sulfate, Z. Krist. 80, 402-415 (1931).
 J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemi-cal analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).

Sodium Iodate, NaIO₃ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0916	$\begin{array}{c} 2. \ 93 \\ 4. \ 25 \\ 3. \ 19 \end{array}$	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [2] 1928	Copper	K_{lpha}

NBS sample. The sample of sodium iodate was obtained from the City Chemical Corp., New York, N.Y. The sample was recrystallized and dried at 130° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium and silicon; 0.001 to 0.01 percent each of aluminum, iron, potassium, and magnesium; and 0.0001 to 0.001 percent each of barium, chromium, copper, lithium, manganese, lead, tin, and strontium.

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

Interplanar spacings and intensity measurements. The d-values reported by Hanawalt, Rinn, and Frevel, and by Zachariasen were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel. Zachariasen National Bureau of Standards.	$021, 112 \\ 021, 112 \\ 021$	110 312,204 110	020 132 020

Structural data. MacGillavry and Panthaleon [3] in 1943 determined that sodium iodate has the space group D_{2h}^{16} -Pbnm and 4(NaIO₃) per unit cell.

The "c" measurement reported by Zachariasen has been doubled, and all of the unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

hkl	1938 Hanawalt, Zac Rinn, and Frevel Mo, 0.7107 A Cu,		192 Zachar Cu, 1.54	8 iasen 418 A	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι	d	Ι	d	Ι	
$110 \\ 002 \\ 111 \\ 020 \\ 021 \\ 112$	$ \begin{array}{c} A \\ 4. 27 \\ 4. 06 \\ 3. 21 \\ 2. 95 \end{array} $	$50 \\ 20 \\ \bar{3}0 \\ 100$	$ \begin{array}{r} A \\ 4. 28 \\ 4. 05 \\ \overline{3.23} \\ 2. 98 \\ \end{array} $	$50 \\ 20 \\ \bar{2}0 \\ 100$	$\begin{array}{c} A\\ 4.\ 28\\ 4.\ 07\\ 3.\ 784\\ 3.\ 202\\ \{2.\ 978\\ 2.\ 947\\ \end{array}$	$ \begin{array}{r} $	
$200 \\ 210 \\ 022 \\ 103 \\ 202$	$2.88 \\ 2.52 \\ 2.33 $	9 $\overline{2}5$ $\overline{9}$	$ \begin{array}{r} 2.89 \\ 2.52 \\ 2.36 \end{array} $	$20 \\ \bar{4}0 \\ \bar{4}0$	$\begin{array}{c} 2.\ 875\\ 2.\ 623\\ 2.\ 516\\ 2.\ 4525\\ 2.\ 3486 \end{array}$	$1 \\ 3 \\ 20 \\ 2 \\ 11$	
$122 \\ 220 \\ 004 \\ 130 \\ 131$	2. 12 2. 02 1. 98		2. 13 2. 03 1. 993	$50 \\ 30 \\ 10 \\ -$	$\begin{array}{c} 2. \ 3041 \\ 2. \ 1391 \\ 2. \ 0342 \\ 1. \ 9993 \\ 1. \ 9414 \end{array}$	$ < 1 \\ 22 \\ 9 \\ 6 \\ 3 \\ 3$	
$222 \\ 301 \\ 114 \\ 132 \\ 024$	$ \begin{array}{r} 1.88\\ 1.82\\ 1.78\\ 1.78\\ 1.70 \end{array} $	$10 \\ \bar{13} \\ 25 \\ 10$	$ \begin{array}{c} 1.893\\ 1.839\\ 1.794\\ 1.714 \end{array} $	$ \begin{array}{r} 20 \\ \bar{30} \\ 60 \\ 20 \end{array} $	$\begin{array}{c} 1.\ 8926\\ 1.\ 8664\\ 1.\ 8360\\ 1.\ 7948\\ 1.\ 7163 \end{array}$	$egin{array}{c} 14 \\ 1 \\ 17 \\ 26 \\ 12 \end{array}$	
$312 \\ 204 \\ 040 \\ 042 \\ 224$	$ \begin{cases} 1. \ 66 \\ 1. \ 60 \\ 1. \ \overline{470} \end{cases} $	$30\\1\\\bar{1}0$	$ \begin{array}{r} 1. \ 669 \\ 1. \ 602 \\ 1. \ \overline{476} \end{array} $	$70 \\ 5 \\ \bar{3}0$	$\begin{cases} 1.\ 6732 \\ 1.\ 6606 \\ 1.\ 5999 \\ 1.\ 4886 \\ 1.\ 4731 \end{cases}$	$\begin{array}{c} 21\\7\\4\\3\\9\end{array}$	
$\begin{array}{c} 400 \\ 330 \\ 331 \\ 240 \\ 043 \end{array}$	$ \Big\} 1. \ 431 \\ \overline{1. \ 393} \\ $	8 -4 -	1. 428 1. 400	30 10 -	$\begin{cases} 1.\ 4373\\ 1.\ 4257\\ 1.\ 4037\\ 1.\ 3977\\ 1.\ 3787 \end{cases}$	2 8 3 5 3	
$314 \\ 006 \\ 332 \\ 242 \\ 420$	$ \begin{array}{c}\\ \overline{1.351}\\ \overline{1.314} \end{array} $	- - 8 -4	$ \begin{array}{r} 1. 361 \\ 1. 346 \\ 1. 323 \\ 1. 315 \end{array} $	$30\\ \bar{3}0\\ 20\\ 10$	$\begin{array}{c} 1.\ 3627\\ 1.\ 3558\\ 1.\ 3454\\ 1.\ 3222\\ 1.\ 3114 \end{array}$	$ \begin{array}{c} 4 \\ 4 \\ 6 \\ 3 \\ 7 \end{array} $	
$116 \\ 044 \\ 026 \\ 152 \\ 404$	$ \begin{array}{c} 1. 287 \\ 1. 251 \\ \overline{1. 191} \\ 1. 171 \end{array} $		$1. 291 \\ 1. 249 \\$	30 30 - -	$\begin{array}{c} 1.\ 2923\\ 1.\ 2576\\ 1.\ 2481\\ 1.\ 1937\\ 1.\ 1739 \end{array}$	$5 \\ 3 \\ 10 \\ 3 \\ 2$	
$334 \\ 244 \\ 226 \\ 510 \\ 117$	$ \begin{array}{c c} \overline{1.149} \\ \overline{1.122} \\ \overline{1.122} \end{array} $	- - - 2			$\begin{array}{c} 1.\ 1675\\ 1.\ 1519\\ 1.\ 1449\\ 1.\ 1318\\ 1.\ 1218 \end{array}$	$\overset{2}{\underset{4}{\overset{2}{\overset{2}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{1$	
$\begin{array}{r} 424 \\ 316 \\ 512 \\ 440 \\ 060 \end{array}$	1. 103 }1. 091	1 2 -			1. 1018 1. 0903 1. 0692 1. 0666	$\begin{array}{c} 4\\7\\-4\\<1\end{array}$	

hkl	193 Hana Rinn, Frey Mo, 0.7	8 walt, and vel 107 A	192 Zachar Cu, 1.5	8 iasen 418 A	195 National of Stan Cu, 1.54 25°	7 Bureau dards 405 A, C
	d	Ι	d	Ι	d	Ι
$154 \\ 350 \\ 442 \\ 352 \\ 530 \\ 260 \\ 261 \\ 063 \\ 118 \\ 514$	A } } 		A 		A 1. 0645 1. 0339 1. 0295 1. 0121 1. 0001 0. 9922 . 9890	<1 3 4 3 <1 <1 <1 1
$336 \\ 532 \\ 246 \\ 262 \\ 208 \\ 600 \\ 444 \\ 354$	} } 				. 9824 . 9727 . 9710 . 9587 . 9464 . 9432	$4 \\ 2 \\ 2 \\ 2 \\ 1 \\ 2$

Sodium Iodate, NaIO₃ (orthorhombic)--Con.

Lattice constants

		a	<i>b</i>	с
$\begin{array}{c} 1928\\ 1943 \end{array}$	Zachariasen [2] MacGillavry and	$egin{array}{c} A \\ 5.\ 76 \\ 5.\ 75 \end{array}$	$\begin{array}{c} A \\ 6.\ 38 \\ 6.\ 38 \end{array}$	A 8. 12 8. 13
1947	Naráy-Szabó and Neugebauer [4].	5. 76	6. 38	8. 12
1957	National Bureau of Standards.	5. 749	6. 399	8. 134 at 25° C

The density of sodium iodate calculated from the NBS lattice constants is 4.392 at 25° C.

References

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- Anal. Ed. 10, 457-512 (1936).
 W. H. Zachariasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO₃, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. 1928, No. 4, (1928).
 C. H. MacGillavry and C. L. Van Eck Panthaleon, The crystal structure of sodium and ammonium isodate Result des Travay Chim des Pays-Bas 62
- [3] C. H. MacGillavry and C. L. Van Eck Panthaleon, The crystal structure of sodium and ammonium iodate, Recucil des Travaux Chim. des Pays-Bas, 62, 729-735 (1943).
 [4] I. Naráy-Szabó and J. Neugebauer, The crystal
- [4] I. Naráy-Szabó and J. Neugebauer, The crystal structure of sodium iodate, J. Am. Chem. Soc. 69, 1280-1283 (1947).

Sodium Metaperiodate, NaIO₄ (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of sodium metaperiodate was obtained from the J. T. Baker Chemical Co., Phillipsburg, N. J. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of aluminum, calcium, iron, potassium, magnesium, and silicon.

The sample is colorless and optically positive. The indices of refraction are $N_0=1.705$ and $N_e=1.743$.

Interplanar spacings and intensity measurements. The three strongest lines for the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards	112	101	204

Structural data. Kirkpatrick and Dickinson [1] in 1926 determined that sodium metaperiodate has calcium tungstate-type structure, the space group $C_{4h}^6-I4_1/a$, and $4(NaIO_4)$ per unit cell.

The unit cell measurements reported by Kirkpatrick and Dickinson and by Hazlewood have been converted from kX to angstrom units for comparison with the NBS values.

	Lattice	constants
--	---------	-----------

		a	с
1926	Kirkpatrick and Dickin-	A 5. 333	$egin{array}{c} A \ 11.95 \end{array}$
1938 1957	Hazlewood [2] National Bureau of Standards.	5. 3330 5. 3372	11. 95 11. 952 at 25° C

The density of sodium metaperiodate calculated from the NBS lattice constants is 4.172 at 25° C.

- L. M. Kirkpatrick and R. G. Dickinson, The crystal structure of sodium periodate, J. Am. Chem. Soc. 48, 2327-2334 (1926).
- [2] E. A. Hazlewood, The O parameters in NaIO₄, a determination of the oxygen parameters for NaIO₄, Z. Krist. [A] 98, 439-446 (1938).

hkl	1957 National H of Stand Cu, 1.540 25° C	Bureau ards 05 A,	hkl	1957 National H of Stand Cu, 1.540 25° (Bureau ards 05 A, C	kkl	1957 National E of Stand Cu, 1.540 25° (Bureau ards 2 A, 2
	d	1		d	1		d	1
$\begin{array}{c} 101\\ 112\\ 004\\ 200\\ 202\\ \end{array}\\ 114\\ 105\\ 213\\ 204\\ 220\\ 116\\ 215\\ 303\\ 312\\ 206\\ 224\\ 008\\ 314\\ 321\\ 305\\ 118\\ 217\\ 400\\ 208\\ 109\\ 325\\ 307\\ 413\\ \end{array}$	$\left.\begin{array}{c} A\\ 4, 87\\ 3, 191\\ 2, 988\\ 2, 669\\ 2, 437\\ 2, 343\\ 2, 182\\ 2, 048\\ 1, 991\\ 1, 887\\ 1, 761\\ 1, 689\\ 1, 624\\ 1, 595\\ 1, 494\\ 1, 469\\ 1, 426\\ 1, 3882\\ 1, 3341\\ 1, 3033\\ 1, 2884\\ 1, 2584\\ 1, 2312\\ \end{array}\right.$	$\begin{array}{c} 89\\ 100\\ 12\\ 17\\ 2\\ 21\\ 4\\ 9\\ 38\\ 12\\ 19\\ 10\\ 26\\ 13\\ 2\\ 5\\ 5\\ 8\\ 6\\ 15\\ 12\\ 3\\ 7\\ \end{array}$	$\begin{array}{r} 404\\ 420\\ 228\\ 219\\ 1.1.10\\ 318\\ 327\\ 406\\ 424\\ 309\\ 336\\ 417\\ 503\\ 512\\ 0.0.12\\ 408\\ 2.1.11\\ 329\\ 3.1.10\\ 338\\ 523\\ 440\\ 2.0.12\\ 3.0.11\\ 419\\ 525\\ 1.0.13\\ 507\\ \end{array}$	$\begin{array}{c} A\\ 1, 2184\\ 1, 1936\\ 1, 1716\\ 1, 1608\\ 1, 176\\ 1, 1608\\ 1, 1184\\ 1, 1081\\ 1, 1081\\ 1, 0638\\ 1, 0319\\ 1, 0319\\ 1, 0311\\ 0, 9954\\ 2, 9886\\ 9954\\ 3, 9886\\ 9751\\ 1, 9886\\ 9435\\ 9332\\ 2, 9269\\ 9154\\ 9061\\ 9048\\ \end{array}$	$3 \\ 3 \\ 3 \\ 2 \\ 1 \\ 2 \\ 1 \\ 9 \\ 4 \\ 4 \\ 6 \\ 2 \\ 3 \\ 4 \\ 1 \\ 1 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 5 \\ 2 \\ 2 \\ 2 \\ 4 \\ 4 \\ 4 \\ 4 \\ 5 \\ 4 \\ 4 \\ 4 \\ 5 \\ 4 \\ 4$	$\begin{array}{c} A\\ 444\\ 600\\ 2\cdot2\cdot12\\ 3\cdot2\cdot11\\ 3\cdot3\cdot10\\ 2\cdot1\cdot13\\ 3\cdot1\cdot12\\ 518\\ 527\\ 446\\ 604\\ 620\\ 1\cdot1\cdot14\\ 4\cdot1\cdot11\\ 509\\ 615\\ 543\\ 606\\ 624\\ 4\cdot0\cdot12\\ 448\\ 631\\ 1\cdot0\cdot15\\ 5\cdot1\cdot10\\ \end{array}$	$\left.\begin{array}{c}.8997\\.8896\\.8809\\.8758\\.8665\\.8579\\.8577\\.8571\\.8571\\.8526\\.8326\\.8326\\.8326\\.8320\\.8237\\.8159\\.8122\\.7982\\.7978\\.7938\\.7879\\.7874\end{array}\right.$	$egin{array}{cccccccccccccccccccccccccccccccccccc$
332			532)				

Sodium Metaperiodate, NaIO₄ (tetragonal)

Sodium Perchlorate, NaClO₄ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0552	$\begin{array}{c} 3. \ 53 \\ 3. \ 97 \\ 2. \ 95 \end{array}$	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Patterns for the high temperature cubic form of sodium perchlorate are given on ASTM cards 2-0271 and 2-0375. According to Herrmann and Ilge [2] the orthorhombic form changes to the cubic form above 308° C.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [3] 1930		

NBS sample. The sample of sodium perchlorate was obtained as the hydrate from the Fisher Scientific Co., New York, N. Y. The anhydrous form was obtained by dehydrating the sample at 100° C. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, potassium, lithium, nickel, silicon, strontium, and zirconium; and 0.0001 to 0.001 percent each of silver, barium, chromium, cesium, copper, iron, magnesium, and manganese.

The sample is colorless and optically positive with the indices of refraction $N\alpha = 1.459$, $N\beta = 1.461$, $N\gamma = 1.472$, and $2V \simeq 10^{\circ}$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units, and the *d*-values of the Zachariasen pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Sodium Perchlorate, NaClO₄ (orthorhombic)

Pattern	1	2	3
Hanawalt, Rinn, and Frevel Zachariasen National Bureau of Standards	$020 \\ 020 \\ 020 \\ 020$	$111 \\ 022 \\ 111$	$\begin{array}{c}102\\111\\102\end{array}$

Structural data. Zachariasen [3] in 1930 determined that sodium perchlorate has barium sulfate-type structure, the space group D_{2h}^{17} -Amma, and 4(NaClO₄) per unit cell.

The unit-cell measurements reported by Zachariasen have been converted from kX to angstrom units for comparison with the NBS values.

Lattice	constants

		<i>a</i>	b	c
1930 1957	Zachariasen [3] National Bureau of Standards.	$A \\ 7.\ 07 \\ 7.\ 055$	A 7. 09 7. 088	$\begin{array}{c} & A \\ 6. \ 49 \\ 6. \ 519 \ \text{at} \\ 25^{\circ} \ \text{C}. \end{array}$

The density of sodium perchlorate calculated from the NBS lattice constants is 2.494 at 25° C.

References

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem-Anal. Ed. 10, 457-512 (1938).
 K. Herrmann and W. Ilge, Röntgenographische Struk-
- [2] K. Herrmann and W. Ilge, Röntgenographische Strukturerforschung der kubischen Modification der Perchlorate, Z. Krist. 75, 41–65 (1930).
- [3] W. H. Zachariasen, The crystal structure of sodium perchlorate, NaClO₄, Z. Krist. 73, 141–146 (1930).

hkl	193 Hanav Rinn, Fre Mo, 0.7	38 walt, and vel 7107 A	1930 Zachariasen Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
_	d	Ι	d	Ι	d	Ι
$011 \\ 111 \\ 020 \\ 002 \\ 102$	$\begin{array}{c} A \\ 4.\ 80 \\ 3.\ 98 \\ 3.\ 54 \\ 3.\ 26 \\ 2.\ 96 \end{array}$		$\begin{array}{c} A \\ 4.\ 80 \\ 3.\ 97 \\ 3.\ 55 \\ 3.\ 25 \\ 2.\ 95 \end{array}$	W S VS W S	$\begin{array}{c} A \\ 4.80 \\ 3.97 \\ 3.54 \\ 3.260 \\ 2.960 \end{array}$	
$211 \\ 220 \\ 022 \\ \\ 122 \\ \\ 122 \\ \\ \\ \\ \\$	$2.862.512.40\overline{2.27}$	17 4 40 $\overline{17}$	$\begin{array}{c} 2. \ 85 \\ 2. \ 51 \\ 2. \ 396 \\ 2. \ 390 \\ 2. \ 267 \end{array}$	m m vs vw m	2.8392.4982.400 2.271	$13 \\ 4 \\ 26 \\ \overline{1}\overline{1}$
$\begin{array}{c} 031 \\ 131 \\ 311 \\ 013 \\ 222 \end{array}$	$ \begin{cases} 2.12 \\ 2.07 \\ 1.98 \end{cases} $	- 5 4 7	$\begin{array}{c} 2.\ 220 \\ \{2.\ 117 \\ 2.\ 113 \\ 2.\ 069 \\ 1.\ 982 \end{array}$	mw w w w w	$\begin{array}{c} 2.\ 222\\ 2.\ 118\\ 2.\ 112\\ 2.\ 077\\ 1.\ 983 \end{array}$	5 2 3 2 3
$302 \\ 231 \\ 040 \\ 400 \\ 322$		33 13 20	$\begin{cases} 1. \ 909 \\ 1. \ 881 \\ 1. \ 774 \\ 1. \ 768 \end{cases}$	s w m m	1. 907 1. 879 1. 772 1. 763 1. 680	
$\begin{array}{c} 411 \\ 331 \\ 240 \\ 420 \\ 142 \end{array}$	$ \begin{array}{r} 1. \ 62 \\ 1. \ 58 \\ 1. \ 56 \\ 1. \ 52 \\ \end{array} $	$-1 \\ -3 \\ 11 \\ 5$			$\begin{array}{c} 1.\ 655\\ 1.\ 616\\ 1.\ 584\\ 1.\ 580\\ .\ 1.\ 521 \end{array}$	$\overset{3}{\overset{1}{\underset{4}{\overset{2}{\atop}}}}$
$\begin{array}{c} 024 \\ 233 \\ 124 \\ 242 \\ 422 \end{array}$					$\begin{array}{c} 1.\ 480\\ 1.\ 457\\ 1.\ 450\\ 1.\ 424\\ 1.\ 4211 \end{array}$	$< 1 \\ 1 \\ 2 \\ 3 \\ 2 \\ 2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 2$
$224 \\ 151 \\ 511 \\ 304$					$\begin{array}{c} 1. \ 3651 \\ 1. \ 3590 \\ 1. \ 3536 \\ 1. \ 3395. \end{array}$	$\overset{1}{\underset{<1}{\overset{<1}{}}}$

Strontium Molybdate, SrMoO₄ (tetragonal)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wavelength
Zambonini and Levi [3] 1925. Broch [2] 1929	Copper Copper	Κα Κα

NBS sample. The sample of strontium molybdate was precipitated from solutions of strontium chloride and sodium molybdate. The sample was heated to 800° C to sharpen the X-ray pattern. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of silicon; 0.01 to 0.1 percent each of barium and calcium; 0.001 to 0.01 percent each of aluminum, potassium, and magnesium; and 0.0001 to 0.001 percent each of silver, chromium, cesium, copper, iron, lithium, manganese, and tin. The sample is colorless. The indices of refraction could not be determined because the particle size is too small.

Interplanar spacings and intensity measurements. The *d*-values reported by Zambonini and Levi and by Broch have been converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Zambonini and Levi Broch National Bureau of Standards.	$ \begin{array}{r} 112 \\ 112 \\ 112 \\ 112 \end{array} $	$312, 303 \\ 204 \\ 204 \\ 204$	204 312, 303 312, 303

Structural data. Broch [2] in 1925 determined that strontium molybdate has calcium tungstate-type structure, the space group C_{4h}^6 -I4₁/a, and 4(SrMoO₄) per unit cell.

The unit-cell measurements reported by Zambonini and Levi and by Broch have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	с
$1925 \\ 1929 \\ 1957$	Zambonini and Levi [1] Broch [2]	$\begin{matrix} A \\ 5. 37 \\ 5. 39 \\ 5. 3944 \end{matrix}$	$\begin{array}{c} A \\ 11. \ 96 \\ 11. \ 99 \\ 12. \ 020 \ at \\ 25^{\circ} \ C \end{array}$

The density of strontium molybdate calculated from the NBS lattice constants is 4.700 at 25° C.

References

- F. Zambonini and G. R. Levi, Richerche sull'isomorfismo dei molibdati dei metalli delle terre rare con quello del calcio, dello stronzio, del bario e del piombo. III. De duzioni dall'analisi röntgengrafica dei molibdati di Ca, Sr, Ba, Pb, Rend. accad. Lincei 2, 303-305 (1925).
- [2] E. K. Broch, Untersuchungen über Kristallstrukturen des Wolframittypus und des Scheelittypus, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. 1929, No. 8 (1929).
- [3] F. Zambonini and G. R. Levi, Richerche sull'isomorfismo dei molibdati dei metalli delle terre rare con quello del calcio, dello stronzio, del bario e del piombo. II. Struttura dei molibdati di Ca, Sr, Ba, Pb, Rend. accad. Lincei 2, 225–230 (1925).

Strontium Molybdate, SrMoO₄ (tetragonal)

	1925 Zambonini		1930 Broch		1957 National	
hkl	and L Cu, 1.54	evi 18 A	Cu, 1.54	18 A	Standards Cu, 1.5405 A, 25° C	
	d	Ι	d	I	d	I
$101 \\ 112 \\ 004 \\ 200 \\ 202$	$ \begin{array}{c} A \\ 3. \overline{08} \\ 2. 91 \\ 2. 61 \end{array} $	vs m mw	A 3. 21 3. 01 2. 70	vvs m s	$\begin{array}{c} A \\ 4.92 \\ 3.222 \\ 3.006 \\ 2.698 \\ 2.461 \end{array}$	$3 \\ 100 \\ 16 \\ 21 \\ 1$
$114 \\ 213 \\ 204 \\ 220 \\ 116$	$ \begin{array}{c} \\ 1. 95 \\ 1. 86 \\ 1. 74 \end{array} $	- s m s	2. 37 $2. 010$ $1. 911$ $1. 774$	vvw vvs s vs	$\begin{array}{c} 2. \ 362 \\ 2. \ 067 \\ 2. \ 008 \\ 1. \ 907 \\ 1. \ 774 \end{array}$	$\begin{array}{c} 6 \\ < 1 \\ 30 \\ 12 \\ 17 \end{array}$
$312 \\ 303 \\ 224 \\ 008 $	}1. 61 1. 58 	vs ms -	$ \begin{array}{r} 1. \ 642 \\ 1. \ 611 \\ 1. \ \overline{444} \end{array} $	vvs vs vw	$1. 642 \\ 1. 611 \\ 1. 503 $	$\begin{array}{c} 25\\11\\2\\\end{array}$
$217 \\ 118 \\ 400 \\ 208 \\ 316$	$ \Big\} \begin{array}{c} \\ 1. \ 29 \\ 1. \ 28 \end{array} $	- - - 	1.3501.3121.298	- VW S S	$\begin{array}{c} 1. \ 399 \\ 1. \ 3486 \\ 1. \ 3129 \\ 1. \ 2994 \end{array}$	$\begin{array}{c}1\\4\\7\\11\end{array}$
$332 \\ 413 \\ 404 \\ 420 \\ 228$	$ \Big\} \begin{matrix} 1. \ 23 \\ 1. \ 21 \\ 1. \ 19 \\ 1. \ 17 \end{matrix} \Big)$	mw w mw mw	$\begin{array}{c} 1.\ 244\\ 1.\ 231\\ 1.\ 206\\ 1.\ 1810 \end{array}$	s s m	$\begin{array}{c} 1.\ 2441 \\ 1.\ 2308 \\ 1.\ 2064 \\ 1.\ 1807 \end{array}$	$7 \\ 6 \\ 6 \\ 3$
$1.1.10 \\ 424 \\ 406 \\ 336 \\ 512 \\ 503$	$ \begin{array}{c} 1. 14 \\ 1. 11 \\ 1. 06 \\ \end{array} $	mw m w -	1. 1464 1. 1198 1. 0737 1. 0426	m vs m vs	$\begin{array}{c} 1.\ 1467\\ 1.\ 1193\\ 1.\ 0736\\ 1.\ 0420 \end{array}$	4 7 3 6
$\begin{array}{c} 408 \\ 0{\cdot}0{\cdot}12 \\ 3{\cdot}1{\cdot}10 \\ 440 \\ 428 \end{array}$	1. 03 0. 999 . 977 	mw mw m -	$ \begin{array}{c} 1. \ 0039 \\ 0. \ \overline{9830} \\ . \ \overline{9413} \end{array} $	m - s - vs	$\begin{array}{c} 1.\ 0036\\ 1.\ 0011\\ 0.\ 9826\\ .\ 9536\\ .\ 9406 \end{array}$	$\begin{vmatrix} 3\\2\\4\\<1\\5\end{vmatrix}$
2.0.12 516 532 444 600	. 937 . 911	mw m			$\begin{array}{c} .9389\\ .9355\\ .9143\\ .9089\\ .8990\end{array}$	$2 \\ 4 \\ 5 \\ 3 \\ < 1$
$2 \cdot 2 \cdot 12$ $3 \cdot 3 \cdot 10$ 604 446 620	$\left. \begin{array}{c} -\overline{871} \\ 860 \\ 853 \end{array} \right.$	w w mw			$. 8868 \\ . 8735 \\ . 8614 \\ . 8529 $	3 2 2 2
$536 \\ 1 \cdot 1 \cdot 14 \\ 606 \\ 624 \\ 448$. 840 } . 820 	ms - ms -			. 8399 . 8376 . 8205 . 8051	5 4 5 3
$\substack{4\cdot0\cdot12\\545}$. 806 . 795	ms m		-	. 8041 . 7950	$\frac{3}{5}$

ASTM cards

Card number	Index lines	Radiation	Source
2-0659	$\begin{array}{c} 3. \ 00 \\ 2. \ 12 \\ 3. \ 47 \end{array}$	Molyb- denum	General Electric Co., Wembley, England.

Additional published patterns

Source	Radiation	Wavelength
Holgersson [1] 1923	Copper	Kα

NBS sample. The sample of strontium sulfide was obtained from the City Chemical Corp., New York, N. Y. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of aluminum, barium, iron, and sodium; 0.01 to 0.1 percent each of calcium, potassium, magnesium, titanium, vanadium, and zirconium; 0.001 to 0.01 percent each of copper, lithium, manganese, nickel, and lead.

The sample has a tan color. The refractive index is too high to be determined by the conventional liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by the General Electric Co., England, have been converted from kX to angstrom units. The *d*-values of the Holgersson pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
General Electric Co., England Holgersson National Bureau of Standards	$200 \\ 200 \\ 200 \\ 200$	$220 \\ 220 \\ 220 \\ 220$	$111 \\ 420 \\ 111$

Structural data. Holgersson [1] in 1923 determined that strontium sulfide has sodium chloride-type structure, the space group O_h^5 -Fm3m, and 4(SrS) per unit cell.

hkl	General Electric Co. Mo, 0.7107 A			I C	1923 Holgerssor u, 1.5418	n A	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι	a	d	Ι	a	d	Ι	a
$111 \\ 200 \\ 220 \\ 311 \\ 222 \\ 400 \\ 331 \\ 420 \\ 422 \\ 511 \\ 440 \\ 531 \\ 600 \\ 620 \\ 533 \\ 622 \\ 444 \\ 711 \\ 640 \\ 642 \\ 731 \\ $	A 3. 48 3. 01 2. 12 1. 816 1. 738 1. 506 1. 381 1. 347 1. 229 1. 158 1. 064 1. 019 1. 005 	70 100 100 50 60 40 20 70 60 20 20 20 50 	A 6. 03 6. 02 6. 00 6. 023 6. 021 6. 024 6. 024 6. 021 6. 024 6. 021 6. 024 6. 021 6. 024 6. 021 6. 017 6. 019 6. 030	$\begin{array}{c} A \\ \hline 2. 91 \\ 2. 06 \\ 1. 759 \\ 1. 689 \\ \hline 1. 460 \\ 1. 343 \\ 1. 310 \\ 1. 199 \\ 1. 125 \\ 1. 039 \\ \hline 0. 985 \\ . 935 \\ . 893 \\ \hline . 858 \\ . 826 \\ \hline \hline \\$	vs vs m s m vs s w w w w s w w w w u s	A 5. 81 5. 83 5. 83 5. 85 5. 85 5. 85 5. 85 5. 85 5. 88 5. 91 5. 91 5. 91 5. 90	$\begin{array}{c} A\\ 3.\ 479\\ 3.\ 007\\ 2.\ 129\\ 1.\ 814\\ 1.\ 7378\\ 1.\ 5045\\ 1.\ 3814\\ 1.\ 3814\\ 1.\ 3464\\ 1.\ 2290\\ 1.\ 1584\\ 1.\ 0641\\ 1.\ 0174\\ 1.\ 0034\\ 0.\ 9519\\ .\ 9182\\ .\ 9075\\ .\ 8691\\ .\ 8430\\ .\ 8346\\ .\ 8044\\ .\ 7837\\ \end{array}$	$\begin{array}{c} 29\\ 100\\ 51\\ 14\\ 16\\ 11\\ 6\\ 14\\ 12\\ 4\\ 4\\ 4\\ 4\\ 8\\ 6\\ <1\\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	$\begin{array}{c} A\\ 6, 03\\ 6, 02\\ 6, 02\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 021\\ 6, 021\\ 6, 021\\ 6, 021\\ 6, 021\\ 6, 019\\ 6, 019\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ 6, 020\\ \end{array}$
Average of last five lines		6. 023			5. 90			6. 020	

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

The density of strontium sulfide calculated from the NBS lattice constant is 3.643 at 25° C.

References

- S. Holgersson, Die Struktur der Sulfide von Mg, Ca, Sr, und Ba, Z. anorg. u. allgem. Chem. **126**, 179–192 (1923).
- [2] V. M. Goldschmidt, Geochemische Verteilungsgesetze der Elemente VIII. Untersuchungen über Bau und Eigenschaften von Krystallen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. 1926, No. 8 (1926).
- [3] E. Rumpf, Über die Gitterkonstante der CaS-und SrS-Samariummischphore, Ann. Physik 84, 313–322 (1927).
- [4] W. Primak, H. Kaufman, and R. Ward, X-ray diffraction studies of systems in the preparation of alkaline earth sulfide and selenide phosphors, J. Am. Chem. Soc. 70, 2043-2046 (1948).
- [5] O. J. Güntert and A. Faessler, Präzisionsbestimmung der Gitterkonstanten der Erdalkalisulfide MgS, CaS, SrS und BaS, Z. Krist. 107, 357–361 (1956).

Strontium Tungstate, SrWO₄ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
2-0507	$\begin{array}{c} 3.\ 23\\ 2.\ 71\\ 2.\ 01 \end{array}$	Molyb- denum	General Electric Co., Wembley, Eng- land.

Additional published patterns

Source	Radiation	Wavelength
Broch [1] 1929	Chro- mium	Κα

NBS sample. The sample of strontium tungstate was precipitated from solutions of strontium chloride and sodium tungstate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of barium, calcium, potassium, sodium, and silicon; 0.001 to 0.01 percent each of aluminum, copper, lithium, magnesium, and antimony; and 0.0001 to 0.001 percent each of silver, chromium, cesium, iron, and rubidium.

The sample is colorless. The indices of refraction could not be determined because the particle size is too small.

Interplanar spacings and intensity measurements. The *d*-values of the Broch pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
General Electric Co., England Broch National Bureau of Standards	$112 \\ 112 \\ 112 \\ 112$	$200 \\ 204 \\ 204 \\ 204$	$204 \\ 312 \\ 312 \\ 312$

Structural data. Broch [1] in 1929 determined that strontium tungstate has the calcium tungstate-type structure, the space group $C_{4h}^{6}-I4_{1}/a$, and 4(SrWO₄) per unit cell.

The unit-cell measurements reported by Broch have been converted from kX to angstrom units for comparison with the NBS values.

Launce con	star	nts
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		a	с
$1929 \\ 1957$	Broch [1] National Bureau of Standards.	$A \\ 5.405 \\ 5.4168$	$\begin{array}{c} A \\ 11. \ 90 \\ 11. \ 951 \ \mathrm{at} \\ 25^{\circ} \ \mathrm{C} \end{array}$

The density of strontium tungstate calculated from the NBS lattice constants is 6.353 at 25° C:

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

Strontium Tungstate, SrWO₄ (tetragonal)

hkl	General Electric Co. Mo, 0.7107 A		1929 Broch Cr, 2.2909 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C		hkl	Gene Electri Mo, 0 A	eral ic Co. .7107	192 Broo Cr, 2.29	9 ch 909 A	195 National of Stan Cu, 1.54 25°	7 Bureau dards 405 A, C
	d	Ι	d	Ι	d	Ι		d	Ι	d	Ι	d	Ι
$101 \\ 112 \\ 004 \\ 200 \\ 211$	$\begin{array}{c} A \\ 4. \ 93 \\ 3. \ 23 \\ 2. \ 99 \\ 2. \ 71 \\ 2. \ 37 \end{array}$	$ \begin{array}{r} 60 \\ 100 \\ 50 \\ 70 \\ 30 \end{array} $	A 3. 22 2. 99 2. 72 2. 38	vvs m s vw	A 4. 93 3. 223 2. 987 2. 707 2. 373	$19 \\ 100 \\ 16 \\ 24 \\ 7$	$336 \\ 512 \\ 408 \\ 0.0.12 \\ 505$	A 		A 1. 076 1. 047 1. 005 	w vs m -	$\begin{array}{c} A\\ 1.\ 0749\\ 1.\ 0462\\ 1.\ 0033\\ 0.\ 9959\\ .\ 9868 \end{array}$	37 3 <1 <1
$114 \\ 105 \\ 213 \\ 204 \\ 220$	$ \begin{array}{c}\\ 2. 07\\ 2. 01\\ 1. 92 \end{array} $	$-10 \\ 70 \\ 50$	$\begin{array}{c}\\\\ 2.\ 01\\ 1.\ 916 \end{array}$	- - vvs s	2. 355 2. 187 2. 069 2. 007 1. 915	$\begin{array}{c} 1 \\ < 1 \\ 3 \\ 30 \\ 14 \end{array}$	$3.1.10 \\ 440 \\ 428 \\ 516 \\ 2.0.12$			0. 982 . 941 	s - s -	$\begin{array}{c} .9801\\ .9576\\ .9408\\ .9374\\ .9349\end{array}$	
$301 \\ 116 \\ 215 \\ 312 \\ 224$	$ \begin{array}{r} 1.77\\ 1.70\\ 1.64\\ 1.61 \end{array} $		$\begin{array}{c} 1.\ 790\\ 1.\ 767\\ 1.\ 700\\ 1.\ 649\\ 1.\ 612 \end{array}$	$\begin{array}{c} \rm vw \\ \rm vs \\ \rm vw \\ \rm vvs \\ \rm s \end{array}$	$\begin{array}{c} 1.\ 786\\ 1.\ 768\\ 1.\ 702\\ 1.\ 646\\ 1.\ 612 \end{array}$	$1 \\ 19 \\ 4 \\ 27 \\ 14$	$525 \\ 532 \\ 444 \\ 600 \\ 2 \cdot 2 \cdot 12$.9275 .9180 .9118 .9028 .8835	$<^{1}_{6}$
$\begin{array}{c} 008 \\ 321 \\ 305 \\ 323 \\ 217 \end{array}$	$ \Big\} 1. \ 49 \\ 1. \ 44 \\ 1. \ 40 \\ 1. \ 39 \Big] $	$20 \\ 10 \\ 10 \\ 10 \\ 10$	1. 490 	W - - -	$\begin{cases} 1. \ 493 \\ 1. \ 490 \\ 1. \ 4411 \\ 1. \ 4059 \\ 1. \ 3953 \end{cases}$	$egin{array}{c} 4 \\ 4 \\ 2 \\ 2 \\ 2 \\ 2 \end{array}$	$3 \cdot 3 \cdot 10 \\ 604 \\ 620 \\ 536 \\ 4 \cdot 1 \cdot 11$				- - -	.8724 .8642 .8564 .8419 .8371	$egin{array}{c} 3 \\ 2 \\ 4 \\ 6 \\ 3 \end{array}$
$\begin{array}{c} 400 \\ 208 \\ 316 \\ 332 \\ 404 \end{array}$	$\begin{array}{c} 1. \ 35 \\ 1. \ 31 \\ 1. \ 28 \\ 1. \ 25 \\ 1. \ 23 \end{array}$	$10 \\ 20 \\ 30 \\ 10 \\ 10 \\ 10$	$\begin{array}{c} 1.\ 356\\ 1.\ 307\\ 1.\ 299\\ 1.\ 248\\ 1.\ 234 \end{array}$	w s vs s m	$\begin{array}{c} 1.\ 3542\\ 1.\ 3077\\ 1.\ 2989\\ 1.\ 2488\\ 1.\ 2335 \end{array}$	$ \begin{array}{c} 4 \\ 10 \\ 16 \\ 7 \\ 6 \end{array} $	$615 \\ 528 \\ 1 \cdot 1 \cdot 14 \\ 624 \\ 448$	} 			- - -	.8345 .8331 .8233 .8061	2 3 7 3
$\begin{array}{c} 420\\ 228\\ 1\cdot1\cdot10\\ 424\\ 431 \end{array}$			1. 212 1. 178 1. 140 1. 123	s s W vs -	$\begin{array}{c} 1.\ 2112\\ 1.\ 1781\\ 1.\ 1411\\ 1.\ 1226\\ 1.\ 0790 \end{array}$	7 4 4 7 1	$529 \\ 4.0.12 \\ 545 \\ 5.1.10 \\ 633$	}	-		-	. 8023 . 7974 . 7939 . 7913	$ \begin{array}{c} 3 \\ 1 \\ 5 \\ 2 \end{array} $

Sulfamic Acid, NH₃SO₃ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
3-0268	4. 06 3. 70 2. 73	Molybde- num.	Michigan Alkali Co., Wyandotte, Mich.

Additional published patterns. None.

NBS sample. The sample of sulfamic acid was obtained from the Fisher Scientific Co. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent of silicon; and 0.0001 to 0.001 percent each of aluminum, calcium, and magnesium. The sample is colorless and optically negative. The indices of refraction are $N\alpha=1.551$, $N\beta=1.561$, $N\gamma=1.564$, and $2V \cong 60^{\circ}$.

Interplanar spacings and intensity measurements. The *d*-values reported by the Michigan Alkali Co. were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Michigan Alkali Co National Bureau of Standards.	200, 120 112	$\begin{array}{c} 012\\012\end{array}$	212, 313 120

Structural data. Brunt [1] in 1945 reported that sulfamic acid has the space group D_{2h}^{o} -Pbam and $8(NH_3SO_3)$ per unit cell. However, Brown, Cox, and Llewellyn [2] reported in 1940 that it has the space group D_{2h}^{o} -Pcab. The indexing of the NBS pattern is in agreement with the conditions of this second space group designation.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	ь	с
$1940 \\ 1945 \\ 1955 \\ 1957$	Brown [2] Brunt [1] Osaki, Tadokoro, and Nitta [3]. National Bureau of Standards.	$\begin{array}{c} A\\ 8.\ 08\\ 8.\ 04\\ 8.\ 115\\ 8.\ 109\end{array}$	$\begin{matrix} A \\ 9. 24 \\ 9. 08 \\ 9. 255 \\ 9. 240 \end{matrix}$	A 8. 07 7. 96 8. 066 8.068 at 25° C

The density of sulfamic acid calculated from the NBS lattice constants is 2.133 at 25° C.

References

- N. A. Brunt, De structuur der thiosulfaatgroep, dissertation, Leiden, pp. 64 (S. R. 10, 149–150 (1945–1946)).
- [2] C. J. Brown, E. G. Cox, and F. J. Llewellyn, The crystal structure of potassium sulphamate, J. Chem. Soc. 1-10 (1940).
- [3] K. Osaki, H. Tadokoro, and I. Nitta, Structure of sulfamic acid molecule from a three-dimensional Fourier analysis, Bull. Chem. Soc. Japan 28, 524–528 (1955).

Sulfamic Acid, NH₃SO₃ (orthorhombic)

hkl	Michigan Co Mo,	Alkali	1957 National Bureau of Standards Cu, 1.5405 A, 25° C			
	d	Ι	d	Ι		
$111 \\ 020 \\ 200 \\ 120 \\ 012$	$ \begin{array}{c} A \\ -4.62 \\ 4.07 \\ 3.71 \end{array} $	20 100 100	$\begin{cases} A \\ 4.86 \\ 4.62 \\ 4.05 \\ 4.01 \\ 3.699 \end{cases}$	$18 \\ 25 \\ 79 \\ 84 \\ 86$		
$201 \\ 121 \\ 112 \\ 220 \\ 022$	 3. 37 3. 13 	80 20	$\begin{array}{c} 3.\ 627\\ 3.\ 594\\ 3.\ 366\\ 3.\ 048\\ 3.\ 038 \end{array}$	$38 \\ 20 \\ 100 \\ 9 \\ 7$		
$122 \\ 212 \\ 131 \\ 222 \\ 231$	$ \begin{array}{c} 2.88\\ 2.74\\ 2.45\\ 2.35 \end{array} $	$20 \\ 100 \\ 5 \\ 5$	$\begin{cases} 2.848 \\ 2.735 \\ 2.712 \\ 2.4325 \\ 2.3486 \end{cases}$	$33 \\ 59 \\ 37 \\ 13 \\ 12$		
$320 \\ 040 \\ 321 \\ 203 \\ 123$	}		2. 3363 2. 3109 2. 2418 2. 2354	$11\\8\\4\\2$		
$312 \\ 141 \\ 004 \\ 223 \\ 331$	} 2.01	 10	$\begin{array}{c} 2. \ 1831 \\ 2. \ 1425 \\ 2. \ 0158 \\ 1. \ 9705 \end{array}$	3 1 6 4		
$133 \\ 401 \\ 241 \\ 142 \\ 411$	<pre>} } 1. 94</pre>	 10 	$\begin{cases} 1. \ 9664 \\ 1. \ 9481 \\ 1. \ 9465 \\ 1. \ 9224 \end{cases}$	$\begin{array}{c} 7\\6\\5\\2\end{array}$		
$114\\420\\421\\204\\412$	} 1. 82	 25 	$\left\{\begin{array}{c} 1.\ 9152\\ 1.\ 8578\\ 1.\ 8094\\ 1.\ 8057\\ 1.\ 7765\end{array}\right.$			
$323 \\ 151 \\ 341 \\ 143 \\ 034$			$\begin{array}{c} 1.\ 7615\\ 1.\ 7583\\ 1.\ 7157\\ 1.\ 7128\\ 1.\ 6871 \end{array}$	$9\\10\\4\\6\\1$		
$\begin{array}{r} 431 \\ 134 \\ 251 \\ 403 \\ 342 \end{array}$	} 1.66	10 	$\left\{\begin{array}{c} 1.\ 6570\\ 1.\ 6515\\ 1.\ 6461\\ 1.\ 6198\\ 1.\ 6096\end{array}\right.$	$\overset{1}{\overset{5}{}}_{7}$		
413	1. 58 (*)	5	1. 5943	4		

· Seven additional lines are omitted.

Tellurium(IV) Oxide, TeO₂ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0870	$\begin{array}{c} 2. \ 99 \\ 3. \ 40 \\ 1. \ 87 \end{array}$	Molybde- num.	New Jersey Zinc Co.

The powder data on card 1–0870 is for the tetragonal form of TeO_2 , but the structural and optical data, and the unit-cell measurements are for tellurite, the orthorhombic form of TeO₂. A pattern for tellurite is on card 1–0117.

Additional published patterns. A pattern published by Inuzuka [1] was found in the literature, but because it was not similar to the other patterns it was not included in the *d*-value table.

NBS sample. The sample of tellurium oxide was obtained from the Johnson Matthey Co., Ltd., Their spectrographic analysis showed London. the following impurities: 0.001 to 0.01 percent each of bismuth, lead, and copper; and 0.0001 to 0.001 percent of cadmium.

The sample is colorless and optically positive. The indices of refraction were too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measure**ments.** The *d*-values reported by the New Jersey Zinc Co. were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
New Jersey Zinc Co National Bureau of Standards	$\begin{array}{c} 102 \\ 102 \end{array}$	$\begin{array}{c} 110\\ 110 \end{array}$	$\begin{array}{c} 212\\ 212 \end{array}$

Structural data. Stehlik and Balak [2] in 1948 determined that tetragonal tellurium oxide has either the space group D₄⁴-P4₁2₁ or the space group $D_4^8 - P4_3 2_1$. There are $4(TeO_2)$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units, and the "c" value reported by Goldschmidt has been doubled for comparison with the NBS values.

		a	с
$1926 \\ 1949 \\ 1957$	Goldschmidt [3] Stehlik and Balak [2] National Bureau of Standards.	$\begin{matrix} A \\ 4.80 \\ 4.805 \\ 4.809 \end{matrix}$	$\begin{array}{c} A \\ 7.56 \\ 7.609 \\ 7.614 \text{ at} \\ 25^{\circ} \text{ C} \end{array}$

The density of tellurium oxide calculated from the NBS lattice constants is 6.019 at 25° C.

References

- [1] H. Inuzuka, The crystal structure of Tellurite, TeO₂,
- J. Geol. Soc. Tokyo 41, 131–138 (1934).
 B. Stehlik and L. Balak, The crystal structure of tellurium dioxide, Coll. Czech Chem. Commun. 14, 595-607 (1949).

hkl	New Je Zinc Mo,	ersey Co.	1957 National H of Stand Cu, 1.5405	Bureau ards A, 25°C
	d	Ι	d	Ι
 $101 \\ 110 \\ 111 \\ 102 \\ 112$	A 	- <u>80</u> 100	$\begin{array}{c} A \\ 4.\ 07 \\ 3.\ 40 \\ 3.\ 10 \\ 2.\ 98 \\ 2.\ 536 \end{array}$	$9\\88\\13\\100\\1$
$200 \\ 201 \\ 210 \\ 211 \\ 113 \\ 202$	2. 41 }	16 	2. 407 2. 293 2. 151 2. 071 2. 034	$\begin{array}{c} 20\\2\\2\\6\\1\end{array}$
$\begin{array}{c} 004 \\ 212 \\ 203 \\ 220 \\ 114 \\ 221 \end{array}$	$ \begin{array}{c} \overline{1.87} \\ \overline{1.70} \\ 1.66 \end{array} $	56 	1. 903 1. 872 1. 745 1. 700 1. 660	
$213 \\ 301 \\ 310 \\ 204 \\ 302$	1.52 1.49	 8 25 	$\begin{array}{c} 1.\ 6401\\ 1.\ 5684\\ 1.\ 5210\\ 1.\ 4923\\ 1.\ 4775 \end{array}$	$4 \\ 3 \\ 12 \\ 15 \\ 9$
$223 \\ 312 \\ 303 \\ 321 \\ 313$	}		1. 4127 1. 3554 1. 3139 1. 3048	$egin{array}{c} 2 \ 1 \ 2 \ < 1 \ \end{array}$
$224 \\ 322 \\ 215 \\ 106 \\ 304$	$\left. \begin{array}{c} 1.26\\\\ 1.22 \end{array} \right\}$	-14 10	1. 2681 1. 2590 1. 2433 1. 2270	4 4 1 5
$\begin{array}{c} 400 \\ 116 \\ 314 \\ 323 \\ 411 \end{array}$	}	14	1. 2020 1. 1881 1. 1806 1. 1531	$< 1 \\ 6 \\ \leq 1 \\ 1$
$225 \\ 331 \\ 412 \\ 216 \\ 324$	 1. 11 } 1. 09	$\frac{}{4}$	1. 1341 1. 1212 1. 1158 1. 0928	$\begin{array}{c} \leq 1\\ 1\\ 2\\ 4 \end{array}$
$\begin{array}{c} 403 \\ 332 \\ 315 \\ 240 \\ 421 \end{array}$	}		1. 0866 1. 0753 1. 0647	<1 <1 <1
$107 \\ 413 \\ 226 \\ 404$	}		$1.\ 0601\\1.\ 0164$	<1 1

[3] V. M. Goldschmidt, Geochemische Verteilungsgesetze Über die Kristallstrukturen vom der Elemente VI. Rutiltypus, mit Bemerkungen zur Geochemie zweiwertiger und vierwertiger Elemente, Skrifter Norske Videnskaps-Akad. Olso I. Mat.-Naturv. Kl. 1926, No. 1 (1926).

Thallium Bromide, TlBr (cubic)

ASTM cards

Card number ^a	Index lines	Radiation	Source
3-0732	$2.82 \\ 1.63 \\ 1.07$	Copper	Van Arkel [1] 1924.

•A pattern by Wagner and Lippert [2] of thallium bromide at 415° C is given on ASTM card 4-0680.

Additional published patterns

Source	Radiation	Wavelength
Lunde [3] 1925	Copper	Kα

NBS sample. The sample of thallium bromide was prepared at the NBS. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of silver, aluminum, calcium, copper, iron, magnesium, manganese, and silicon. The sample is yellow. The index of refraction is too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by Van Arkel and by Lunde were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Van Arkel Lunde. National Bureau of Standards	$110 \\ 110 \\ 110 \\ 110$	$211 \\ 211 \\ 211 \\ 211$	$321 \\ 321 \\ 100$

Structural data. Van Arkel [1] in 1924 determined that thallium bromide has cesium chloridetype structure, the space group O_h^1 -Pm3m, and 1(TlBr) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Thallium Bromide, TIBr (cubic)

hkl	C	1924 Van Arkel u, 1.5418	l A	1925 Lunde Cu, 1.5418 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι	a	d	Ι	a	d	I	a
$100\\110\\111\\200\\210\\211\\220\\300\\310\\311\\222\\320\\321\\400\\410\\411\\420\\421\\332\\422\\510$	$\begin{array}{c} A\\ \hline 2.83\\ 2.31\\ 1.99\\ 1.78\\ \hline 1.63\\ 1.41\\ 1.33\\ 1.26\\ 1.20\\ \hline 1.15\\ 1.11\\ 1.07\\ 0.999\\ .969\\ \hline .942\\ .893\\ .872\\ .853\\ .816\\ \hline 784 \end{array}$	vs vw m w vs m w s vw vw vw vw vw vw vw vw vw vw vw vw vw	$\begin{array}{c} A\\ \hline 4.00\\ 4.00\\ 3.98\\ 3.98\\ 3.98\\ \hline 4.00\\ \hline 4.00\\ \hline 3.996\\ \hline 3.995\\ \hline 3.997\\ \hline 3.994\\ \hline 3.996\\ \hline 4.001\\ \hline 3.998\\ \hline 3.908\\ $	$\begin{array}{c} A\\ 4. 0\\ 2. 81\\ 2. 29\\ 1. 99\\ 1. 78\\ 1. 62\\ 1. 40\\ 1. 32\\ 1. 26\\ 1. 20\\ 1. 15\\ 1. 10\\ 1. 06\\ 0. 996\\ . 965\\ . 937\\ . 890\\$	VW VVS VW S S VVS S W VS VW VVS VW VVS VW VVS VS VS VS VS VS VS VS VS VS VS VS S VVS S VVS S VVS S VS V	A 4. 0 3. 97 3. 98 3. 98 3. 98 3. 98 3. 96 3. 96 3. 96 3. 96 3. 98 3. 98 3. 98 3. 98 3. 98 3. 97 3. 98 3. 97 3. 97 3. 97 3. 97 3. 98 4. 97 97 5. 980	$\begin{array}{c} A\\ 3, 98\\ 2, 818\\ 2, 300\\ 1, 9926\\ 1, 7820\\ \hline 1, 7820\\ \hline 1, 6268\\ 1, 4091\\ 1, 3287\\ 1, 2604\\ 1, 2015\\ \hline 1, 1509\\ 1, 1058\\ 1, 0653\\ 0, 9965\\ ., 9667\\ 0395\\ ., 9965\\ ., 9965\\ ., 9965\\ ., 9965\\ ., 9965\\ ., 9965\\ ., 9965\\ ., 8911\\ ., 8696\\ ., 8495\\ ., 8135\\ 7815\\ \end{array}$	$\begin{array}{c} 25\\ 100\\ 7\\ 18\\ 7\\ 27\\ 7\\ 2\\ 8\\ 1\\ 2\\ 2\\ 8\\ 1\\ 2\\ 1\\ 6\\ <1\\ 2\\ 1\\ \\ 1\\ 2\\ 1\\ 3\end{array}$	$\begin{array}{c} A\\ 3. 98\\ 3. 986\\ 3. 988\\ 3. 988\\ 3. 9852\\ 3. 9852\\ 3. 9847\\ 3. 9848\\ 3. 9855\\ 3. 9861\\ 3. 9855\\ 3. 9861\\ 3. 9857\\ 3. 9868\\ 3. 9857\\ 3. 9860\\ 3. 9860\\ 3. 9850\\ 3. 9858\\ 3. 9850\\ 3. 9850\\ 3. 9850\\ 3. 9853\\ 3. 9849\\ \end{array}$
Average	of last five lin	nes	3. 997			3. 978			3. 9850

Lattice constants

1924Van Arkel [1]1925Lunde [3]1939Straumanis, Ieviņš, and Karlsons [4].1957National Bureau of Stand- ards.	$\begin{array}{c} A\\ 3. 99\\ 3. 976\\ 3.98582 \text{ at}\\ 25^{\circ} \text{ C}\\ 3.9850 \text{ at}\\ 25^{\circ} \text{ C} \end{array}$
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The density of thallium bromide calculated from the NBS lattice constant is 7.458 at 25° C.

References

- [1] A. E. Van Arkel, Over den Bouw van Mengkristallen,
- [1] I. L. Physica 4, 33-41 (1924).
 [2] G. Wagner and L. Lippert, Über polymorphe Umwandlung bei einfachen Ionengittern. I. Versuche zur Umwandlung von CsCI- in NaCl-Gitter durch Die Generation 24, 262, 267 (1925, 269).
- Erhitzen, Z. physik. Chem. **31**, 263–267 (1935–36). [3] G. Lunde, Bemerkungen über die Kristallstruktur von Thalliumchlorür und Thalliumbromür, Z. phys. Chem. 117, 51-56 (1925).
- [4] M. Straumanis, A. Ievinš, and K. Karlsons, Hängt die Gitterkonstante von der Wellenlänge ab? Präzions-bestimmungen von Gitterkonstanten des LiF, NaF, As₂O₃, TlČl, TlBr, Z. physik. Chem. 42B, 143-152 (1939).

Thallium(I) Phosphate, Tl_3PO_4 (hexagonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of thallium phosphate was prepared at the NBS by Alvin Perloff. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, barium, bismuth, sodium, silicon, and strontium; 0.001 to 0.01 percent each of arsenic, beryllium, iron, mercury, indium, magnesium, manganese, and nickel; and 0.0001 to 0.001 percent each of silver, chromium, copper, and lead.

The sample is colorless. The indices of refraction are too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Stand- ards.	111	201	311, 212

Structural data. The structure for thallous phosphate has not been published. The NBS pattern was indexed by the cell and space group proposed by Bernard Borie ⁵ in 1949: C⁶₆-P6₃ with $2(Tl_3PO_4)$ per unit hexagonal cell.

Lattice constants

		a	с
$1949 \\ 1957$	Borie National Bureau of Stand- ards.	A 8. 35 8. 355	A 5. 12 5. 112 at 25° C

The density of thallous phosphate calculated from the NBS lattice constants is 7.608 at 25° C.

⁵ M. S. Thesis (1949), Physics Dept., Tulane University.

Thallium (I) Phosphate, Tl_3PO_4 (hexagonal)

hkl	1957 National H of Stands Cu, 1.540 25° (Bureau ards 05 A, C
	d	Ι
100 110 101 200 111	$ \begin{array}{c} A \\ 7. 24 \\ 4. 18 \\ 3. 62 \\ 3. 236 \end{array} $	7 44 25 100
$201 \\ 210 \\ 002 \\ 300 \\ 211$	$\left.\begin{array}{c} 2. \ 954 \\ 2. \ 735 \\ 2. \ 557 \\ 2. \ 412 \end{array}\right\}$	88 47 25 14
$301 \\ 112 \\ 220 \\ 202 \\ 310$	$ \left. \left. \begin{array}{c} \textbf{2. 181} \\ \textbf{2. 089} \\ \textbf{2. 006} \end{array} \right. \right. \right. $	12 9 24
$221 \\ 311 \\ 212 \\ 400 \\ 302$	$\left. \begin{array}{c} 1.\ 9336 \\ 1.\ 8681 \\ 1.\ 8093 \\ 1.\ 7533 \end{array} \right.$	$6\\54\\4\\7$
$\begin{array}{r} 401 \\ 320 \\ 410 \\ 321 \\ 312 \\ 113 \end{array}$	$\left. \begin{array}{c} 1.\ 7060 \\ 1.\ 6606 \end{array} \right\} \\ 1.\ 5786 \end{array} \right\}$	3 6 40
$203 \\ 411 \\ 500 \\ 213$	$\left. \begin{array}{c} 1.5421 \\ 1.5091 \\ 1.4471 \end{array} \right\}$	9 5 3
$330 \\ 501 \\ 322 \\ 303 \\ 420$	$\left. \right\} 1.3926$	13 6

hkl	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		hkl	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι		d	I	
$331 \\ 412 \\ 421 \\ 223 \\ 510 \\ 313$	$\begin{array}{c} A \\ 1. 3436 \\ 1. 3209 \\ 1. 2995 \end{array}$	7 4 7	$701 \\ 612 \\ 620 \\ 414 \\ 115$	$\begin{array}{c} A \\ 1.\ 0132 \\ 1.\ 0043 \\ 0.\ 9934 \end{array}$	3 2 4	
$502 \\ 104 \\ 332 \\ 600 \\ 422 \\ 204$	$\left. \begin{array}{c} 1. \ 2588 \\ 1. \ 2231 \\ 1. \ 2058 \end{array} \right.$	4 1 5	$\begin{array}{c} 621 \\ 603 \\ 205 \\ 433 \\ 710, 702 \\ 523, 504 \\ 215 \end{array}$	$\left. \begin{array}{c} .9846 \\ .9751 \\ \end{array} \right\} \ .9583 \\ \end{array} \right\}$	6 4 4	
$\begin{array}{r} 430\\323\\601\\520,431\\512,413\end{array}$	$\left. \begin{array}{c} 1. \ 1896 \\ 1. \ 1739 \\ 1. \ 1586 \end{array} \right. \right\}$	4 4 10	$711 \\ 334 \\ 305 \\ 622 \\ 424$	$\left. \begin{array}{c} . \ 9419 \\ \end{array} \right\} \ . \ 9338 \\ \end{array} \right\}$	4 4	
$ 521 \\ 304 \\ 610 \\ 503 \\ 602 $	$ \left. \left. \right\} \begin{array}{l} 1. \ 1298 \\ 1. \ 1033 \end{array} \right\} $	3 3	$540 \\ 613 \\ 630, 541 \\ 514, 315 \\ 800$	$\left. \begin{array}{c} . \ 9266 \\ . \ 9115 \\ . \ 9045 \end{array} \right.$	4 5 1	
$ \begin{array}{r} 502 \\ 224 \\ 611, 432 \\ 333, 314 \\ 522 \\ (a) \\ \end{array} $	$\left. \begin{array}{c} 1.\ 0905 \\ 1.\ 0781 \\ 1.\ 0551 \\ 1.\ 0411 \end{array} \right.$	2 5 5	$\begin{array}{r} 631 \\ 712 \\ 801 \\ 443 \\ 405 \end{array}$	$\left. \begin{array}{c} . \ 8975 \\ . \ 8905 \end{array} \right\}$	5 2	
700 513 441	$\left. \begin{array}{c} 1.0411 \\ 1.0336 \\ 1.0230 \end{array} \right.$	2 3 4	$720 \\ 703 \\ 721, 542 \\ 434, 325$	$\left. \begin{array}{c} . \ 8839 \\ . \ 8709 \end{array} \right\}$	5 4	

Thallium(I) Phosphate, Tl₃PO₄ (hexagonal)-Con.

^a This line could not be indexed by using the proposed hexagonal cell.

Thallium(III) Phosphate, TIPO₄ (orthorhombic)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wavelength
Mooney [1] 1956	Copper	$K \alpha_1$

NBS sample. The thallium phosphate was prepared at NBS by Alvin Perloff. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, mercury, indium, sodium, nickel, and zirconium; 0.001 to 0.01 percent each of aluminum, gold, copper, iron, gallium, magnesium, molybdenum, lead, and titanium; and 0.0001 to 0.001 percent each of silver, barium, chromium, manganese, tin, platinum, and strontium.

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

Interplanar spacings and intensity measurements. The *d*-values of the Mooney pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Mooney National Bureau of Standards	$\begin{array}{c} 112\\112\end{array}$	110 110	$\begin{array}{c} 020\\ 020 \end{array}$

Structural data. Mooney [1] in 1956 determined that thallium phosphate has the space group D_{2h}^{17} -Cmcm, and 4(TIPO₄) per unit cell. The unit-cell measurements of the Mooney pat-

The unit-cell measurements of the Mooney pattern have been converted from kX to angstrom units.

Lattice constants

1	1	1	1	
		a	b	с
$1956 \\ 1957$	Mooney [1] National Bureau of Standards.	$egin{array}{c} A \\ 5. \ 406 \\ 5. \ 408 \end{array}$	${}^{A}_{8.\ 026}_{8.\ 027}$	A 7.085 7.087 at 25° C

The density of thallium phosphate calculated from the NBS lattice constants is 6.461 at 25° C.

References

 R. C. L. Mooney, Crystal structure of anhydrous indium phosphate and thallic phosphate by X-ray diffraction, Acta Cryst. 9, 113-117 (1956).

Thallium(III) Phosphate, TlPO₄ (orthorhombic)

hkl	195 Moor Cu, 1.54	6 ney 405 A	195 National of Stan Cu, 1.54 25°	7 Bureau dards 405 A, C	hkl	195 Moor Cu, 1.54	6 ney 405 A	195 National of Stan Cu, 1.54 25°	7 Bureau dards 405 A, C
	d	Ι	d	Ι		d	Ι	d	Ι
$110 \\ 020 \\ 111 \\ 002 \\ 021$	$\begin{array}{c} A \\ 4. \ 48 \\ 4. \ 01 \\ 3. \ 786 \\ 3. \ 545 \\ 3. \ 493 \end{array}$	$99 \\ 55 \\ 8 \\ 22 \\ 3$	$\begin{array}{c} A \\ 4. \ 48 \\ 4. \ 01 \\ 3. \ 789 \\ 3. \ 542 \\ 3. \ 491 \end{array}$	$96 \\ 51 \\ 12 \\ 28 \\ 9$	$243 \\ 044 \\ 420 \\ 333 \\ 402$	$ \begin{array}{c} A \\ 1.3280 \\ 1.2811 \\ 1.2627 \end{array} $	$3 \\ 2 \\ <1$	$\begin{array}{c} A \\ 1. \ 3284 \\ 1. \ 2811 \\ 1. \ 2630 \end{array}$	6 3 3
$112 \\ 200 \\ 022 \\ 130 \\ 220$	2. 779 2. 702 2. 656 2. 399 2. 238	$100 \\ 28 \\ 23 \\ 38 \\ 10$	$\begin{array}{c} 2.\ 780\\ 2.\ 703\\ 2.\ 656\\ 2.\ 398\\ 2.\ 242 \end{array}$	$100 \\ 28 \\ 24 \\ 40 \\ 11$	$\begin{array}{c} 062 \\ 314 \\ 422 \\ 260 \\ 350 \\ 225 \end{array}$	$\left.\begin{array}{c}1.\ 2508\\1.\ 2478\\1.\ 2074\\1.\ 1988\end{array}\right.$	1 5 4 6	$\begin{array}{c} 1.\ 2509\\ 1.\ 2481\\ 1.\ 2046\\ 1.\ 1989 \end{array}$	$< 1 \\ 5 \\ 4 \\ 5 \\ 5$
$202 \\ 023 \\ 040 \\ 132 \\ 222$	$\begin{array}{c} 2. \ 149 \\ 2. \ 036 \\ 2. \ 007 \\ 1. \ 985 \\ 1. \ 8937 \end{array}$	$27 < 1 \\ 11 \\ 25 \\ 33$	$\begin{array}{c} 2. \ 149 \\ 2. \ 036 \\ 2. \ 006 \\ 1. \ 986 \\ 1. \ 8949 \end{array}$	$27 < 1 \\ 11 \\ 26 \\ 33$	$229 \\ 244 \\ 006 \\ 154 \\ 334 \\ 116 \\$	1. 1919 1. 1814 1. 1615 }	$<^{3}_{1}_{5}_{}$	$\begin{array}{c} 1. \ 1922 \\ 1. \ 1814 \\ 1. \ 1617 \\ 1. \ 1423 \end{array}$	$\overset{3}{\overset{1}{\overset{4}{\overset{1}{12}}}}$
$\begin{array}{c} 004 \\ 310 \\ 042 \\ 311 \\ 133 \end{array}$	$\begin{array}{c} 1.\ 7717\\ 1.\ 7583\\ 1.\ 7458\\ 1.\ 7072\\ 1.\ 6817 \end{array}$	${ \begin{array}{c} 11 \\ 9 \\ 14 \\ < 1 \\ < 1 \end{array} }$	$\begin{array}{c} 1.\ 7720\\ 1.\ 7593\\ 1.\ 7461\\ 1.\ 7072\\ 1.\ 6822 \end{array}$	$\overset{11}{\underset{\scriptstyle 14}{\overset{\scriptstyle 14}{\underset{\scriptstyle <1}{\overset{\scriptstyle 1}}}}$	$ \begin{array}{r} 262 \\ 352 \\ 026 \\ 170 \\ 440 \end{array} $	} } } 		$\begin{array}{c} 1. \ 1356 \\ 1. \ 1329 \\ 1. \ 1214 \end{array}$	$8 \\ 6 \\ 5$
$114 \\ 024 \\ 240 \\ 312 \\ 150$	$\begin{array}{c} 1.\ 6477\\ 1.\ 6205\\ 1.\ 6111\\ 1.\ 5744\\ 1.\ 5381 \end{array}$	$ \begin{array}{r} 16 \\ 10 \\ 6 \\ 18 \\ 7 \end{array} $	$\begin{array}{c} 1.\ 6480\\ 1.\ 6207\\ 1.\ 6114\\ 1.\ 5754\\ 1.\ 5391 \end{array}$	$15 \\ 12 \\ 7 \\ 17 \\ 8$	$ \begin{array}{r} 315 \\ 206 \\ 404 \\ 510 \\ 172 \end{array} $, 		$\begin{array}{c} 1. \ 1030 \\ 1. \ 0822 \\ 1. \ 0747 \\ 1. \ 0718 \end{array}$	$<^{1}_{2}$ $^{3}_{10}$
$330 \\ 204 \\ 242 \\ 124$	$\begin{array}{c} 1. \ 4946 \\ 1. \ 4813 \\ 1. \ 4666 \\ 1 \ 4946 \end{array}$	$9 \\ 6 \\ 20 \\ 12$	$\begin{array}{c} 1. \ 4949 \\ 1. \ 4822 \\ 1. \ 4671 \\ 1 \ 4250 \end{array}$	$ \begin{array}{c} 10 \\ 8 \\ 15 \\ 12 \end{array} $	$ \begin{array}{r} 112 \\ 263 \\ 353 \\ 442 \\ 064 \end{array} $	}		1. 0690	6
154	1. 4240	8	1. 4250	13 9	511	}		1. 0597	3
$224 \\ 332 \\ 400 \\ 115$	$ \begin{array}{c} 1.3902\\ 1.3771\\ 1.3513 \end{array} $	6 6 4	$\begin{array}{c} 1. \ 3902 \\ 1. \ 3771 \\ 1. \ 3520 \end{array}$	7 7 5	$ \begin{array}{r} 130 \\ 226 \\ 424 \\ 512 \end{array} $			$\begin{array}{c} 1.\ 0451\\ 1.\ 0382\\ 1.\ 0260 \end{array}$	$egin{array}{c} 6 \\ 4 \\ 2 \end{array}$
$\begin{array}{c} 115 \\ 060 \end{array}$	1. 3369	2	1. 3381	3	046			1. 0180	3

ASTM cards.

Cards number	Index lines	Radiation	Source
6–0603	$2.22 \\1.41 \\1.29$	Iron	American Smelting and Refining Co., N. J.

Additional published patterns. None.

NBS sample. The sample of tin telluride was prepared at NBS by D. E. Roberts. Spectrographic analysis of the sample showed the following impurities: 0.001 to 0.01 percent each of lead and silicon; and 0.0001 to 0.001 percent each of copper, iron, and magnesium.

The sample has a gray metallic luster and is opaque.

Interplanar spacings and intensity measurements. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
American Smelting and Refining Co. National Bureau of Standards	220 200	420 220	422 222

Structural data. Goldschmidt [1] in 1927 determined that tin telluride has sodium chloridetype structure, the space group O_h^5 -Fm3m, and 4(SnTe) per unit cell.

The unit-cell measurement reported by Goldschmidt has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

$1927 \\ 1957$	Goldschmidt [1] National Bureau of Stand- ards.	A 6. 298 6. 303 at 25° C

The density of tin telluride calculated from the NBS lattice constant is 6.532 at 25° C.

hkl	Amer. Smeltin Refining C Fe, 1.9373		Amer. Smelting and N Refining Co. Fe, 1.9373 A C		Nationa Sta Cu, 1.54	1957 National Bureau of Standards Cu, 1.5405 A, 25°C		
;	d	Ι	a	d	Ι	a		
$\begin{array}{c} 200\\ 220\\ 222\\ 400\\ 420\\ \end{array}\\ \begin{array}{c} 422\\ 440\\ 600\\ 622\\ 444\\ 640\\ 642\\ 800\\ \end{array}$	A 3. 13 2. 22 1. 82 1. 58 1. 41 1. 28 1. 12 1. 06 0. 999 	70 100 60 40 90 80 30 70 60 - - - -	A 6. 26 6. 28 6. 30 6. 32 6. 31 6. 30 6. 34 6. 36 6. 32 	$\begin{array}{c} A\\ 3.\ 15\\ 2.\ 23\\ 1.\ 822\\ 1.\ 577\\ 1.\ 410\\ 1.\ 2870\\ 1.\ 1147\\ 1.\ 0511\\ 0.\ 9969\\ .\ 9502\\ .\ 9098\\ .\ 8741\\ .\ 8423\\ .\ 7878\\ \end{array}$	$ \begin{array}{c} 100 \\ 52 \\ 15 \\ 10 \\ 15 \\ 8 \\ 3 \\ 4 \\ 4 \\ 2 \\ 1 \\ 2 \\ 4 \\ 1 \end{array} $	$\begin{array}{c} A\\ 6, 31\\ 6, 309\\ 6, 310\\ 6, 308\\ 6, 306\\ 6, 306\\ 6, 306\\ 6, 306\\ 6, 307\\ 6, 303\\ 6, 303\\ 6, 303\\ 6, 303\\ 6, 303\\ 6, 303\\ 6, 302\\ \end{array}$		
Average of last five lines		6. 33		-	6. 303			

References

Urea, $CO(NH_2)_2$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0444	4. 00 3. 04 3. 61	Molybde- num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. A pattern by Becker and Jancke [2] was found in the literature, but because it was in poor agreement with other patterns, it was not included in the *d*-value table. **NBS sample.** The sample of urea was obtained from the City Chemical Corp., New York, N. Y. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of barium, copper, magnesium, and silicon.

The sample is colorless and optically positive. The indices of refraction are N_0 =1.480 and N_e = 1.601.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The three strongest lines of each pattern are as follows:

V. M. Goldschmidt, Geochemische Verteilungsgesetze der Elemente IV. Untersuchungen über Bau und Eigenschaften von Kristallen, Skrifter Norske Videnskaps-Akad. Olso I. Mat.-Naturv. Kl. 1927, No. 8 (1927).

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	110	$\frac{111}{111}$	101
National Bureau of Standards	110		101

Structural data. Mark and Weissenberg [3] in 1923 determined that urea has the space group $D_{2d}^3 - P42_1m$ and $2[CO (NH_2)_2]$ per unit cell. Urea is used as a structure-type.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	с
1923 1928 1957	Mark and Weissenberg [3]_ Hendricks [4] National Bureau of Standards.	$\begin{array}{c} A \\ 5.\ 64 \\ 5.\ 75 \\ 5.\ 645 \end{array}$	$\begin{matrix} A \\ 4.71 \\ 4.78 \\ 4.704 \text{ at} \\ 25^{\circ} \text{ C} \end{matrix}$

The density of urea calculated from the NBS lattice constants is 1.330 at 25° C.

References

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemi-cal analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938).
 K. Becker and W. Jancke, Röntgenspektroskopisch Ustersveibungen an Weibindungen L. Z. physik
- Untersuchungen an Verbindungen. I., Z. physik. Chem. 99, 242–266 (1921). [3] H. Mark and K. Weissenberg, Röntgenographische
- [3] H. Mark and R. Weissenberg, Hongenographische Bestimmung der Struktur des Harnstoffs und des Zinntetrajodids, Z. Physik. 16, 1-22 (1923).
 [4] S. B. Hendricks, Crystal structure of urea, and the molecular symmetry of thiourea, J. Am. Chem. Soc. 70 (2017) 100 (1000)
- 50. 2455-2464 (1928).

hkl	193 Hanawalt and Fr Mo, 0.7	8 c, Rinn, evel 107 A	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	Ι	d	Ι	
110 101 111 200 210	$\begin{matrix} A \\ 4. \ 01 \\ 3. \ 62 \\ 3. \ 05 \\ 2. \ 83 \\ 2. \ 53 \end{matrix}$	$100 \\ 40 \\ 53 \\ 11 \\ 20$	$\begin{array}{c} A \\ 4.\ 01 \\ 3.\ 62 \\ 3.\ 048 \\ 2.\ 826 \\ 2.\ 528 \end{array}$	$100 \\ 25 \\ 29 \\ 6 \\ 12$	
201 002 211 102	$\begin{array}{c} 2. \ 41 \\ 2. \ 34 \\ 2. \ 23 \\ 2. \ 17 \\ 2. \ 08 \end{array}$	$20 \\ 3 \\ 8 \\ 20 \\ 1$	2. 422 2. 349 2. 229 2. 171	10 3 5 5	
$112 \\ 220 \\ 221 \\ 310 \\ 301$	$ \begin{array}{r} 2.01 \\ \hline 1.84 \\ \hline 1.75 \\ \end{array} $		$\begin{array}{c} 2.\ 025\\ 1.\ 996\\ 1.\ 837\\ 1.\ 786\\ 1.\ 747 \end{array}$	2224 <111	
$212 \\ 311 \\ 003 \\ 222 \\ 103$	1. 67 1. 51	 8	$\begin{array}{c} 1.\ 721\\ 1.\ 669\\ 1.\ 568\\ 1.\ 5219\\ 1.\ 5090 \end{array}$	$\overset{{\color{red}}{\scriptstyle <1}}{\underset{\scriptstyle 1}{\overset{\scriptstyle 1}{\scriptstyle <1}}}_1$	
$312 \\ 401 \\ 330 \\ 420 \\ 421$	$ \begin{array}{r} 1.370\\ 1.331\\ 1.261\\ 1.232 \end{array} $	$\begin{array}{c} \\ 3 \\ 7 \\ 1 \\ 1 \end{array}$	$\begin{array}{c} 1.\ 4209\\ 1.\ 3518\\ 1.\ 3304\\ 1.\ 2622\\ 1.\ 2190 \end{array}$	$\begin{matrix} \leqslant 1 \\ 1 \\ 1 \\ \leqslant 1 \\ 1 \end{matrix}$	
$004 \\ 323 \\ 431$	1. 179 	4	1. 1771 1. 1076 1. 0979	$\overset{1}{\underset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{$	

Zinc Orthosilicate, (willemite), Zn_2SiO_4 (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-1412	1. 42 2. 84 2. 63	Copper	Schütz [1] 1936.*
2–1413	$\begin{array}{c} 1.\ 42\\ 2.\ 63\\ 2.\ 31 \end{array}$	Copper	Schütz [1] 1936. ^b
2-0813	$\begin{array}{c} 2.\ 81\\ 2.\ 61\\ 3.\ 44 \end{array}$	Copper	British Museum.
1-1076	$\begin{array}{c} 2. \ 64 \\ 3. \ 49 \\ 2. \ 83 \end{array}$	Molyb- denum	New Jersey Zinc Co.

*Natural willemite. ^bSynthetic willemite.

Additional published patterns. None.

NBS sample. The sample of zinc orthosilicate was synthesized at the Geophysical Laboratory, Washington, D. C. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of aluminum, calcium, and niobium; 0.01 to 0.1 percent each of cobalt, iron, magnesium, manganese, molybdenum, and titanium; 0.001 to 0.01 percent each of barium, beryllium, chromium, copper, nickel, lead, and antimony; and 0.0001 to 0.001 percent each of silver and boron.

The sample is colorless and optically positive. The refractive indices are $N_0 = 1.691$ and $N_e =$ 1.719.

Interplanar spacings and intensity measurements. The *d*-values reported by the British Museum and the New Jersey Zinc Co. were converted from kX to angstrom units and the dvalues of the Schütz pattern were calculated from reported Bragg angle data. The three strongest

Urea, $CO(NH_2)_2$ (tetragonal)

lines of each pattern are as follows:

Pattern	1	2	3
Schütz, natural Schütz, synthetic British Museum New Jersey Zinc Co National Bureau of Standards	$713 \\713 \\113 \\140 \\140$	$113 \\ 140 \\ 140 \\ 220 \\ 113$	$140 \\ 223 \\ 220 \\ 113 \\ 220$

Structural data. Gottfried [2] in 1927 determined that zinc orthosilicate has phenacite-type structure, the space group C_{3i}^2 -R3, and $18(Zn_2SiO_4)$ per unit hexagonal cell or $6(Zn_2SiO_4)$ per unit rhombohedral cell. Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	С
$1927 \\ 1929 \\ 1930$	Gottfried [2] Pabst [3] Bragg and Zachariasen	$\begin{matrix} A \\ 14. \ 17 \\ 13. \ 898 \\ 13. \ 97 \end{matrix}$	$\begin{array}{c} A \\ 9.60 \\ 9.337 \\ 9.36 \end{array}$
1936 1957	Schütz [1] National Bureau of Standards.	13. 97 13. 94	9.36 9.309 at 25° C

The density of zinc orthosilicate calculated from the NBS lattice constants is 4.251 at 25° C.

Zinc Orthosilicate (willemite),	Zn_2SiO_4	(trignoal)
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hkl	1936 Schütz (natural) Cu, 1.5418 A		1936 Schütz (synthetic) Cu, 1.5418 A		British Museum Cu, 1.5418 A		New Jersey Zine Co. Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405, 25° C	
	d	Ι	d	I	d	Ι	d	Ι	d	Ι
110 012 211 300	<u>A</u> <u>-4.40</u> <u></u> 	40	A 	40	$\begin{array}{c} A \\ 6.85 \\ 4.45 \\ \hline \\ 4.04 \\ 3.82 \end{array}$	$ \begin{array}{r} 60 \\ 40 \\ -\overline{} \\ -\overline{} \\ 60 \\ 40 \\ \end{array} $	A 4. 05 		$\begin{array}{c} A \\ 6.98 \\ 4.35 \\ 4.10 \\ 4.026 \\ \hline \end{array}$	$\begin{array}{c} 22\\ 4\\ 17\\ 33\\\end{array}$
220 122 131 113	3. 49 2. 85	60 80	3. 48 2. 85	20 60	$ \begin{array}{c} 3.45\\\\ 3.12\\ 2.93\\ 2.82 \end{array} $		3. 50 2. 84	75 75	3. 486 3. 264 3. 153 2. 834	$81 \\ 4 \\ 7 \\ -\overline{97}$
$312 \\ 140 \\ 042 \\ 232 \\ 223$	2. 63 2. 32	 80	2. 63 2. 32	80 -80	2. 62	100 70	$ \begin{array}{c} -2.65 \\ \\ -2.32 \end{array} $	100 -50	$\begin{array}{c} 2.\ 720\\ 2.\ 634\\ 2.\ 533\\ 2.\ 381\\ 2.\ 318 \end{array}$	
$104 \\ 241 \\ 502 \\ 214 \\ 422$	2. 22 2. 18	10 10 	2. 22 2. 18	10 10 	2. 23 2. 13 2. 07	20 20 40 		 	$\begin{array}{c} 2. \ 287 \\ 2. \ 215 \\ 2. \ 144 \\ 2. \ 074 \\ 2. \ 049 \end{array}$	$\begin{array}{c} 2\\ 1\\ 4\\ 1\\ 5\end{array}$
$\begin{array}{c} 600 \\ 413 \\ 152 \\ 250 \\ 333 \end{array}$	$ \left. \begin{array}{c} 2.01 \\ \hline 1.94 \\ 1.85 \end{array} \right $	20 40 80	2. 01 1. 93 1. 85	20 20 80	2. 01 1. 93 1. 86	40 40 80	$2.01 \\ \\ 1.93 \\ 1.86$	5 -15 75	$\left\{\begin{array}{l} 2.\ 013\\ 2.\ 0111\\ 1.\ 9656\\ 1.\ 9332\\ 1.\ 8592\end{array}\right.$	$7 \\ 9 \\ 2 \\ 9 \\ 36$
$342 \\ 161 \\ 324 \\ 125 \\ 603$	 1. 74 1. 70	 10 10	1. 74 1. 70	 10 10	$ \begin{array}{c}$	$\frac{1}{20}$ $\frac{1}{40}$	1. 69		$\begin{array}{c} 1.\ 8260\\ 1.\ 8074\\ 1.\ 7817\\ 1.\ 7235\\ 1.\ 6882 \end{array}$	$< 1 \\ 1 \\ 1 \\ 3 \\ 7 \\ 1 \\ 3 \\ 7 \\ 1 \\ 3 \\ 7 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$
$\begin{array}{c} 054 \\ 621 \\ 523 \\ 315 \\ 710 \end{array}$	1. 63 1. 60	$\begin{array}{c c}\\ -20\\ -20\\ -20 \end{array}$	1. 63 1. 60	 20 20	 1. 64 1. 60		1. 64 1. 60	 8 	$\begin{array}{c} 1. \ 6752 \\ 1. \ 6491 \\ 1. \ 6404 \\ 1. \ 6273 \\ 1. \ 5986 \end{array}$	$ \begin{array}{c} 1 \\ 2 \\ 7 \\ 10 \\ 10 \end{array} $

hkl	1936 Schütz (natural) Cu, 1.5418 A		1936 Schütz (synthetic) Cu, 1.5418 A		British Museum Cu, 1.5418 A		New Jersey Zine Co. Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405, 25° C	
	d	Ι	d	Ι	d	Ι	d	Ι	d	Ι
$514 \\ 006 \\ 630 \\ -271$	$\begin{array}{c} A \\ \hline 1.56 \\ 1.52 \\ \hline \\ \hline \end{array}$	20 20	$\begin{array}{c} A \\ \hline 1.56 \\ 1.52 \\ \hline \end{array}$	20 20	$\begin{matrix} A \\ 1.57 \\ 1.55 \\ 1.52 \\ 1.49 \end{matrix}$	$40 \\ 60 \\ 60 \\ 20 \\$	$\begin{array}{c} A \\ \hline 1.55 \\ 1.52 \\ \hline \\ \hline \end{array}$	8 8 	$\begin{array}{c} A \\ 1.5863 \\ 1.5516 \\ 1.5203 \\ \overline{1.4570} \end{array}$	$ \begin{array}{c} <1 \\ 11 \\ 9 \\ \hline <1 \end{array} $
$306 \\ 713 \\ 550 \\ 633 \\ 900 \\ 416$	$\left. \begin{array}{c} 1. \ 42 \\ 1. \ 397 \\ 1. \ 357 \\ \end{array} \right\} \ 1. \ 342 \\ \end{array} \right\}$		$1. 42 \\ 1. 395 \\ 1. 354 \\ 1. 341$	$ \begin{array}{r} 100\\ 20\\ 60\\ 60 \end{array} $	$ \begin{array}{r} 1. 42 \\ 1. 39 \\ 1. 37 \\ 1. 34 \end{array} $		$ \begin{array}{r} 1.42 \\ \overline{1.36} \\ 1.34 \end{array} $	$\begin{array}{c} 75\\ -\overline{25}\\ 25\\ 25\end{array}$	$\begin{array}{c} 1. \ 4475 \\ 1. \ 4205 \\ 1. \ 3937 \\ 1. \ 3656 \\ \left\{ \begin{array}{c} 1. \ 3411 \\ 1. \ 3369 \end{array} \right.$	$<\!$
$\begin{array}{c} 820 \\ 553 \\ 740 \\ 606 \\ 823 \end{array}$	1. 255 1. 233	 10 10	 1. 232	 10 	$ \begin{array}{c} \\ 1. 25\\ 1. 23\\ 1. 21 \end{array} $	20 20 20 40			$\begin{array}{c} 1.\ 3171\\ 1.\ 2716\\ 1.\ 2518\\ 1.\ 2284\\ 1.\ 2112 \end{array}$	< 1 1 1 2 4
$526 \\ 743 \\ 10 \cdot 1 \cdot 0 \\ 716 \\ 636$	$ \begin{array}{c} 1. \ 206 \\ 1. \ 165 \\ 1. \ 148 \\ \hline 1. \ 091 \end{array} $	$20 \\ 20 \\ 20 \\ 40$	$\begin{array}{c} 1. \ 201 \\ 1. \ 162 \\ 1. \ 148 \\ 1. \ 117 \\ 1. \ 090 \end{array}$	$20 \\ 20 \\ 20 \\ 40 \\ 40$	$ \begin{array}{r} 1.16\\ 1.15\\ 1.12\\ 1.09 \end{array} $	$ \begin{array}{r} 40 \\ 40 \\ 60 \\ 40 \end{array} $	$ \begin{array}{c} 1.16\\ 1.14\\ 1.11\\ 1.09 \end{array} $	 5 8 8	$\begin{array}{c} 1.\ 2106\\ 1.\ 1610\\ 1.\ 1458\\ 1.\ 1136\\ 1.\ 0862 \end{array}$	$\begin{array}{c} 4\\4\\3\\4\\1\end{array}$
$850 \\ 933 \\ 556 \\ 119 \\ 906$	1. 066 1. 056 1. 040	10 20 20 	1. 056 1. 040	20 20	$ \begin{array}{c} 1.05\\ 1.04\\ 1.02\\ 1.01 \end{array} $	$ \begin{array}{c} 40 \\ 40 \\ 20 \\ 60 \end{array} $	1. 02	 8	$\begin{array}{c} 1.\ 0629\\ 1.\ 0503\\ 1.\ 0370\\ 1.\ 0232\\ 1.\ 0147 \end{array}$	$2 \\ 2 \\ 2 \\ 1 \\ 2$
853	1. 009 (ª)	60	1. 009 (^b)	60					1. 0056	2

Zinc Orthosilicate (willemite), Zn₂SiO₄ (trigonal)—Continued

^a Seven additional lines are omitted. ^b Four additional lines are omitted.

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- W. Schütz, Die kristallchemische Verwandtschaft zwischen Germanium und Silicum, Z. physik. Chem. 31, 292-308 (1936).
- [2] C. Gottfried, Über die Struktur der Phenakit-Dioptasgruppe, Neues Jahrb. Mineral Geol., Beilage Bd. 55A, 393-400 (1927).

[3] A. Pabst, Röntgenuntersuchung über die Bildung von

[4] W. L. Bragg and W. H. Zachariasen, The crystalline structure of phenacite, Be₂SiO₄ and willemite, Zn₂SiO₄, Z. Krist. **72**, 518–528 (1930).

Zinc Sulfate (zinkosite), $ZnSO_4$ (orthorhombic)

ASTM cards

Cards numbers	Index lines	Radiation	Source
2-0274	$\begin{array}{c} 4. \ 17 \\ 3. \ 54 \\ 2. \ 65 \end{array}$	Iron	Sehiff [1] 1934.
1–1086	2. 61 4. 16 3. 53	Molyb- denum	New Jersey Zinc Co.

Additional published patterns. None.

NBS sample. The sample of zinc sulfate was obtained from Johnson, Matthey, and Co., Ltd., London. Their spectrographic analysis showed less than 0.01 percent of copper, less than 0.001 percent of magnesium and silicon, and less than 0.0001 percent of iron.

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

Interplanar spacings and intensity measure**ments.** The *d*-values reported by the New Jersey Zinc Co. were converted from kX to angstrom units, and the *d*-values of the Schiff pattern were calculated from reported Bragg angle data. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Schiff New Jersey Zinc Co National Bureau of Stand- ards.	$101 \\ 220, 121 \\ 111$	$111 \\ 101 \\ 101$	$220 \\ 111 \\ 220$

Structural data. Schiff [1] in 1934 determined that zinc sulfate has barium sulfate-type structure, the space group D_{2h}¹⁶-Pnma, and 4(ZnSO₄) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	Ь	с
1934 1936 1957	Schiff [1] Hammel [2] National Bureau of Standards.	A 8. 60 8. 53 8. 588	$\begin{matrix} A \\ 6.74 \\ 6.74 \\ 6.74 \\ 6.740 \end{matrix}$	A 4. 77 4. 72 4.770 at 25° C

The density of zinc sulfate calculated from the NBS lattice constants is 3.883 at 25° C.

References

- [1] K. Schiff, Bestimmung des Kristallsystems und der Gitterkonstanten des wasserfreien Zinksulfates, Z. Krist. 87, 379–386 (1934). [2] F. Hammel, Sur les sulfates anhydres de la série mag-
- nésienne, Compt. rend. 202, 57-59 (1936).

hkl	1934 Schiff hkl Fe,		1934 SchiffNew Jersey Zinc Co.Fe,Mo,		195 Natic Burea Stand Cu, 1.5 26°	7 onal u of ards 405 A, C	hkl		1 S Fe
	d	Ι	d	Ι	d	Ι			d
$\begin{array}{c} 200\\ 101\\ 210\\ 111\\ 020 \end{array}$	$\begin{matrix} A \\ 4.\ 25 \\ 4.\ 17 \\ 3.\ 63 \\ 3.\ 55 \\ 3.\ 38 \end{matrix}$	VW S W S .W	$ \begin{array}{c} A \\ \overline{4.17} \\ 3.62 \\ 3.54 \\ 3.38 \end{array} $		$\begin{array}{c} A \\ 4. 29 \\ 4. 17 \\ 3. 616 \\ 3. 543 \\ 3. 371 \end{array}$	$27\\82\\48\\100\\6$		$013 \\ 113 \\ 203 \\ 431 \\ 521$	A 1. 4
$220 \\ 121 \\ 301 \\ 002 \\ 221$	$\begin{array}{c} 2. \ 65 \\ 2. \ 62 \\ 2. \ 45 \\ 2. \ 38 \\ 2. \ 30 \end{array}$	s ms s m W	$\left. \begin{array}{c} 2. \ 62 \\ 2. \ 44 \\ 2. \ 37 \\ 2. \ 30 \end{array} \right.$	$ \begin{array}{r} 100 \\ 33 \\ 10 \\ 10 \\ 10 \end{array} $	$\begin{cases} 2. 650 \\ 2. 620 \\ 2. 451 \\ 2. 383 \\ 2. 316 \end{cases}$	$76 \\ 72 \\ 59 \\ 18 \\ 14$		$\begin{array}{c} 422 \\ 600 \\ 123 \\ 341 \\ 303 \end{array}$	}
$102 \\ 202 \\ 031 \\ 321 \\ 022$	 1. 98 	- - m -	2. 08 2. 03 1. 98		$\begin{array}{c} 2. \ 296 \\ 2. \ 084 \\ 2. \ 032 \\ 1. \ 984 \\ 1. \ 947 \end{array}$	$\begin{array}{c}13\\10\\4\\25\\2\end{array}$		$\begin{array}{c} 042 \\ 242 \\ 323 \\ 602 \\ 630 \\ 612 \end{array}$	 }
$302 \\ 420 \\ 222 \\ 040 \\ 501$	$ \begin{array}{c} \overline{1.81} \\ 1.77 \\ 1.69 \\ \\ \end{array} $	w w m -	$ \begin{array}{c c} \hline 1.80 \\ 1.76 \\ 1.68 \\ 1.61 \\ \end{array} $	$\begin{bmatrix} 15\\25\\13\\2\end{bmatrix}$	$\begin{array}{c} 1.\ 832\\ 1.\ 810\\ 1.\ 773\\ 1.\ 686\\ 1.\ 616 \end{array}$	$ \begin{array}{c} 2 \\ 16 \\ 32 \\ 15 \\ 3 \end{array} $		$143 \\ 523 \\ 640 \\ 702 \\ 260 \\ 224$	 } }
$132 \\ 402 \\ 511 \\ 103 \\ 430$	$\overline{1.59}$ $\overline{1.56}$	w m	$\overline{1.59}$ $\overline{1.56}$	$\overline{5}$ $\overline{23}$	$\begin{array}{c} 1,606\\ 1,5958\\ 1,5713\\ 1,5632\\ 1,5520 \end{array}$	$\begin{array}{c c}2\\10\\7\\17\\2\end{array}$		343 731 811 820	

Zinc Sulfate (zinkosite), ZnSO₄ (orthorhombic)

hkl	1934 Schiff Fe,		New Je Zinc Mo, _	- ersey Co.	1957 National Bureau of Standards Cu, 1.5405 A, 26° C			
	d	Ι	d	Ι	d	Ι		
$013 \\113 \\203 \\431 \\521$	A 1. 49 	- m -	A 1. 45	- - - 15	$\begin{matrix} A \\ 1.\ 5482 \\ 1.\ 5228 \\ 1.\ 4916 \\ 1.\ 4761 \\ 1.\ 4572 \end{matrix}$	$\begin{array}{c}2\\2\\2\\3\\19\end{array}$		
$\begin{array}{c} 422 \\ 600 \\ 123 \\ 341 \\ 303 \end{array}$	 }		${1.41}$ 1.38	- 10 15	$\begin{array}{c} 1.\ 4421\\ 1.\ 4312\\ 1.\ 4182\\ 1.\ 3899 \end{array}$	$10 \\ 6 \\ 12 \\ 14$		
$\begin{array}{c} 042 \\ 242 \\ 323 \\ 602 \\ 630 \\ 612 \end{array}$	 }	- - - -	$ 1. 28 \\ 1. 22 \\ 1. 19 $	$\begin{bmatrix} -\\ 2\\ 1\\ 1\\ 1 \end{bmatrix}$	$\begin{array}{c} 1.\ 3767\\ 1.\ 3109\\ 1.\ 2852\\ 1.\ 2274\\ 1.\ 2078 \end{array}$	$7 \\ 2 \\ 8 \\ 5 \\ 2$		
$143 \\ 523 \\ 640 \\ 702 \\ 260 \\ 224$	 }		1. 15 1. 08 	1 - 5 -	1. 1458 1. 1027 1. 0908 1. 0872	$ \begin{array}{c} 1 \\ 3 \\ 4 \\ 5 \end{array} $		
$343 \\731 \\811 \\820$					$\begin{array}{c} 1.\ 0728\\ 1.\ 0502\\ 1.\ 0349\\ 1.\ 0229 \end{array}$	$4 \\ 1 \\ 1 \\ 2$		

Zirconium Sulfate Tetrahydrate, Zr(SO₄)₂·4H₂O (orthorhombic)

ASTM cards. None. Additional published patterns

Source	Radiation	Wavelength
Staritzky and Singer [1] 1956.	Copper	1.5418 A

An unpublished pattern sent to us by L. K. Rinn of the Dow Chemical Co. has been included in the *d*-value table.

NBS sample. The sample of zirconium sulfate tetrahydrate was prepared at the NBS by W. S. Clabaugh and R. Gilchrist [2]. Chemical analysis at the NBS showed that the sample contained 0.01 percent of chloride ion and less than 0.00001 percent each of iron and copper. Spectrographic analysis showed the following impurities: 0.7 percent of hafnium; and 0.0001 to 0.001 percent each of calcium, magnesium, sodium, and silicon. The theoretical composition of this compound compares with the experimental values as follows:

Component	Theoretical	Analyzed
$\begin{array}{c} HfO_2 + ZrO_2 \\ SO_3 \\ H_2O \end{array}$		35. 0 44. 5 20. 5 100. 0

The sample is colorless and optically positive. The indices of refraction are $N\alpha = 1.618$, $N\beta = 1.646$, $N\gamma = 1.676$, and $2V \approx 70^{\circ}$.

Interplanar spacings and intensity measurements. The *d*-values reported by Staritzky and Singer and those sent by Rinn were expressed in angstrom units. The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Staritzky and Singer Rinn National Bureau of Standards	$311 \\ 311 \\ 311 \\ 311$	$331 \\ 331 \\ 331 \\ 331$	$400 \\ 400 \\ 400$

hkl	1953 Rinn hkl Cu, 1.5418		195 Starit and Si Cu, 1.54	6 zky nger 418 A	1957 National Bu- reau of Stand- ards Cu, 1.5405 A, 25° C		
	d	Ι	d	Ι	d	Ι	
$400 \\ 220 \\ 111 \\ 311 \\ 620$	$\begin{array}{c} A \\ 6.50 \\ 5.30 \\ 4.90 \\ 4.32 \\ 3.46 \end{array}$	$50 \\ 4 \\ 30 \\ 100 \\ 40$	$\begin{array}{c} A \\ 6. \ 49 \\ 5. \ 30 \\ 4. \ 90 \\ 4. \ 32 \\ 3. \ 47 \end{array}$	$\begin{array}{c ccc} A & & \\ 6. \ 49 & \ 45 \\ 5. \ 30 & \ 5 \\ 4. \ 90 & \ 25 \\ 4. \ 32 & \ 100 \\ 3. \ 47 & \ 30 \end{array}$		$44 \\ 3 \\ 27 \\ 100 \\ 37$	
	$\begin{array}{c} 3. \ 31 \\ 3. \ 23 \\ 3. \ 14 \\ 2. \ 96 \\ 2. \ 89 \end{array}$	$2 \\ 2 \\ 4 \\ 80 \\ 20$	3. 24 3. 15 2. 98 2. 91	$5 \\ 5 \\ 75 \\ 15$	3. 2383. 1482. 9772. 902	$2 \\ 5 \\ 88 \\ 19$	
$531 \\ 202 \\ 911 \\ 731 \\ 10 \cdot 2 \cdot 0$		$egin{array}{c} 6 \ 6 \ 6 \ 4 \end{array}$	2. 71 2. 50 2. 408 2. 373	$5 \\ 10 \\ 20 \\ 10$	$\begin{array}{c} 2.\ 705\\ 2.\ 495\\ 2.\ 410\\ 2.\ 368\end{array}$	6 5 6 6	
$\begin{array}{c} 422 \\ 602 \\ 622 \\ 12 \cdot 0 \cdot 0 \end{array}$	$ \Big\} 2. \ 32 \\ \Big\} 2. \ 15 $	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		2. 332 35 2. 164 5		31 7	
$151 \\ 931 \\ 11 \cdot 1 \cdot 1 \\ 351 \\ 551 \\ 242$		25 6 30	 2. 134 2. 080 1. 980 	30 5 25	2. 133 2. 080 1. 979	19 3 22	
$ \begin{array}{r} 11.3.1\\ 10.0.2\\ 751\\ 642\\ 113 \end{array} $		$-25 \\ 10 \\ 14$	1. 916 1. 894 1. 855 1. 818	<5 15 5 10	1. 893 1. 854 1. 818	12 4 8	
$\begin{array}{c} 10 \cdot 2 \cdot 2 \\ 313 \\ 660 \\ 12 \cdot 4 \cdot 0 \\ 951 \\ 513 \end{array}$	$\begin{array}{c}\\ 1. \ 76\\ 1. \ 73\\ \end{array}$	- 30 8 8			$\begin{array}{c} 1.\ 798\\ 1.\ 783\\ 1.\ 7666\\ 1.\ 7332\\ 1.\ 7190 \end{array}$	$< 1 \\ 2 \\ 18 \\ 4 \\ 4 \\ 4 $	
$13.3.1 \\ 133 \\ 333 \\ 713 \\ 12.2.2$	$\left. \begin{array}{c} 1.\ 682 \\ 1.\ 654 \\ 1.\ 637 \end{array} \right\}$	30 2 35			$ \begin{array}{c} 1. \ 6885 \\ 1. \ 6612 \\ 1. \ 6342 \end{array} $	$10 \\ 2 \\ 13$	
$\begin{array}{c} 16 \cdot 0 \cdot 0 \\ 11 \cdot 5 \cdot 1 \\ 533 \\ 10 \cdot 4 \cdot 2 \\ 371 \end{array}$	 }1. 57 	-			 1. 6202 1. 5848 1. 5632 	<1 13 5	
$\begin{array}{c c} 10 \cdot 6 \cdot 0 \\ 462 \\ 913 \\ 733 \\ 14 \cdot 2 \cdot 2 \end{array}$	}				1. 5513 1. 5400 1. 5185 1. 4875	$\begin{vmatrix} 3\\2\\-4\\<1 \end{vmatrix}$	

hkl	1953 Rinn Cu, 1.5418 A d I		195 Starit and Si Cu, 1.5	6 zky nger 418 A	1957 National Bu- reau of Stand- ards Cu, 1.5405 A, 25° C	
			d	I	<i>d</i>	Ι
13.5.1 17.1.1 933	A }	-	A 		A 1. 4590	6
	} 	-			1. 4411 1. 4160	$\frac{4}{3}$
$16 \cdot 4 \cdot 0 \\ 18 \cdot 2 \cdot 0 \\ 971$	·	-			$\begin{array}{c} 1.\ 4148 \\ 1.\ 3981 \end{array}$	$\frac{2}{3}$
$\begin{array}{c} 553\\004\end{array}$	} - 	-			$1. \ 3913 \\1. \ 3826$	$\frac{3}{2}$
17.3.1 11.3.3		-			1. 3748	< 1
$14.4.2 \\ 16.2.2$	}	-			1. 3590	3
$753 \\ 15 \cdot 5 \cdot 1 \\ 13 \cdot 1 \cdot 3 \\ 14 \cdot 6 \cdot 0$	}	-			1. 3450	1
224	}	-			1. 3379	<1
$19 \cdot 1 \cdot 1 \\ 20 \cdot 0 \cdot 0 \\ 624$		-	 		$\begin{array}{c} 1.\ 3160 \\ 1.\ 2956 \\ 1.\ 2843 \end{array}$	\leq^1_1
$15.1.3 \\ 19.3.1$	}	-			1. 2536	1
$044 \\ 13.7.1$	۱	-			1. 2491	6
$244 \\ 591 \\ 12.8.0$	} 	-			1. 2428 1. 2214 1. 2059	4
882)	-			1. 2032	< 1
$ \begin{array}{r} 10 \cdot 2 \cdot 4 \\ 791 \end{array} $	} 	-			1. 1942 1. 1940	$< 1 \\ 2$
20.4.0		-			1. 1841	<1

Structural data. Staritzky and Singer [1] in 1956 determined that zirconium sulfate tetrahydrate has the space group D_{2h}^{24} -Fddd and 8[Zr(SO₄)₂·4H₂O] per unit cell.

The unit-cell measurements reported by Staritzky and Singer are compared to the NBS values.

Lattice constants

			b	с
1956 1957	Staritzky and Singer [1]. National Bureau of Standards.	A = 26.11 = 25.92	$\begin{matrix}A\\11.\ 62\\11.\ 62\end{matrix}$	$\begin{matrix} A \\ 5.56 \\ 5.532 \text{ at} \\ 25^{\circ} \text{ C} \end{matrix}$

The density of zirconium sulfate tetrahydrate calculated from the NBS lattice constants is 2.833 at 25° C.

- E. Staritzky and J. Singr, Zirconium disulfate tetrahydrate, Zr(SO₄)₂·4H₂eO Anal. Chem. 28, 553-554 (1956).
 W. S. Clabaugh and R. Gilchrist, Method for freeing
- [2] W. S. Clabaugh and R. Gilchrist, Method for freeing zirconium of common impurities and for preparing zirconium sulfate and oxide J. Am Chem. Soc. 74, 2104 (1952).

CUMULATIVE INDEX TO VOLUMES 1, 2, 3, 4, 5, 6, AND 7 6

	Volume	Page		Volume	Page
Aluminum, Al	1	11	Calcium nitrate, Ca(NO ₃) ₂	7	14
Aluminum antimony, AlSb	4	72	Calcium oxide, CaO	. 1	43
Aluminum chloride hexahvdrate (chloralu-			Calcium sulfate (anhydrite), CaSO4	4	65
minite), AlCl ₂ ·6H ₂ O	7	3	Calcium sulfide (oldhamite), CaS	7	15
Aluminum oxide alpha (corundum) Al ₂ O ₂	2	20	Calcium tungstate (scheelite) CaWO	6	23
Aluminum oxide monohydrate alpha	_	-0	Carbon (diamond). C	2	- 5
(böhmite) AleO.H.O	, 3	38	Carium(IV) ovide (carianita) CaO.	1	56
Aluminum ovide monohydrate bete (die-	0	00	Cosium aluminum sulfate dedesehudrate	T	00
Alo HO		41	$C_{a} \Lambda (S_{a}) = 1011 O$	· · ·	05
spore), $A_{12}O_{3} \cdot \Pi_{2}O_{$	э	41	$O_{4}(SO_{4})_{2} \cdot 12 \Pi_{2}O_{2}$	0	25
Ammonium aluminum sulfate dodecany-		0	Cesium bromide, CSBr	3	49
drate, $NH_4AI(SO_4)_2 \cdot 12H_2O_{}$	6	3	Cesium chloride, CsCl	2	44
Ammonium bromide, NH ₄ Br	2	49	Cesium chloroplatinate, Cs ₂ PtCl ₆	5	14
Ammonium bromoosmate, $(NH_4)_2OsBr_{6}$	3	71	Cesium chlorostannate, Cs ₂ SnCl ₆	5	16
Ammonium chloride (sal-ammoniac), NH ₄ Cl_	. 1	59	Cesium dichloroiodide, CsICl ₂	3	50
Ammonium chloropalladite, (NH ₄) ₂ PdCl ₄	6	6	Cesium fluogermanate, Cs ₂ GeF ₆	5	17
Ammonium chloroplatinate, (NH ₄) ₂ PtCl ₆	5	3	Cesium fluoplatinate, Cs ₂ PtF ₆	6	27
Ammonium chlorostannate (NH ₄) ₂ SnCl ₆	5	4	Cesium fluosilicate, Cs ₂ SiF ₆	5	19
Ammonium chromium sulfate dodecahy-			Cesium iodide, Csl	4	47
drate, NH ₄ Cr(SO ₄) ₂ ,12H ₂ O	6	7	Cesium iron sulfate dodecahydrate		~.
Ammonium dihydrogen phosphate NH ₄ H ₂ PO ₄	4	64	$C_{s}F_{e}(SO_{t}) = 12H_{s}O_{t}$	6	28
Ammonium fluogermanate (NH ₄) ₂ GeF ₂	6	ŝ	Cosium sulfate Cs-SO	7	17
Ammonium fluogiliaato (aruptobalita)	0	0	Chromium Cr	5	20
(NH) SE	5	5	Chromium/III) avida Cr O		20
(10114) 2011 6	0	0	Characteristic char	5	22
Mill G (GO) 1911 O	C	0	Chromium sincide, Cr ₃ Si	. 0	29
$N \pi_4 Ga(SO_4)_2 \cdot 12 \pi_2 O_{$	0	9	Copper, Cu	. I	15
Ammonium iodide, NH ₄ I	4	50	Copper(1) bromide, CuBr	. 4	36
Ammonium iron sulfate dodecahydrate,			Copper(I) chloride (nantokite), CuCl	. 4	35
$N H_4 Fe(SO_4)_2 \cdot 12 H_2 O_{$	6	10	Copper(I) iodide (marshite), Cul	4	- 38
$Ammoniumnitrate(ammonia-niter), NH_4NO_3$. 7	4	Copper(I) oxide (cuprite), Cu ₂ O	2	23
Ammonium oxalate monohydrate (oxam-			Copper(II) oxide (tenorite), CuO	. 1	49
mite), $(NH_4)_2C_2O_4H_2O_{$	7	5	Copper(II) sulfide (covellite), CuS	. 4	13
Ammonium perchlorate, NH4ClO4, (ortho-			Gallium, Ga	2	9
rhombic)	7	6	Gallium antimonide, GaSb	6	30
Ammonium sulfate (mascagnite), (NH ₄) ₂ SO ₄	6	12	Gallium oxide, alpha, Ga ₂ O ₂	. 4	25
Ammonium zirconium fluoride $(NH_4)_2 ZrF_7$	Ğ	14	Germanium Ge	î	18
Antimony Sh	3	14	Germanium (IV) jodide GeL	5	25
Antimony, DD	6	16	Germanium avida GaO		51
Antimony (III) rounde, Soligeneerse Antimony (III) gulfide (stibuite) Sh.S.	5	10	Cold An	1	22
Antimony (111) sumde (submite), 50 ₂ S ₃	. J 9	21	Gold, Au	. 17	00 10
Antimony trioxide (senarmonule), SD_2O_3	3	51	Gold antimony 1:2 (aurostibite), $AuSD_{2}$	4	18
Arsenic, As	ತ	17	Gold tin 1:1, Ausn	(19
Arsenic (111) iodide, $As1_3$	6	17	Hafnium, Hf	. 3	18
Arsenic trioxide (arsenolite), As_2O_3	Ţ	51	Indium, In	. 3	12
Barium, Ba	4	7	Indium antimony, InSb	4	73
Barium carbonate (witherite), BaCO ₃	2	54	Indium oxide, In ₂ O ₃	5	26
Barium fluoride, BaF ₂	1	70	Iodic acid, HIO ₃	5	28
Barium molybdate, BaMoO ₄	7	7	Iodine, I ₂	3	16
Barium nitrate (nitrobarite), Ba(NO ₃) ₂	1	81	Iridium, Ir	4	9
Barium peroxide, BaO ₂	6	18	Iron. alpha. Fe	4	3
Barium sulfate (barite). BaSO4	3	65	Iron sulfide (pyrite), FeS ₂	5	29
Barium sulfide, BaS	7	8	Lanthanum fluoride, LaF ₂	7	21
Barium titanate, BaTiO ₂	3	45	Lanthanum oxide La.O.	3	33
Barium tungstate BaWO	7	Ĩĝ	Lanthanum oxychloride LaOCl	7	22
Barium zirconate BaZrO	5	Ř	Lord Ph	i	34
Baryllium oxida (bromallita) BaO	1	36	Lead bromide PhBr	2	47
Derymum Oxide (Dromenite), Deo	2	20	Lead profilide, 1 pp12	2	56
Dismuth, Di	6	20	Lead carbonate (cerussite), 1 b003	5	45
Dismuth (111) Iodide, Dil3	0	20	Lead chloride (cotunnite), $rbCl_{2}$	2	40
Bismuth oxychioride (bismociite), bioci	4	04	Lead fluochloride (matlockite) PDF Cl	1	10
Bismuth sulfide (bismuthinite), Bi ₂ S ₃	4	23	Lead fluoride, alpha, PDF ₂	5	31
Cadmium, Cd	3	10	Lead fluoride, beta, PbF ₂	5	33
Cadmium carbonate (otavite), CdCO ₃	7	11	Lead (II) iodide, PbI ₂	5	34
Cadmium molybdate, CdMoO ₄	6	21	Lead molybdate (wulfenite), PbMoO ₄	7	23
Cadmium oxide, CdO	2	27	Lead monoxide (litharge), PbO (red)	2	30
Cadmium selenide, CdSe, (hexagonal)	7	12	Lead monoxide (massicot), PbO (yellow)	2	32
Cadmium sulfide (greenockite), CdS	4	15	Lead nitrate, Pb(NO ₃) ₂	5	36
tri-Calcium aluminate, 3CaO·Al ₂ O ₃	5	10	Lead selenide (clausthalite), PbSe	5	- 38
Calcium carbonate (aragonite), CaCO ₂	3	53	Lead sulfate (anglesite), PbSO4	3	67
Calcium carbonate (calcite). CaCO ₂	2	51	Lead sulfide (galena), PbS	2	18
Calcium chromate. CaCrO	7	13	Lead titanate PhTiO	5	39
Calcium fluoride (fluorite) CaF.	i	69	Load tungstate (stolzite) PhWO.	7	24
Calcium hydroxide (nortlandite) Ca(OH).	ĩ	58	Lithium bromide LiBr	4	30
Calaium molybdata (nowallita) CaMoO	6	22	Lithium ablarida LiC	1	62
Calcium morybuate (powenite), Camou4	0	22	Lithium fuorido LiF	1	61
			Lithium indote LiD	7	26
6 Further work on this program is in programs, and it i	s anticipat	ted that	Lithium idate, Lito3	7	20
additional volumes will be issued. Therefore, the accum	ulative inc	lex here	Lithium nitrate, LINO ₃	1	21
is not necessarily the concluding index for the project			Magnesium, Mg	1	10

additional volumes will be issued. Therefore, the accumulative index here is not necessarily the concluding index for the project.
	volume	1 age
Magnesium aluminate (spinel) MgAl ₂ O ₄	2	35
Magnesium aanhanata (magnagita) MaCO	7	00
Magnesium carbonate (magnesite), $MgCO_{3-}$	4	28
Magnesium fluoride (sellaite), MgF ₂	4	- 33
Magnesium hydroxide (brucite), Mg (OH).	6	- 30
Magnosium avido (norielezo) MgO	1	97
Magnesium oxide (periciase), MgO	Ţ	31
Magnesium silicate (enstatite), $MgSiO_{3}$	6	-32
Magnesium silicate (forsterite), Mg ₂ SiO ₄	1	83
Magnasium sulfate hantahydrate (ansomite)	-	00
Magnesium sunate neptanyurate (epsonite),	_	00
$MgSO_4 \cdot I H_2O_{$	(30
Magnesium sulfide, MgS	7	- 31
Magnesium tin Mg.Sn	5	41
Magnesium tit, Mg2011	្ទ	11
Magnesium titanate (geikielite), $Mg11O_{3}$	Э	43
Magnesium tungstate, MgWO ₄	1	84
Manganese (II) carbonate (rhodochrosite)		
Maco	7	20
MINCO3-	4	32
Manganese (11) oxide (manganosite), MnO_	5	45
Manganese sulfide, alpha (alabandite), q-		
Mng	4	11
MIND	4	11
Mercury (1) bromide, Hg_2Br_2	7	- 33
Mercury (I) chloride (calomel), Hg ₂ Cl ₂	1	72
Moreury (II) chlorido HaCl	1	72
Mercury (11) chloride, fig 012	1	10
Mercury (11) cyanide, $Hg(CN)_{2}$	6	- 35
Mercury (I) iodide, HgI	4	49
Moreury (II) jodido Hal	ĩ	74
Mercury (II) Ioulde, Iigi2	1	14
Mercury (11) oxide (montroydite), HgO	3	-35
Mercury (II) selenide (tiemannite), HgSe	7	35
Noodymium oxido Nd O	Å	96
Neouyinnun Oxide, Nu_2O_3	4	- 40
Nickel, Ni	1	13
Nickel (II) oxide (bunsenite), NiO	1	47
Nickel gulfate herebydrate NiSO 6H O	7	26
Nickel sulfate nexallyulate, NiSO4.01120		30
Osmium, Os	4	8
Palladium, Pd	1	21
Palladium oxida PdO	A	27
Di ti Di	1	01
Platinum, Pt	T	31
Potassium aluminum sulfate dodecahydrate.		
KA1(SO.). 19H.O	6	36
$\mathbf{R}_{11}(004) = 1211_{20}$	e e e e e e e e e e e e e e e e e e e	00
Potassium bromate, KBrO ₃		38
Potassium bromide, KBr	1	66
Potassium chloride (sylvite) KCl	1	65
D (in 11 a mlati ata K DtOl	÷	40
Potassium chloroplatinate, K ₂ PtOl ₆	Э	49
Potassium chlorostannate K ₂ SnCl ₆	6	- 38
Potassium chromium sulfate dodecabydrate		
$IO_{-}(O_{-})$ 1011 ()	C	20
$ROr(SO_4)_2 \cdot 12H_2O_{$	ō	39
Potassium cyanate, KCNO	7	-39
Potassium evanide KCN	1	77
Detersions dihudronen nhaanhata VU DO	5	60
Potassium dinydrogen phosphate, KH ₂ PO ₄	3	09
Potassium fluogermanate, K_2GeF_{6}	6	41
Potassium fluoplatinate, K ₂ PtF ₆	6	42
Potessium fluorido KF	ĭ	64
Fotassium nuoride, AF	Ť	04
Potassium fluosilicate (hieratite), K_2SiF_{6}	ъ	50
Potassium fluotitanate, K ₂ TiF ₆	7	40
Potessium iodide KI	i	69
D / ! I I I I I I I I I I I I I I I I I I	-	41
Potassium metaperiodate, $IXIO_{4}$	6	41
Potassium nitrate (niter), KNO ₃	3	58
Potassium perchlorate KClO	6	43
Potossium perenerate VM-0	7	49
Potassium permanganate, KMnO ₄	(42
Potassium sulfate (arcanite), K ₂ SO ₄	3	62
Potassium zine fluoride, KZnF ₂	5	51
Prozoodumium fluorido DrF	Ĕ	50
Traseodymnum nuoride, TTF3	0	04
Rhenium, Re	2	13
Rhodium, Rh	3	9
Rubidium aluminum sulfate dedeeshudrate	0	v
DI ALCON 1011 O	0	
$RbAI(SO_4) \sim 12H \sim 0$	6	44
Rubidium bromide, RbBr	7	43
Rubidium chloride RhCl	4	41
Dabidian allowalstin to DI D(C)	4	11
Rubidium chloroplatinate, Rb ₂ PtCl ₆	Э	53
Rubidium chlorostannate, Rb ₂ SnCl ₆	6	46
Rubidium chromium sulfate dodecabydrate		
DhCr(CO) 1911 O	C	17
$ROUT(SU_4)_2 \cdot 12H_2U_{$	0	47
Rubidium fluoplatinate, Rb ₂ PtF ₆	6	48
Rubidium fluosilicate Rh.SiF.	6	40
Dubidium iodide DhI	4	12
Rubidium iodide, Rb1	4	43
Ruthenium, Ru	4	5
Scandium oxide, Sc.O.	3	27
Solonium So	E	54
belemum, be	9	04

	volume	Page
Selenium diavide (selenalite) SeQ.	1	50
Cilian Ci	1	- 33
Silicon, Si	2	6
Silicon dioxide (alpha or low quartz), SiO_{2}	3	24
Silicon dioxide (alpha or low cristobalite)		
Sio	1	
	1	- 39
Silicon dioxide (beta or high cristobalite),		
SiO_2	1	42
Silver Ag	1	
Silver engenete Ar AgO	Ê	20
Silver alsenate, Aganso4	5	90
Silver bromate, AgBrO ₃	5	57
Silver bromide (bromyrite), AgBr	4	46
Silver chlorate, AgClO ₂	7	44
Silver chloride (cerergyrite) Ag(1	4	4.4
Cilian and halfs An MaO	14 17	44
Silver molybdate, Ag ₂ MoO ₄		45
Silver nitrate, AgNO ₃	5	-59
Silver nitrite, AgNO ₂	5	60
Silver (ID) oxynitrate Ag-O.NO.	4	61
Silver phembers Ar DO	Ţ	01
Silver phosphate, Ag ₃ r O ₄	5	02
Silver sulfate, Ag ₂ SO ₄	7	-46
Sodium acid fluoride, NaHF ₂	5	63
Sodium bromate NaBrO ₂	5	65
Sodium bromido NaBr	2	47
d l' ll A Man	3	41
Sodium chlorate, NaClO ₃	3	51
Sodium chloride (halite), NaCl	2	41
Sodium evanide, NaCN (cubic)	1	78
Sodium evanide NaCN (orthorhombia)	î	70
Sodium fuorido (villioumita) N-E	1	19
Sodium nuoride (vinaumite), NaF	1	63
Sodium iodate, NaIO ₃	7	47
Sodium iodide, NaI	4	31
Sodium metaperiodate NaIO	7	48
Sodium nitrato (godo nitor) NoNO	c .	10
Sodium mitrate (soda-inter), NanO ₃	0	50
Sodium nitrite, NaNO ₂	4	62
Sodium perchlorate, NaClO ₄ , (orthorhom-		
bic)	7	49
Sodium sulfate (thenardite). Na ₂ SO ₄	2	59
Sodium sulfite Na.SO.	2	60
$S \neq a = t + i = b = a = i d = b = b = d = t$	9	00
Strontium bromide nexanydrate,		
$\mathrm{SrBr}_{2}\cdot\mathrm{6H}_{2}\mathrm{O}$	4	60
Strontium carbonate (strontianite) $SrCO_{3}$	3	56
Strontium chloride, SrCl ₂	4	40
Strontium chloride beyabydrate SrCl.		- 0
6H.O	А	59
Oli 20	4	00
Strontium nuoride, SFF 2	5	01
Strontium molybdate, SrMoO ₄	7	50
Strontium nitrate, Sr(NO ₃) ₂	1	80
Strontium oxide SrO	5	68
Strontium penavida SnO	c C	500
Strontium peroxide, SrO ₂	0	02
Strontium sulfate (celestite), $SrSO_{4}$	2	61
Strontium sulfide, SrS	7	-52
Strontium titanate, SrTiO ₂	3	44
Strontium tungstate SrWO.	7	53
Sulfamia and NIL CO	:-	50
Sunamic aciu, NII 3003	1	04
Tantalum, Ta	1	29
Tellurium, Te	1	26
Tellurium (IV) oxide, TeO ₂ (tetragonal)	7	56
Thellium eluminum sulfate dodeeehydrate		
TIAL(SO), 19U O	G	5.0
$\Pi AI(SO_4) 2 \cdot 12 \Pi 2 O_{}$	ō	- 23
Thallium bromide, TIBr	1	57
Thallium (I) chloride, TlCl	4	51
Thallium chloroplatinate, Tl ₂ PtCl ₆	5	70
Thallium chlorostannate Tl.SnCl.	6	54
Thallium abromium culfate dedeeshedret	U	04
Tion (SO) 1911 O	0	
$\Pi Or(SO_4)_2 \cdot 12H_2O_{$	0	55
Thallium fluosilicate, Tl ₂ SiF ₆	6	56
Thallium gallium sulfate dodecahvdrate.		
$TIGa(SO_4) = 12H_2O_1$	6	57
Thallium (I) iodide TIL (orthorhombic)	4	53
Thallium (I) nitrate (III, (Orthornomole)	4	00
Thanium (1) nitrate, TINO ₃	6	58
Thallium (III) oxide, Tl_2O_{3}	2	28
Thallium (I) phosphate, Tl ₃ PO ₄	7	58
Thallium (III) phosphate. TIPO.	7	59
Thallium (I) sulfate TLSO	6	50
Thorium orido (thoria-ita) Tho	1	59
Thorium oxide (thorianite), InO_{2}	1	01
Tin, alpha, Sn	2	12
Tin, beta, Sn	1	24

	Volume	Page
Tin (IV) iodide, SnI ₄	5	71
Tin (II) oxide, SnO	4	28
Tin (IV) oxide (cassiterite), SnO ₂	1	54
Tin (II) telluride, SnTe	7	61
Titanium, Ti	3	1
Titanium dioxide (anatase), TiO ₂	1	46
Titanium dioxide (rutile), TiO ₂	1	44
Tungsten, W	1	28
Uranium dioxide, UO ₂	2	- 33
Urea, $CO(NH_2)_{2}$	7	61
Yttrium, oxide, Y ₂ O ₃	3	28
Zinc, Zn	1	16
Zinc aluminate (gahnite), ZnAl ₂ O ₄	2	- 38
Zinc borate, ZnB ₂ O ₄	1	83

	volume	Page
Zinc cyanide, Zn (CN) ₂	5	73
Zinc fluoride, ZnF ₂	6	60
Zinc orthosilicate (willemite), Zn ₂ SiO ₄	7	62
Zinc oxide (zincite), ZnO	2	25
Zinc pyrosilicate hydrate (heminorphite),		
$Zn_4(OH)_2Si_2O_7 \cdot H_2O_1$	2	62
Zinc senenide, ZnSe	3	23
Zinc sulfate (zinkosite), ZnSO ₄	7	64
Zinc sulfide, alpha (wurtzite), ZnS	2	14
Zinc sulfide, beta (sphalerite), ZnS	2	16
Zirconium alpha, Zr	2	11
Zirconium silicate (zircon), ZrSiO ₄	4	68
Zirconium sulfate tetrahydrate,		
$Zr(SO_4)_2 \cdot 4H_2O_{$	7	66

THE NATIONAL BUREAU OF STANDARDS

The scope of activities of the National Bureau of Standards at its headquarters in Washington, D. C., and its major field laboratories in Boulder, Colorado, is suggested in the following listing of the divisions and sections engaged in technical work. In general, each section carries out specialized research, development, and engineering in the field indicated by its title. A brief description of the activities, and of the resultant publications, appears on the inside front cover.

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Electricity and Electronics. Resistance and Reactance. Electron Devices. Electrical Instruments. Magnetic Measurements. Dielectrics. Engineering Electronics. Electronic Instrumentation. Electrochemistry.

Optics and Metrology. Photometry and Colorimetry. Optical Instruments. Photographic Technology. Length. Engineering Metrology.

Heat and Power. Temperature Physics. Thermodynamics. Cryogenic Physics. Rheology. Engine Fuels. Free Radicals Research.

Atomic and Radiation Physics. Spectroscopy. Radiometry. Mass Spectrometry. Solid State Physics. Electron Physics. Atomic Physics. Neutron Physics. Nuclear Physics. Radioactivity. X-rays. Betatron. Nucleonic Instrumentation. Radiological Equipment. AEC Radiation Instruments.

Chemistry. Organic Coatings. Surface Chemistry. Organic Chemistry. Analytical Chemistry. Inorganic Chemistry. Electrodeposition. Gas Chemistry. Physical Chemistry. Thermochemistry. Spectrochemistry. Pure Substances.

Mechanics. Sound. Mechanical Instruments. Fluid Mechanics. Engineering Mechanics. Mass and Scale. Capacity, Density, and Fluid Meters. Combustion Controls.

Organic and Fibrous Materials. Rubber. Textiles. Paper. Leather. Testing and Specifications. Polymer Structure. Plastics. Dental Research.

Metallurgy. Thermal Metallurgy. Chemical Metallurgy. Mechanical Metallurgy. Corrosion. Metal Physics.

Mineral Products. Engineering Ceramics. Glass. Refractories. Enameled Metals. Concreting Materials. Constitution and Microstructure.

Building Technology. Structural Engineering. Fire Protection. Air Conditioning, Heating, and Refrigeration. Floor, Roof, and Wall Coverings. Codes and Specifications. Heat Transfer.

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Data Processing Systems. SEAC Engineering Group. Components and Techniques. Digital Circuitry. Digital Systems. Analog Systems. Application Engineering.

• Office of Basic Instrumentation

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Cryogenic Engineering. Cryogenic Equipment. Cryogenic Processes. Properties of Materials. Gas Liquefaction.

Radio Propagation Physics. Upper Atmosphere Research. Ionospheric Research. Regular Propagation Services. Sun-Earth Relationships.

Radio Propagation Engineering. Data Reduction Instrumentation. Modulation Systems. Navigation Systems. Radio Noise. Tropospheric Measurements. Tropospheric Analysis. Radio Systems Application Engineering.

Radio Standards. High Frequency Electrical Standards. Radio Broadcast Service. High Frequency Impedance Standards. Calibration Center. Microwave Physics. Microwave Circuit Standards.

