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VOLUME 7

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

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Standard X-ray Diffraction Powder Patterns

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

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Contents

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[$(NH_4)_2GeF_6$] per rhombohedral cell.
Page 27, under Structural data, delete 3(Cs_2PtF_6) per unit rhombohedral cell.
Page 31, under Structural data, delete 3[$Mg(OH)_2$] per unit rhombohedral cell.
Page 41, under Structural data, space group D^3z should read $D^{33}z$-, delete 3(K_2GeF_6) per unit rhombohedral cell.
Page 48, under Structural data, delete 3(Rb_2PtF_6) per unit rhombohedral cell.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. 7—Data for 53 Substances

Howard E. Swanson, Nancy T. Gilfrich,[1] and Marlene I. Cook [1]

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, comparison 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 calculated 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, $AuSb_2$, AuSn, 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, $NaIO_3$, $NaIO_4$, $NaClO_4$, $SrMoO_4$, SrS, $SrWO_4$, NH_3SO_3, TeO_2, TlBr, Tl_3PO_4, $TlPO_4$, 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 program [2] 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 Diffraction 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 *d*-values and intensities.

NBS sample. Many of the samples used to make the NBS patterns were special preparations (of exceptionally high purity) obtained or prepared 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 determination. Another excellent check of phase-purity 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

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[1] 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 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 large-angle 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 unit-cell 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.

References

[1] Cumulative alphabetical and grouped numerical index 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, 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), $AlCl_3 \cdot 6H_2O$ (trigonal)

ASTM Cards

Card number	Index lines	Radiation	Source
1–0682	3. 29 2. 30 2. 05	Molybdenum	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.	113, 122	321	134
National Bureau of Standards.	113	122	321

Lattice constants. Andress and Carpenter [2] in 1934 determined that aluminum chloride hexahydrate has chromium chloride hexahydrate-type structure, the space group D_{3d}^6–$R\bar{3}c$, 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.

Lattice constants

		a	*c*
		A	*A*
1934	Andress and Carpenter[2]	11. 78	11. 84
1957	National Bureau of Standards.	11. 831	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 Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
110	6. 0	17	5. 95	26
012	5. 2	20	5. 14	26
202	3. 90	13	3. 89	40
211	3. 70	27	3. 68	37
300	3. 42	11	3. 416	25
113	3. 30	100	3. 297	100
122			3. 246	57
220	2. 96	12	2. 949	13
131	2. 76	11	2. 764	40
312	2. 57	40	2. 565	27
321	2. 30	53	2. 308	48
232	2. 18	27	2. 188	15
134	2. 05	53	2. 056	20
125	1. 99	8	2. 030	8
006			1. 985	6
413	1. 94	27	1. 948	14
404			1. 941	15
422	------	----	1. 842	1
511	1. 82	8	1. 818	3
152	1. 76	27	1. 758	9
054	1. 68	13	1. 688	1
235			1. 673	4
226	1. 65	11	1. 648	4
244	------	----	1. 623	<1
514	------	----	1. 5664	<1
161	------	----	1. 5487	2
523	1. 51	11	1. 5158	2
416	1. 478	17	1. 4839	2
440			1. 4801	3
434			1. 4660	2
155	------	----	1. 4566	1
072	------	----	1. 4215	<1
621	1. 415	11	1. 4106	<1
336	------	----	1. 3996	<1
262	1. 383	13	1. 3819	<1
327	------	----	1. 3789	<1
170	1. 358	5	1. 3573	1
318	1. 319	9	1. 3184	<1
354	------	----	1. 3139	<1
713	1. 293	5	1. 2843	1
526	------	----	1. 2648	<1
633	1. 227	13	1. 2274	3
722	------	----	1. 2247	2

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] K. R. Andress and C. Carpenter, Kristallhydrate. II. Die Struktur von Chromiumchlorid und Aluminumchlorid hexahydrat, Z. Krist. **87**, 446–463 (1934).

Ammonium Nitrate (form IV) (ammonia-niter), NH_4NO_3 (orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–0809	3. 09 2. 72 2. 25	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
3–1239	[a]	[a]	West [2] 1932.

[a] 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 $2V\cong35°$.

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	111	020	112, 210
National Bureau of Standards.	111	020	011

Structural data. West [2] in 1932 determined that the orthorhombic form of ammonium nitrate has the space group D_{2h}^{13}–Pnmm, and $2(NH_4NO_3)$ per unit cell. Ammonium nitrate is used as a structure-type. This form is the IV modification which is stable from −18° to +32° 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

[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] 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*	*c*
		A	*A*	*A*
1932	West [2]	4. 938	5. 449	5. 744
1932	Hendricks, Posnjak, and Kracek [3].	4. 97	5. 46	5. 76
1957	National Bureau of Standards.	4. 942	5. 438	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), NH_4NO_3 (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
100	4. 94	40	4. 95	45
011	3. 96	50	3. 96	67
110	-----	-----	3. 66	1
111	3. 10	100	3. 087	100
002	2. 87	5	2. 879	10
020	2. 73	75	2. 722	75
102	2. 48	13	2. 485	10
120	2. 38	10	2. 380	8
112	2. 25	75	2. 260	44
210			2. 249	1
211	2. 10	5	2. 094	2
022	1. 97	5	1. 978	4
122	1. 83	5	1. 835	1
103	1. 78	6	1. 786	4
212	-----	-----	1. 769	<1
031	1. 73	5	1. 730	3
131	1. 63	9	1. 631	5
310	1. 57	10	1. 578	5
303	1. 51	10	1. 513	1
123	1. 498	10	1. 492	2
132	1. 467	15	1. 464	1
230			1. 461	2
004	1. 433	5	1. 434	<1
302			1. 423	1
312	-----	-----	1. 383	<1
104	-----	-----	1. 380	1

Ammonium Oxalate Monohydrate (oxammite), $(NH_4)_2C_2O_4 \cdot H_2O$ (orthorhombic)

ASTM cards

Cards numbers	Index lines	Radiation	Source
1–0825	3. 06 2. 67 3. 81	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
5–0192*	6. 37 2. 88 2. 68	--------	Winchell and Benoit [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 $2V \cong 60°$.

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	021	211	001
Winchell and Benoit	211	230	110
National Bureau of Standards	211	110	021

Structural data. Hendricks and Jefferson [3] in 1936 determined that ammonium oxalate monohydrate had the space group D_2^3–$P2_12_12$ and $2[(NH_4)_2C_2O_4 \cdot H_2O]$ 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

		a	*b*	*c*
		A	*A*	*A*
1926	Wood [4]	8. 08	10. 36	3. 83
1936	Hendricks and Jefferson [3].	8. 06	10. 29	3. 83
1957	National Bureau of Standards.	8. 035	10. 31	3.801 at 25°C

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

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1951 Winchell and Benoit ----		1957 National Bureau of Standards Cu, 1·5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
110	6. 3	60	6. 46	80	6. 32	99
020	5. 1	10	-------	------	5. 15	37
120	-------	-----	-------	------	4. 23	10
200	-------	-----	-------	------	4. 02	3
001	3. 82	80	3. 83	70	3. 80	72
210	-------	-----	-------	------	3. 74	9
011	3. 58	10	-------	------	3. 564	15
101	3. 44	10	3. 49	------	3. 437	16
111	3. 27	60	3. 29	60	3. 256	60
130	-------	-----	-------	------	3. 158	3
021	3. 07	100	3. 07	60	3. 057	95
121	2. 87	80	2. 88	60	2. 858	60
----	2. 77	10	-------	------	-------	------
211	2. 68	100	2. 68	100B	2. 666	100
230	2. 59	60	2. 62	100B	2. 606	50
310					2. 592	43
140	2. 43	60	2. 47	60B	2. 453	33
131					2. 429	27
320	2. 36	60	2. 40	60B	2. 374	26
240	-------	-----	-------	------	2. 169	7
311	2. 14	30	2. 16	50	2. 142	23
330	-------	-----	-------	------	2. 113	1
141	-------	-----	-------	------	2. 061	2
321	2. 01	20	2. 02	30	2. 014	10
400	-------	-----	-------	------	2. 008	1
420	1. 86	20	1. 89	40B	1. 871	6
331	-------	-----	1. 84	40B	1. 846	6
250	1. 82	20	-------	------	1. 836	9
112	-------	-----	-------	------	1. 822	5
022	-------	-----	-------	------	1. 784	1
151	-------	-----	-------	------	1. 768	1
411	-------	-----	1. 75	20	1. 750	1
122	-------	-----	-------	------	1. 739	1
430	-------	-----	1. 69	10	1. 735	1
212	-------	-----	-------	------	1. 696	1
160	-------	-----	-------	------	1. 680	1
341	-------	-----	-------	------	1. 668	1
061	-------	-----	-------	------	1. 565	1
161	-------	-----	-------	------	1. 536	3
232						
142	-------	-----	-------	------	1. 502	2
501	-------	-----	-------	------	1. 483	2
441	-------	-----	-------	------	1. 463	3
332	-------	-----	-------	------	1. 413	2

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] H. Winchell and R. J. Benoit, Taylorite, mascagnite, aphthitalite, lecontite, and oxammite from guano, Am. Mineralogist **36**, 590–602 (1951).

[3] S. B. Hendricks and M. E. Jefferson, Electron distribution in $(NH_4)_2C_2O_4 \cdot H_2O$ and the structure of the oxalate group, J. Chem. Phys. **4**, 102–107 (1936).

[4] J. F. Wood, The crystal structure of some oxalates, Proc. Univ. Durham Phil. Soc. **7**, 111–116 (1926).

Ammonium Perchlorate, NH_4ClO_4 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0315	4. 61 3. 60 3. 25	Molybde-num.	Hanawalt, Rinn, and Frevel [1] 1938.

ASTM card 2–0232 gives a cubic pattern for NH_4ClO_4 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 $2V \cong 70°$.

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	011	210	211
National Bureau of Standards	011	210	211

Structural data. Büssem and Herrmann [2] in 1930 determined that ammonium perchlorate has barium sulfate-type structure, the space group D_{2h}^{16}–Pnma, and $4(NH_4ClO_4)$ 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 constants

		a	*b*	*c*
		A	*A*	*A*
1928	Bussem and Herrmann [5].	9. 24	5. 81	7. 43
1932	Gottfried and Schusterius [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.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
101	5. 8	16	5. 80	26
011	4. 62	100	4. 58	100
201	3. 94	30	3. 922	43
002	3. 71	30	3. 724	33
210	3. 61	60	3. 611	61
102	-------	----	3. 455	9
211	3. 26	60	3. 249	51
112	2. 98	60	2. 970	42
202	2. 91	40	2. 899	26
121 212	2. 61	40	2. 595	29
311	-------	----	2. 552	3
302	-------	----	2. 374	3
221	-------	----	2. 334	1
400	-------	----	2. 305	3
122	-------	----	2. 243	1
401	2. 21	35	2. 205	12
312	-------	----	2. 191	16
222	-------	----	2. 054	<1
213	-------	----	2. 047	3
402	-------	----	1. 961	1
303	-------	----	1. 933	1
412	-------	----	1. 859	12
123	1. 85	20	1. 850	12
313	-------	----	1. 834	4
421	-------	----	1. 756	<1
114	-------	----	1. 742	2
403 132	1. 68	25	1. 690	11
323 232	1. 60	2	1. 611	3
124	-------	----	1. 546	1
600 314	1. 54	2	1. 538	3
431	1. 45	8	1. 4562	5
513	-------	----	1. 4361	2
602	-------	----	1. 4217	1
414	-------	----	1. 4076	1
324	1. 395	6	1. 3977	4
432	-------	----	1. 3792	1
333	1. 365	2	1. 3680	2
134	-------	----	1. 3287	2
523	-------	----	1. 3206	1
504	1. 314	4	1. 3112	1
---	1. 214	2	-------	----

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Barium Molybdate, $BaMoO_4$ (tetragonal)

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	Kα

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	112	200	204
Zambonini and Levi	112	204	116
National Bureau of Standards	112	204	200

Structural data. Vegard and Refsum [2] in 1928 determined that barium molybdate has calcium tungstate-type structure, the space group C_{4h}^6–$I4_1/a$, 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, $BaMoO_4$ (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	*I*	*d*	*I*	*d*	*I*
	A		A		A	
101	----	---	-----	---	5. 11	2
112	3. 37	100	3. 26	vs	3. 357	100
004	3. 21	40	3. 15	vw	3.202	20
200	2. 80	50	2. 72	w	2. 789	24
202	----	---	-----	---	2. 557	3
114	----	---	-----	---	2. 4866	3
211	2. 45	10	-----	---	2. 4492	3
105	2. 33	10	-----	---	2. 3293	2
213	----	---	-----	---	2. 1537	3
204	2. 10	50	2. 08	s	2. 1035	30
220	1. 97	30	-----	---	1. 9721	10
116	1. 88	40	1. 863	s	1. 8779	18
312	1. 70	40	1. 693	s	1. 7007	23
224	1. 68	30	1. 679	m	1. 6797	12
008	----	---	-----	---	1. 6024	2
400	1. 39	10	1. 392	m	1. 3946	2
208	----	---	-----	---	1. 3899	7
316	1. 36	20	1. 364	ms	1. 3606	10
332	1. 28	10	1. 290	m	1. 2885	3
404	----	---	-----	---	1. 2795	3
420	1. 24	10	1. 252	m	1. 2478	3
228	----	---	-----	---	1. 2444	5
1·1·10	----	---	-----	---	1. 2195	4
424	----	---	1. 170	ms	1. 1631	4
336	----	---	1. 126	mw	1. 1201	4
512	----	---	1. 085	s	1. 0788	4
0·0·12	----	---	-----	---	1. 0688	5
408	----	---	1. 043	vw	1. 0523	3
3·1·10	----	---	-----	---	1. 0373	2
2·0·12	----	---	0. 991	w	0. 9978	4
440	----	---	. 983	w	. 9865	2
428					. 9846	3
516	----	---	-----	---	. 9741	3
532	----	---	. 952	ms	. 9465	2
444	----	---	-----	---	. 9427	3
2·2·12	----	---	-----	---	. 9395	2
600	----	---	-----	---	. 9301	<1
3·3·10	----	---	-----	---	. 9181	1
604	----	---	. 901	mw	. 8930	3
1·1·14	----	---	. 890	vw	. 8920	1
620	----	---	-----	---	. 8823	1
622	----	---	-----	---	. 8735	4
536						
624	----	---	. 858	m	. 8508	<1
4·0·12	----	---	. 847	w	. 8484	3
448	----	---	. 840	m	. 8401	2
5·1·10	----	---	-----	---	. 8324	4

Lattice constants

		a	*c*
		A	*A*
1925	Zambonini and Levi [3]	5. 61	12. 89
1928	Vegard and Refsum [2]	5. 567	12. 781
1957	National Bureau of Standards.	5. 5802	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	3. 18 2. 25 3. 67	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Holgersson [2] 1923	Copper	K_α

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 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	200	220	111
Holgersson	200	220	420
National Bureau of Standards	200	220	111

Structural data. Holgersson [2] in 1923 determined that barium sulfide has sodium chloride-type structure, the space group O_h^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.

Lattice constants

		A
1923	Holgersson [2]	6.359
1927	Goldschmidt [3]	6.381
1956	Güntert and Faessler [4]	6.3877 at 21° C
1957	National Bureau of Standards.	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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Barium Sulfide, BaS (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1923 Holgersson Cu, 1.5418 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	3. 68	53	6. 37	3. 65	w	6. 32	3. 688	72	6. 388
200	3. 19	100	6. 38	3. 16	vs	6. 32	3. 194	100	6. 388
220	2. 25	83	6. 36	2. 24	vs	6. 34	2. 258	80	6. 387
-----	--------	--	--------	2. 08	s	--------	--------	--	--------
311	1. 91	40	6. 33	1. 90	m	6. 30	1. 9258	40	6. 387
222	1. 83	27	6. 34	1. 82	s	6. 30	1. 8433	27	6. 384
400	1. 59	15	6. 36	--------	--	--------	1. 5970	14	6. 388
331	1. 463	11	6. 377	1. 46	m	6. 36	1. 4652	12	6. 387
420	1. 424	45	6. 368	1. 42	vs	6. 35	1. 4285	33	6. 388
422	1. 302	25	6. 378	1. 30	vs	6. 37	1. 3037	22	6. 387
511	1. 227	10	6. 376	1. 22	m	6. 34	1. 2291	10	6. 387
440	1. 127	5	6. 375	1. 125	m	6. 364	1. 1286	6	6. 384
531	1. 078	5	6. 378	1. 073	m	6. 348	1. 0801	8	6. 381
600	1. 063	8	6. 378	1. 060	s	6. 360	1. 0641	13	6. 385
620	1. 007	4	6. 369	1. 006	m	6. 363	1. 0094	9	6. 384
533	--------	--	--------	--------	--	--------	0. 9734	5	6. 383
622	0. 962	4	6. 381	0. 9592	s	6. 363	. 9627	8	6. 386
444	--------	--	--------	. 9180	w	6. 360	. 9217	<1	6. 386
711	. 893	1	6, 377	. 8914	m	6. 366	. 8941	6	6. 385
640	. 885	1	6. 381	. 8819	m	6. 359	. 8856	7	6. 386
642	. 853	5	6. 383	. 8503	vs	6. 363	. 8534	12	6. 386
731	. 831	1	6. 383	. 8288	s	6. 366	. 8313	8	6. 385
800	--------	--	--------	. 7958	w	6. 366	. 7984	<1	6. 387
Average of last five lines--			6. 381	--------	--	6. 364	--------	--	6. 386

Barium Tungstate $BaWO_4$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0658	3. 34 2. 08 1. 70	Molybdenum.	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	112	204	312
National Bureau of Standards	112	204	312

Structural data. Navarro and Palacios [2] in 1929 determined that barium tungstate has calcium tungstate-type structure, the space group C_{4h}^6–$I4_1/a$, and 4($BaWO_4$) per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1928	Vegard and Refsum [3]	5. 60	12. 71
1931	Navarro and Palacios [2]	5. 65	12. 72
1931	Aanerud [4]	5. 60	12. 74
1932	Jimenez [5]	5. 65	12. 72
1957	National Bureau of Standards.	5. 6134	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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[2] I. Navarro and J. Palacios, Crystalline structure of barium tungstate II, Anal. soc. españ. fís. quím. **29**, 21–32 (1931).

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Barium Tungstate, $BaWO_4$ (tetragonal)

hkl	New Jersey Zinc 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	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
101	5. 05	4	---	-	5. 13	7
112	3. 34	100	3. 39	-	3. 367	100
004	3. 14	30	3. 20	-	3. 178	23
200	2. 78	26	2. 82	-	2. 805	31
114	--	-	2. 48	-	2. 483	1
211	--	-	---	-	2. 464	2
204	2. 08	50	2. 11	-	2. 104	33
220	1. 97	14	1. 99	-	1. 985	14
116	1. 85	30	1. 880	-	1. 870	24
215	--	-	1. 787	-	1. 787	1
312	1. 68	50	1. 706	-	1. 710	32
206	--	-	---	-	1. 6908	2
224	1. 67	10	1. 685	-	1. 6836	16
008	1. 58	4	---	-	1. 5898	3
---	--	-	1. 485	-	----	--
400	--	-	---	-	1. 4037	4
208	1. 37	6	---	-	1. 3835	7
316	1. 35	20	---	-	1. 3611	13
332	1. 28	8	---	-	1. 2955	7
404			---	-	1. 2840	6
420	1. 25	8	---	-	1. 2553	5
228	1. 23	8	---	-	1. 2411	7
1·1·10	1. 20	12	---	-	1. 2114	4
424	1. 16	16	---	-	1. 1677	6
336	1. 12	4	---	-	1. 1226	3
512	1. 08	10	---	-	1. 0849	3
0·0·12	--	-	---	-	1. 0603	<1
408	1. 05	6	---	-	1. 0523	2
3·1·10	1. 03	10	---	-	1. 0340	3
440	--	-	---	-	0. 9927	1
2·0·12	--	-	---	-	. 9915	1
428	--	-	---	-	. 9852	3
516	--	-	---	-	. 9771	2
532	--	-	---	-	. 9520	3
444	--	-	---	-	. 9473	2
600	--	-	---	-	. 9358	2
2·2·12	--	-	---	-	. 9350	3
3·3·10	--	-	---	-	. 9171	2
604	--	-	---	-	. 8978	3
620	--	-	---	-	. 8877	2
1·1·14	--	-	---	-	. 8856	3
536	--	-	---	-	. 8766	5
624	--	-	---	-	. 8550	3
4·0·12	--	-	---	-	. 8460	3
448	--	-	---	-	. 8419	3
5·1·10	--	-	---	-	. 8325	4
4·2·12	--	-	---	-	. 8099	1
3·1·14	--	-	---	-	. 8088	4
608	--	-	---	-	. 8065	3
712	--	-	---	-	. 7879	7

Cadmium Carbonate (otavite), $CdCO_3$ (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	104	018, 116	112
National Bureau of Standards.	104	012	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–$R\bar{3}c$ with $2(CdCO_3)$ per unit rhombohedral cell or $6(CdCO_3)$ per unit hexagonal cell.

Two unit-cell measurements have been converted from the rhombohedral to the hexagonal cell values and from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1928	Zachariasen [2]	4. 923	16. 28
1947	Vegard [4]	5. 014	16. 37
1957	National Bureau of Standards.	4. 930	16. 27 at 25° C

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

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1928 Zachariasen Cu, ----		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
012	3. 78	80	3. 65	50	3. 78	78
104	2. 95	100	2. 85	100	2. 95	100
006	---		2. 65	10–20	2. 72	3
110	2. 47	50	2. 40	50	2. 46	35
113	2. 23	3	2. 20	5	2. 245	7
202	2. 06	45	2. 02	50	2. 066	27
024	1. 88	33	1. 85	40	1. 890	14
018	1. 83	80	1. 80	100	1. 838	23
116			1. 78		1. 825	34
122	1. 58	40	1. 55	60	1. 582	15
1·0·10	---		1. 49	20	1. 522	4
214	1. 50	17	1. 47	50	1. 500	11
208	1. 473	5	1. 44	20–30	1. 473	5
300	1. 422	15	1. 39	40	1. 423	7
0·0·12	1. 358	5	1. 33	20	1. 357	2
0·2·10	1. 297	5	1. 27	20–30	1. 293	3
128	1. 263	17	1. 24	50	1. 263	6
306					1. 260	3
220	1. 232	5	1. 20	20	1. 232	2
1·1·12	1. 192	8	1. 17	40	1. 189	4
312	---		1. 15	30	1. 171	3
2·1·10	1. 144	8	1. 13	30	1. 146	4
134	---		1. 12	30–40	1. 137	5
226	1. 122	8	1. 10	30	1. 121	5
042	---		1. 02	30	1. 057	<1
404	1. 024	8	1. 01	50	1. 032	3
318					1. 0231	4
1·1·15	---		0. 979	20	0. 9900	1
3·0·12	0. 978	7	. 970	40	. 9825	2
232	---		. 959	30	. 9725	<1
1·3·10	---		. 947	10	. 9571	<1
324	---		. 941	20	. 9522	<1
048	. 944	7	. 933	40	. 9446	1
140	---		. 920	40	. 9310	<1
413	---		. 911	20	. 9191	<1
2·2·12	---		. 902	30	. 9126	<1
4·0·10	---		---	--	. 8928	<1
238	. 882	7	---	--	. 8814	3
416						

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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----	100	110	101
Zachariasen----------	110	100	112
National Bureau of Standards----	100	110	101

Structural data. Zachariasen [1] in 1926 determined that cadmium selenide has wurtzite-type structure with the space group C_{6v}^4–$P6_3mc$ 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.

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[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	*c*
		A	*A*
1926	Goldschmidt [2]----------	4. 31	7. 03
1926	Zachariasen [1]----------	4. 31	7. 02
1957	National Bureau of Standards.	4. 299	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 --------		1926 Zachariasen Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
100	3. 74	100	3. 74	80	3. 72	100
002	3. 52	80	3. 49	30	3. 51	70
101	3. 305	90	3. 30	60	3. 290	75
102	2. 563	40	2. 57	20	2. 554	36
110	2. 157	100	2. 160	100	2. 151	85
103	1. 988	70	1. 989	70	1. 980	70
200	1. 866	30	1. 872	20	1. 863	12
112	1. 839	80	1. 842	80	1. 834	51
201	1. 807	20	1. 812	20	1. 800	11
202	1. 649	30	1. 649	10	1. 645	8
203	1. 459	50	1. 460	70	1. 456	20
210	1. 409	30	1. 411	20	1. 407	8
211	1. 383	30	1. 384	30	1. 380	8
105	1. 315	40	1. 315	50	1. 3120	13
212	-----	--	-----	--	1. 3059	5
300	1. 244	30	1. 245	40	1. 2411	10
301	-----	--	-----	--	1. 2218	<1
213	-----	--	1. 209	70	1. 2055	18
302	-----	--	1. 174	40	1. 1700	8
205	-----	--	1. 123	40	1. 1201	7
106	-----	--	-----	--	1. 1144	2
220	-----	--	1. 078	40	1. 0748	6
310	-----	--	-----	--	1. 0327	3
222	-----	--	1. 031	80	1. 0273	6
116	-----	--	-----	--	1. 0267	4
311	-----	--	-----	--	1. 0219	2
215	-----	--	0. 997	80	0. 9932	9
312	-----	--	-----	--	. 9906	6
313	-----	--	. 948	80	. 9446	6
400	-----	--	-----	--	. 9307	<1
401	-----	--	-----	--	. 9226	<1
402 216	-----	--	-----	--	. 8992	1
207	-----	--	-----	--	. 8820	<1
008	-----	--	-----	--	. 8761	<1
403	-----	--	-----	--	. 8648	3
320	-----	--	-----	--	. 8542	1
306	-----	--	-----	--	. 8508	2
315	-----	--	-----	--	. 8314	5

Calcium Chromate, $CaCrO_4$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0516	3. 63 2. 70 1. 86	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Clouse [2] 1932	Molybdenum	K_α

NBS sample. The sample of calcium chromate was prepared at NBS by melting $CaCl_2$ 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 yellow color. 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 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	200	112	312
Clouse	200	312	112
National Bureau of Standards	200	112	312

Structural data. Clouse [3] in 1930 determined that calcium chromate has zirconium silicate-type structure, the space group D_{4h}^{19}–$I4_1/amd$ 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.

Lattice constants

		a	*c*
		A	*A*
1930	Clouse [3]	7. 11	6.20
1932	Clouse [2]	7. 26	6.35
1957	National Bureau of 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		1932 Clouse Mo, ------		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
101	4. 81	6	4. 77	10	4. 75	10
200	3. 64	100	3. 60	100	3. 62	100
211	2. 91	15	2. 90	30	2. 880	15
112	2. 71	75	2. 68	80	2. 679	54
220	2. 58	15	2. 58	30	2. 562	11
202	2. 39	20	2. 38	50	2. 375	16
301	2. 27	8	2. 27	20	2. 254	7
103	-----	---	2. 025	10	2. 013	6
321	-----	---	----	---	1. 913	5
312	1. 86	75	1. 862	100	1. 8510	45
400	1. 81	20	1. 818	50	1. 8100	15
411	-----	---	1. 699	10	1. 6926	2
420	1. 62	15	1. 619	40	1. 6195	10
004	1. 58	2	1. 573	20	1. 5722	5
332	1. 50	23	1. 500	60	1. 4999	13
323	1. 45	18	1. 446	60	1. 4499	5
204	-----	---	----	---	1. 4423	6
224	1. 348	13	1. 341	80	1. 3397	8
521	-----	---	----	---	1. 3146	4
512	1. 296	10	1. 297	80	1. 2946	10
440	-----	---	----	---	1. 2809	4
600	1. 212	6	1. 207	30	1. 2069	4
404	1. 190	5	1. 192	40	1. 1877	4
532	1. 156	8	1. 1630	60	1. 1554	6
620	-----	---	----	---	1. 1446	6
424	1. 132	8	----	---	1. 1281	8
116	1. 029	8	----	---	1. 0270	4
640	1. 002	5	----	---	1. 0040	3
534 712	0. 975	8	----	---	0. 9738	4
316	-----	---	----	---	. 9533	4
624	-----	---	----	---	. 9258	5
732	-----	---	----	---	. 9100	4
406	-----	---	----	---	. 9077	2
800	-----	---	----	---	. 9051	4

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).

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Calcium Nitrate, $Ca(NO_3)_2$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–1215	2. 19 2. 29 4. 39	Molybdenum.	Hanawalt, 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	222	311	111
Vegard	311	222	210
National Bureau of Standards	222	111	210

Structural data. Jaeger and Melle [3] in 1928 determined that calcium nitrate has the space group T_h^6–Pa3 and 4[$Ca(NO_3)_2$] per unit cell. Calcium nitrate is used as a structure type.

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

		A
1922	Vegard [2]	7. 62
1932	Ringdal [4]	7. 615
1955	Menary [5]	7. 590 at 24° C
1957	National Bureau of Standards.	7.600 at 25° C

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

Calcium Nitrate, $Ca(NO_3)_2$ (cubic)

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*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
111	4. 40	60	7. 62	4. 45	w	7. 71	4. 39	97	7. 60
---	-------	---	-------	3. 92	w	-------	-------	---	------
210	3. 40	50	7. 60	3. 46	m	7. 74	3. 40	90	7. 60
211	3. 10	50	7. 59	3. 14	m	7. 69	3. 10	60	7. 60
220	2. 68	2	7. 58	-------	---	-------	2. 69	8	7. 60
221	2. 53	4	7. 59	-------	---	-------	2. 53	14	7. 60
311	2. 29	80	7. 59	2. 31	s	7. 66	2. 292	73	7. 603
222	2. 19	100	7. 59	2. 20	s	7. 62	2. 194	100	7. 601
321	2. 01	2	7. 52	-------	---	-------	2. 032	5	7. 603
400	1. 89	30	7. 56	1. 91	m	7. 64	1. 900	27	7. 599
411	1. 78	12	7. 55	-------	---	-------	1. 791	10	7. 600
331	1. 73	10	7. 54	-------	---	-------	1. 743	8	7. 599
420	1. 69	10	7. 56	-------	---	-------	1. 699	8	7. 599
421	1. 65	2	7. 56	-------	---	-------	1. 658	1	7. 600
332	1. 61	2	7. 55	-------	---	-------	1. 620	1	7. 598
422	1. 54	4	7. 54	-------	---	-------	1. 551	2	7. 596
511	1. 46	10	7. 59	1. 46	w	7. 59	1. 462	6	7. 598
432	1. 408	4	7. 58	-------	---	-------	1. 4110	3	7. 598
440	1. 341	14	7. 59	1. 34	m	7. 59	1. 3432	10	7. 598
531	1. 283	10	7. 59	1. 286	m	7. 61	1. 2846	10	7. 599

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	I	a	d	I	a
	A		A	A		A	A		A
600	-------	----	-------	-------	----	-------	1. 2668	2	7. 601
610	-------	----	-------	-------	----	-------	1. 2497	<1	7. 602
611	-------	----	-------	-------	----	-------	1. 2330	<1	7. 601
620	-------	----	-------	-------	----	-------	1. 2019	<1	7. 602
621	-------	----	-------	-------	----	-------	1. 1871	<1	7. 601
533	-------	----	-------	-------	----	-------	1. 1589	1	7. 599
622	1. 142	4	7. 58	1. 146	m	7. 60	1. 1459	4	7. 601
630	-------	----	-------	-------	----	-------	1. 1332	<1	7. 602
444	-------	----	-------	1. 094	----	7. 58	1. 0969	<1	7. 600
543	-------	----	-------	-------	----	-------	1. 0750	<1	7. 601
711	-------	----	-------	-------	----	-------	1. 0642	1	7. 600
641	-------	----	-------	-------	----	-------	1. 0439	<1	7. 600
642	-------	----	-------	1. 013	----	7. 58	1. 0156	2	7. 600
722	-------	----	-------	-------	----	-------	1. 0064	1	7. 598
731	-------	----	-------	0. 9865	----	7. 58	0. 9894	3	7. 600
650	-------	----	-------	-------	----	-------	. 9730	<1	7. 599
810	-------	----	-------	-------	----	-------	. 9428	<1	7. 601
820	-------	----	-------	-------	----	-------	. 9217	<1	7. 600
821	-------	----	-------	-------	----	-------	. 9150	<1	7. 601
822	-------	----	-------	-------	----	-------	. 8956	<1	7. 599
831	-------	----	-------	-------	----	-------	8835	<1	7. 600
751	-------	----	-------	-------	----	-------	. 8775	<1	7. 599
662	-------	----	-------	-------	----	-------	. 8718	1	7. 600
840	-------	----	-------	-------	----	-------	. 8496	1	7. 599
911	-------	----	-------	. 8347	----	7. 60	. 8342	2	7. 600
842	-------	----	-------	-------	----	-------	. 8293	1	7. 601
Average of last five lines			7. 59	-------	----	7. 59	--------	----	7. 600

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[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).

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[3] F. M. Jaeger and F. A. van Melle, On the symmetry and structure of the cubic nitrates of calcium, strontium, barium, and lead, Proc. Acad. Amsterdam **31**, 651–655 (1928).

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Calcium Sulfide (oldhamite), CaS (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0980	2. 85 2. 00 1. 27	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

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

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 measurements. 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	200	220	420
Holgersson	200	220	420
Oftedal	420	600	620
National Bureau of Standards	200	220	222

Structural data. Kustner [2] in 1922 determined that calcium sulfide has sodium chloride-type 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

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

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

Calcium Sulfide (oldhamite), CaS (cubic)

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*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	---	--	---	---	--	--	---	--	--	---	--	--	3.28	<1	5.70
200	2.85	100	5.70	2.88	--	5.76	2.77	vs	5.54	---	--	--	2.846	100	5.693
220	2.00	100	5.66	2.03	--	5.74	1.98	vs	5.60	---	--	--	2.013	68	5.694
311	---	--	---	---	--	--	1.69	w	--	---	--	--	1.717	<1	5.695
222	1.63	50	5.65	1.66	--	5.75	1.63	s	5.65	---	--	--	1.6439	21	5.695
400	1.422	16	5.688	1.43	--	5.72	1.40	s	5.60	---	--	--	1.4238	9	5.695
331	---	--	---	---	--	--	---	--	--	---	--	--	1.3065	<1	5.696
420	1.271	60	5.684	1.28	--	5.72	1.26	vs	5.63	1.28	s	5.72	1.2737	20	5.696
422	1.160	32	5.683	1.17	--	5.73	1.15	vs	5.63	---	--	--	1.1627	14	5.696
---	---	--	---	---	--	--	1.09	m	--	---	--	--	----	--	----
440	1.006	6	5.691	1.01	--	5.71	0.996	w	5.63	1.01	w	5.71	1.0068	4	5.6953
600	0.948	14	5.688	0.956	--	5.74	.939	vs	5.63	0.950	s	5.70	0.9491	8	5.6946
620	.899	8	5.686	.908	--	5.74	---	--	--	.900	s	5.69	.9005	7	5.6953
622	.858	6	5.691	.867	--	5.75	---	--	--	---	--	--	.8585	7	5.6946
444	---	--	---	---	--	--	---	--	--	---	--	--	.8220	1	5.6950
640	.790 [a]	5	5.697	---	--	--	---	--	--	---	--	--	.7897	7	5.6946
Average of last five lines			5.691	---	--	5.73	---	--	5.62		--	5.71	----	--	5.6948

[a] 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	Molybdenum.	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 $N\alpha=1.561$, $N\beta=1.570$, $N\gamma=1.572$, and $2V\cong 60°$.

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 D_{2h}^{16}–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*	*c*
		A	*A*	*A*
1916	Ogg and Hopwood [3].	6. 231	10. 906	8. 215
1928	Taylor and Boyer [4].	6. 25	10. 94	8. 24
1930	Ogg [5].	6. 261	10. 959	8. 254
1930	Tutton [6].	6. 25	10. 95	8. 25
1957	National Bureau of Standards.	6. 264	10. 95	8. 242 at 25° C

The density of cesium sulfate calculated from the NBS lattice constants is 4.250 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	*I*	*d*	*I*
	A		*A*	
020	----------	---	5. 47	6
111	4. 56	10	4. 54	13
012	----------	---	3. 85	11
121	3. 68	35	3. 684	43
102	----------	---	3. 441	11
031	----------	---	3. 333	14
022	3. 29	100	3. 290	100
112			3. 285	
130	3. 15	100	3. 152	83
200			3. 129	59
131	----------	---	2. 949	4
122	2. 91	5	2. 913	9
040	2. 73	10	2. 736	12
220	----------	---	2. 728	10
013	2. 66	20	2. 665	27
041	2. 59	20	2. 599	10
221			2. 580	18
212	2. 42	10	2. 432	11
141			2. 400	11
042	2. 28	45	2. 279	22
222			2. 270	26
033	2. 20	5	2. 194	11
142	----------	---	2. 143	8
051	2. 11	5	2. 115	11
240	----------	---	2. 062	4
232	2. 04	10	2. 057	7
213			2. 029	12
151	----------	---	2. 004	5
104	----------	---	1. 957	3
052	----------	---	1. 933	2
024	1. 93	5	1. 929	10
321	----------	---	1. 899	3
143	1. 84	15	1. 853	18
124			1. 842	2
312			1. 836	11
060	----------	---	1. 824	4
330	1. 80	5	1. 812	8
233	----------	---	1. 797	4
034	----------	---	1. 794	4
251	1. 75	5	1. 753	9
134	----------	---	1. 724	2
161	1. 71	5	1. 713	2
062	----------	---	1. 668	1
153	----------	---	1. 652	<1
224	----------	---	1. 642	<1
015	----------	---	1. 630	1
341	----------	---	1. 627	2
162	----------	---	1. 612	1
260	1. 57	10	1. 576	4

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] A. Ogg, The crystal structure of the isomorphous sulfates of potassium, ammonium, rubidium, and cesium, Phil. Mag. **5,** 354–367 (1928).

[3] A. Ogg and F. L. Hopwood, A critical test of the crystallographic law of valency volumes; crystalline structures of the alkali sulfates, Phil. Mag. **32,** 518–525 (1916).

[4] W. Taylor and T. Boyer, An investigation into the structure of caesium and ammonium sulphates, Mem. Proc. Manchester Lit. and Phil. Soc. **72,** 125–137 (1928).

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

[6] A. E. H. Tutton, Note by, Phil. Mag. **9,** 667–668 (1930).

Gold Antimony (aurostibite), $AuSb_2$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
5-0718	2. 003 3. 33 2. 98	Copper	Graham and Kaiman [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	311	200	731
Oftedal	311	511	731
Bottema and Jaeger	311	511	200
National Bureau of Standards	311	210	200

Structural data. Oftedal [2] in 1928 determined that gold antimony has pyrite-type structure, the space group T_h^6–Pa3, and 4($AuSb_2$) per unit cell.

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

Lattice constants

		A
1928	Oftedal [2]	6. 649
1931	Nail, Almin, and Westgren [4].	6. 660
1932	Bottema and Jaeger [3]	6. 649
1952	Graham and Kaiman [1]	6. 657
1957	National Bureau of Standards.	6.6589 at 25° C

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

Gold Antimony (aurostibite), $AuSb_2$ (cubic)

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	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A
111	3. 83	10	6. 63	----	---	----	3. 82	30	6. 62	3. 85	32	6. 67
200	3. 33	50	6. 66	3. 32	m	6. 64	3. 31	60	6. 62	3. 33	69	6. 67
210	2. 98	40	6. 66	2. 97	m	6. 64	2. 97	60	6. 64	2. 98	74	6. 66
211	2. 72	30	6. 66	2. 71	m	6. 64	2. 70	50	6. 61	2. 719	55	6. 66
220	2. 34	40	6. 62	2. 35	m	6. 65	2. 34	50	6. 62	2. 356	54	6. 663
---	----	--	----	----	---	----	2. 22	40	----	-----	--	-----
311	2. 003	100	6. 64	1. 97	vs	6. 53	2. 00	100	6. 64	2. 009	100	6. 663
222	1. 918	10	6. 64	1. 92	vvw	6. 65	1. 92	30	6. 65	1. 922	17	6. 659
230	1. 840	10	6. 63	1. 84	w	6. 63	1. 84	40	6. 63	1. 848	16	6. 664
321	1. 777	20	6. 65	1. 77	w+	6. 62	1. 77	50	6. 62	1. 779	30	6. 658
400	----	--	----	1. 64	m+	6. 56	----	--	----	1. 664	6	6. 656
331	1. 524	5	6. 64	1. 52	vw	6. 62	1. 52	10	6. 62	1. 528	11	6. 660
420	1. 485	10	6. 64	1. 48	w—	6. 62	1. 49	30	6. 66	1. 489	12	6. 657
421	1. 448	10	6. 64	1. 45	m+	6. 64	1. 45	20	6. 64	1. 452	7	6. 655
332	1. 417	5	6. 65	1. 41	m	6. 61	1. 42	20	6. 66	1. 419	6	6. 657
422	1. 356	10	6. 64	1. 35	m+	6. 61	1. 36	20	6. 66	1. 359	10	6. 657
----	----	--	----	1. 30	w—	----	1. 30	10	----	-----	--	-----
511	1. 280	30	6. 65	1. 28	vs	6. 65	1. 28	80	6. 65	1. 282	25	6. 659
432	1. 233	10	6. 64	1. 23	m+	6. 62	1. 24	20	6. 68	1. 236	10	6. 657
521	1. 213	5	6. 64	1. 21	m—	6. 63	1. 21	20	6. 63	1. 215	6	6. 656
440	1. 177	20	6. 66	1. 17	s+	6. 62	1. 18	50	6. 68	1. 1769	16	6. 658
531	1. 126	5	6. 66	1. 12	w+	6. 63	1. 13	20	6. 69	1. 1254	2	6. 658
600	1. 109	10	6. 65	1. 11	m	6. 66	1. 11	20	6. 66	1. 1096	2	6. 658
610	1. 080	10	----	1. 09	s—	6. 63	1. 08	20	----	1. 0945	1	6. 568
611				1. 07	m	6. 60				1. 0801	2	6. 658

Gold Antimony (aurostibite), $AuSB_2$ (cubic)—Continued

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	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
620	1.050	5	6.64	1.05	m	6.64	1.05	20	6.64	1.0526	1	6.657
533	1.013	20	6.64	1.01	s	6.62	1.02	30	6.69	1.0153	2	6.658
622	1.003	5	6.65	1.00	s	6.63	1.00	10	6.63	1.0039	<1	6.659
630	0.991	5	6.65	0.989	w	6.63	0.992	10	6.65	0.9925	1	6.658
631	.981	5	6.65	.978	w−	6.63	----	--	----	.9816	<1	6.657
---	----	--	----	.956	w+	----	.960	20	----	-----	--	-----
711	.934	10	6.67	.928	vw	6.63	----	--	----	.9324	<1	6.659
640	.923	5	6.66	.919	w	6.63	----	--	----	.9233	<1	6.658
641	.914	10	6.65	.912	w	6.64	----	--	----	.9148	<1	6.660
721	.906	10	6.66	.903	m	6.64	----	--	----	.9060	1	6.658
642	.890	20	6.66	.887	s	6.64	.888	30	6.64	.8898	1	6.659
731	.867	50	6.66	.863	vs	6.63	.866	60	6.65	.8669	15	6.659
650	.853	10	6.66	----	---	----	----	--	----	.8526	<1	6.659
732	.846	10	6.66	----	---	----	----	--	----	.8459	1	6.660
800	.833	20	6.66	----	---	----	----	--	----	.8324	1	6.6592
820	.808	20	6.66	----	---	----	----	--	----	.8076	2	6.6593
821	.802	20	6.66	----	---	----	----	--	----	.8016	2	6.6588
653	.796	5	6.66	----	---	----	----	--	----	.7959	<1	6.6588
822	.785	40	6.66	----	---	----	----	--	----	.7847	2	6.6586
Average of last five lines			6.66	----	---	6.64	----	--	6.62	-----	--	6.6589

References

[1] A. R. Graham and S. Kaiman, Aurostibite, $AuSb_2$; a new mineral in the pyrite group, Am. Mineralogist **37**, 461–469 (1952).

[2] I. Oftedal, Über die Kristallstrukturen der Verbindungen RuS_2, OsS_2, $MnTe_2$ und $AuSb_2$, 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).

[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	102	110	212
Bottema and Jaeger	102	110	202
National Bureau of Standards	102	110	100

Structural data. Preston and Owen [1] determined that gold tin has nickel arsenide-type structure, the space group D_{6h}^4–$P6_3/mmc$, and 2(AuSn) per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1927	Preston and Owen [1]	4. 318	5.508
1931	Stenbeck and Westgren [3].	4. 323	5.523
1932	Bottema and Jaeger [2]	4. 316	5.507
1957	National Bureau of Standards.	4. 323	5.517 at 25° C.

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

References

[1] G. D. Preston and E. A. Owen, The atomic structure of AuSn, Phil. Mag. **4**, 133–147 (1927).

[2] 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 antimony, Proc. Acad. Sci. Amsterdam **35**, 916–928 (1932).

[3] S. Stenbeck and A. Westgren, Röntgenanalyse der Gold-Zinn, Z. physik. Chem. **14B**, 91–96 (1931).

Gold Tin AuSn (hexagonal)

hkl	1927 Preston and Owen Cu, 1.542 A		1932 Bottema and Jaeger Cu, 1.542 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I* [a]	*d*	*I*	*d*	*I*
	A		*A*		*A*	
100	3. 76	7	3. 75	40	3. 74	51
101	3. 09	6	3. 09	40	3. 09	45
102	2. 22	1	2. 21	100	2. 222	100
110	2. 16	2	2. 15	80	2. 161	65
200	1. 86	22	1. 87	20	1. 870	7
201	1. 77	22	1. 77	20	1. 772	10
112	1. 71	22	---	---	1. 702	4
103	1. 65	22	1. 664	20	1. 652	9
202	1. 55	5	1. 541	50	1. 549	27
210	-----	---	1. 410	10	1. 415	9
---	-----	---	1. 376	20	------	--
211	1. 37	16	1. 363	10	1. 3705	7
203	-----	---	1. 310	10	1. 3120	3
104	1. 28	17	1. 290	20	1. 2950	6
212	1. 25	3	1. 261	50	1. 2592	19
300	-----	---	1. 241	20	1. 2475	8
114	1. 16	4	1. 159	50	1. 1637	14
302	-----	---	-----	---	1. 1372	<1
214	-----	---	1. 117	10	1. 1220	<1
204	-----	---	1. 106	10	1. 1112	2
220	1. 07	18	1. 076	10	1. 0808	4
105 221	-----	---	1. 056	10	1. 0594	<1
310	-----	---	-----	---	1. 0382	<1
311	1. 02	19	1. 018	10	1. 0204	2
222	-----	---	-----	---	1. 0063	2
214	0. 985	19	0. 985	20	0. 9882	2
312	. 964	9	. 970	30	. 9720	6
205	-----	---	-----	---	. 9509	<1
400	-----	---	-----	---	. 9361	<1
304	-----	---	. 923	40	. 9258	4
313	-----	---	-----	---	. 9042	2
106	. 892	8	. 892	40	. 8938	5
402	. 885	10	. 884	10	. 8863	3
215	-----	---	-----	---	. 8706	2
320	-----	---	-----	---	. 8587	1
224	. 848	10	-----	---	. 8509	7
321	-----	---	-----	---	. 8486	3
403	-----	---	-----	---	. 8342	1
314	. 825	22	-----	---	. 8298	2
305 206	-----	---	-----	---	. 8259	4
322	-----	---	-----	---	. 8200	7
410	. 818	10	-----	---	. 8171	11

[a] The intensities of the Preston and Owen pattern are in order of decreasing intensity.

Lanthanum Fluoride, LaF_3 (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	300	113	302
National Bureau of Standards	111	113	300

Structural data. The structure of lanthanum fluoride was redetermined by Oftedal [2] in 1931. The postulated structure is D^3_{6h}–$P6_3/mcm$ with $6(LaF_3)$ per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1929	Oftedal [1]	7. 177	7.344
1957	National Bureau of Standards.	7. 184	7.351 at 25° C

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

References

[1] 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, . . .)F_3, Z. physik. Chem. **B13**, 190–200 (1931).

hkl	1929 Oftedal Cu, 1.5392 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
002	3. 699	w	3. 67	40
110	------	----	3. 59	32
111	3. 250	s	3. 229	100
112	2. 588	w−	2. 569	11
300	2. 092	s+	2. 075	51
113	2. 039	s+	2. 025	54
004	1. 848	w−	1. 8377	5
302	1. 817	s+	1. 8064	33
221	1. 755+	s	1. 7451	20
114	1. 646	w	1. 6364	4
222	1. 622	w−	1. 6142	3
223	1. 457	s	1. 4487	14
304	1. 385+	m+	1. 3755	10
115	1. 369	m+	1. 3604	7
411	1. 344	s+	1. 3354	15
224	1. 294	vw	1. 2849	2
412	1. 281	vw+	1. 2737	4
006	1. 234	w−	1. 2254	2
330	1. 204	w	1. 1974	6
413	1. 194	s	1. 1877	14
116	1. 167	w	1. 1601	2
332, 225	1. 145−	s	1. 1384	10
414	1. 099	w	1. 0921	3
306	1. 062	s−	1. 0549	8
600	1. 042	w−	1. 0370	3
226	------	----	1. 0120	2
117	------	----	1. 0078	3
334	1. 007	w	1. 0033	4
415	1. 002	s+	0. 9978	9
521	0. 9918	m+	. 9872	6
522	------	----	. 9616	2
523	------	----	. 9228	5
416	------	----	. 9094	3
227	------	----	. 9066	3
604	------	----	. 9030	4
441	------	----	. 8913	4
700, 515	------	----	. 8898	2
524	------	----	. 8759	2
336	------	----	. 8564	6
614, 443, 622, 308, 435	------	----	. 8433	4
417	------	----	. 8306	6
710, 525	------	----	. 8249	6
711	------	----	. 8190	6
444	------	----	. 8069	2
712	------	----	. 8042	3

Lanthanum Oxychloride, LaOCl (tetragonal)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wavelength
Sillén and Nylander [1] 1941.	Chromium.	K_α

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	101	110	102
National Bureau of Standards	102	101	110

Structural data. Sillén and Nylander [1] in 1941 determined that lanthanum oxychloride has lead chloride-type structure, the space group D^7_{4h}–P4/nmm and 2(LaOCl) per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1941	Sillén and Nylander [1]	4. 117	6.879
1957	National Bureau of Standards.	4. 120	6.882 at 25° C

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

References

[1] 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		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
001	------	----	6. 89	30
101	3. 52	s	3. 54	89
002	3. 43	w	3. 441	10
110	2. 90	s	2. 914	80
111	------	----	2. 681	7
102	2. 63	s	2. 642	100
003	2. 29	w	2. 294	7
112	2. 22	s	2. 224	28
200	2. 06	s	2. 060	42
103	2. 00	w	2. 005	5
201	1. 971	w	1. 975	6
113	1. 799	m	1. 803	26
211	1. 778	m	1. 780	29
202	1. 765	w	1. 768	7
004	1. 719	vw	1. 720	2
212	1. 622	s	1. 624	39
104	1. 586	m	1. 587	15
203	1. 532	w	1. 533	8
114	1. 481	w	1. 481	4
220	1. 455	m	1. 457	11
213	1. 436	vw	1. 436	2
221	1. 425	vvw	1. 425	2
005	1. 375	vw	1. 376	2
301	1. 346	vw	1. 347	7
222	1. 341	vw	1. 342	4
204	1. 320	vw	1. 321	2
105	1. 305	vvw	1. 306	3
310	1. 302	m	1. 303	10
311	------	----	1. 2805	4
302	1. 275	m	1. 2754	8
214	1. 257	m	1. 2573	13
115	1. 244	w	1. 2444	3
223	1. 229	vw	1. 2295	4
312	1. 218	m—	1. 2186	6
303	1. 178	vw	1. 1778	1
205	------	----	1. 1446	6
313	------	----	1. 1328	8
321	------	----	1. 1275	6
215	------	----	1. 1027	3
322	------	----	1. 0845	10
304	------	----	1. 0733	5
116	------	----	1. 0672	3
314	------	----	1. 0388	3
400	------	----	1. 0302	3
323	------	----	1. 0231	1
206	------	----	1. 0019	3
225	------	----	1. 0003	5
411	------	----	0. 9888	5
402	------	----	. 9868	4
330	------	----	. 9713	3
412	------	----	. 9596	8
107	------	----	. 9568	7
324	------	----	. 9519	7
315	------	----	. 9463	3
403	------	----	. 9399	2
332	------	----	. 9346	1
420	------	----	. 9212	5
226	------	----	. 9010	4

Lead Molybdate (wulfenite), $PbMoO_4$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
2–0544	3. 17 2. 00 1. 77	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	112	303, 312	204
Zambonini and Levi	112	303, 312	204
National Bureau of Standards.	112	204	303, 312

Structural data. Vegard and Refsum [3] in 1925 determined that lead molybdate has calcium tungstate-type structure, the space group C^6_{4h}–$I4_1/a$, and 4($PbMoO_4$) 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.

Lattice constants

		a	*c*
		A	*A*
1925	Zambonini and Levi [4]	5. 501	12. 04
1928	Vegard and Refsum [3]	5. 425	12. 10
1931	Aanerud [5]	5. 430	12. 15
1943	Sillén and Nylander [6]	5. 435	12. 10
1957	National Bureau of Standards.	5. 435	12.11 at 25° C

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

hkl	1942 Harcourt Cu, 1.5418 A		1925 Zambonini and Levi Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
101	---	-	---	-	4. 96	11
112	3. 17	100	3. 09	vs	3. 244	100
004	3. 00	10	2. 91	m	3. 028	22
200	2. 67	20	---	-	2. 718	24
---	---	-	2. 61	mw	----	-
211	2. 35	5	---	-	2. 383	8
---	---	-	2. 30	w	----	-
105	2. 20	2	---	-	2. 212	5
213	----	-	---	-	2. 082	7
204	2. 00	40	1. 97	s	2. 021	31
220	1. 96	20	1. 88	m	1. 920	14
116	1. 77	40	1. 75	s	1. 787	18
303 312	1. 64	50	1. 62	vs	1. 653	25
224	---	-	1. 59	ms	1. 622	12
008	1. 50	2	---	-	1. 515	3
321 314	---	-	1. 48	w	1. 496	2
323 217	---	-	---	-	1. 411	2
400	1. 35	2	---	-	1. 359	3
208	---	---	1. 30	m	1. 3229	7
316	1. 30	40	1. 29	s	1. 3085	12
325	---	-	1. 26	w	1. 2802	2
332 413	---	-	---	-	1. 2535	5
404	1. 24	10	1. 23	m	1. 2400	5
---	---	-	1. 22	w	------	-
420	1. 21	10	1. 20	m	1. 2151	5
228	1. 182	10	1. 17	m	1. 1889	4
415	---	-	---	-	1. 1574	<1
1·1·10	1. 150	10	---	-	1. 1550	3
327 318	---	-	---	-	1. 1354	<1
424 406	1. 120	20	1. 11	ms	1. 1277	6
336	1. 075	10	1. 07	mw	1. 0814	3
512 503	1. 045	20	1. 04	s	1. 0497	5
408 2·1·11	1. 005	10	1. 00	mw	1. 0110 1. 0030	2 <1

Lead Molybdate (wulfenite), $PbMoO_4$ (tetragonal) —Continued

hkl	1942 Harcourt Cu, 1.5418 A		1925 Zambonini and Levi Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
3·1·10	0. 986	20	0. 981	ms	0. 9900	4
525	---	-	---	-	. 9795	<1
440	---	-	---	-	. 9609	<1
428	. 945	30	---	-	. 9475	4
516	---	-	. 941	s	. 9426	4
532	. 918	10	-----	-	. 9212	3
444	---	-	. 915	ms	. 9156	3
600	---	-	---	-	. 9057	1
2·2·12	. 890	5	. 887	mw	. 8935	2
3·3·10	. 880	5	. 875	w	. 8800	2
604 446	. 868	5	. 867	w	. 8678	1
620	. 857	5	. 857	mw	. 8593	1
536 541	. 845	30	. 844	s	. 8462	3
624 606	. 825	30	. 817	vw	. 8267	3
448	. 811	30	---	-	. 8112	2
4·0·12	---	-	---	-	. 8102	2
5·1·10	. 800	30	. 802	ms	. 8002	3

References

[1] G. A. Harcourt, Tables for the identification of ore minerals by X-ray powder patterns, Am. Mineralogist **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).

[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'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 tungstates and molybdates with the scheelite structure, Arkiv Kemi. Mineral. Geol. **A17** No. 4 (1943).

Lead Tungstate (stolzite), $PbWO_4$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
2–0527	3. 21 2. 01 1. 65	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 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	112	204	312
National Bureau of Standards	112	204	312

Structural data. Vegard and Refsum [1] in 1928 determined that lead tungstate, stolzite, has calcium tungstate-type structure, the space group C^6_{4h}–$I4_1/a$, and 4($PbWO_4$) per unit cell. Shaw and Claringbull [2] have reported that the monoclinic form of $PbWO_4$, 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 (stolzite), $PbWO_4$ (tetragonal)

hkl	British Museum Cu, 1.541 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
-------	3. 57	40	------	----
112	3. 21	100	3. 252	100
004	2. 99	40	3. 014	22
200	2. 71	60	2. 732	32
211	2. 21	20	2. 394	1
204	2. 01	80	2. 024	35
-------	1. 95	20	------	----
220	1. 91	50	1. 9309	16
222	1. 82	40	1. 8377	<1
116	1. 76	70	1. 7817	21
312	1. 65	80	1. 6603	33
224	1. 61	60	1. 6255	16
008	1. 50	20	1. 5056	3
-------	1. 44	20	------	----
400	1. 36	20	1. 3653	4
208	------	----	1. 3184	7
316	1. 30	80	1. 3092	8
332	1. 25	60	1. 2590	6
404	1. 23	60	1. 2436	5
420	1. 22	60	1. 2213	5
228	1. 18	60	1. 1872	5
-------	1. 16	20	------	----
1·1·10	1. 15	40	1. 1498	4
424	1. 13	60	1. 1317	7
336	1. 08	40	1. 0836	4
512	1. 05	70	1. 0546	6
408	1. 01	40	1. 0114	3
0·0·12	------	----	1. 0040	1
3·1·10	------	----	0. 9882	6
440	------	----	. 9656	1
428	------	----	. 9486	3
516	------	----	. 9451	5
2·0·12	------	----	. 9423	2
532	------	----	. 9256	4
444	------	----	. 9193	2
600	------	----	. 9104	1
2·2·12	------	----	. 8906	3
3·3·10	------	----	. 8796	3
604	------	----	. 8713	3
620	------	----	. 8635	3
536	------	----	. 8488	5
1·1·14	------	----	. 8398	3
624	------	----	. 8301	5
448	------	----	. 8127	2
4·0·12	------	----	. 8088	3
5·1·10	------	----	. 8004	5

Lattice constants

		a	*c*
		A	*A*
1928	Vegard and Refsum [1]	5. 453	12.034
1931	Aanerud [3]	5. 464	12.055
1943	Sillén and Nylander [4]	5. 459	12.040
1957	National Bureau of Standards.	5. 4616	12.046 at 25° C

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

References

[1] 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 $PbWO_4$), 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, $LiIO_3$ (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
3–0369	3. 49 2. 74 4. 75	Molybdenum	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 measurements. 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	101	112	211
National Bureau of Standards	101	110	100

Structural data. Zachariasen and Barta [1] in 1931 determined that lithium iodate has the space group D_6^6–$P6_322$ and $2(LiIO_3)$ 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	*c*
		A	*A*
1931	Zachariasen and Barta [1]	5. 480	5. 165
1957	National Bureau of Standards.	5. 481	5. 172 at 25° C

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

hkl	1931 Zachariasen and Barta Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
100	4. 74	w+	4. 75	23
101	3. 50	vs	3. 50	100
110	2. 74	ms	2. 741	27
002	2. 58	vw	2. 587	8
111	2. 419	w	2. 422	2
200	2. 369	w	2. 374	8
102	2. 267	w	2. 272	10
201	2. 155	ms	2. 158	18
112	1. 889	s	1. 882	23
210	1. 794	vw	1. 795	3
202	1. 747	vw	1. 750	3
211	1. 695	s	1. 696	19
103	1. 618	m	1. 621	7
300	1. 580	m	1. 583	6
212	1. 4721	----	1. 473	3
-----	1. 4577	----	------	----
203	1. 3929	----	1. 395	5
220	1. 3693	----	1. 370	3
302	1. 3491	----	1. 349	5
-----	1. 3237	----	------	----
310	1. 3163	----	1. 3162	1
311	1. 2749	----	1. 2755	5
104	1. 2457	----	1. 2472	<1
213	1. 2413	----	1. 2430	6
222	1. 2095	----	1. 2109	3
400	1. 1852	----	1. 1865	<1
312	1. 1728	----	1. 1732	4
-----	1. 1715	----	------	----
114	1. 1645	----	1. 1696	2
401	1. 1557	----	1. 1567	1
204	------	----	1. 1354	1
320	------	----	1. 0891	<1
402	------	----	1. 0785	1
321	------	----	1. 0657	3
214	------	----	1. 0489	1
313	------	----	1. 0464	2
410	------	----	1. 0359	1
105	------	----	1. 0109	2
322	------	----	1. 0034	1
304	------	----	1. 0012	1
403	------	----	0. 9775	2
412	------	----	. 9617	2
500	------	----	. 9495	2
205	------	----	. 9484	<1
224	------	----	. 9404	1
501	------	----	. 9398	1
314	------	----	. 9224	1
323	------	----	. 9208	2
330	------	----	. 9134	<1
215	------	----	. 8959	2
502	------	----	. 8911	<1
421	------	----	. 8838	2
404	------	----	. 8742	<1
332	------	----	. 8614	2
510	------	----	. 8525	<1
422	------	----	. 8477	1
511	------	----	. 8413	1
324	------	----	. 8328	<1
503	------	----	. 8316	2
116	------	----	. 8222	<1
315	------	----	. 8133	1
512	------	----	. 8097	<1
414	------	----	. 8083	1
423	------	----	. 7957	1
600	------	----	. 7911	1

References

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

Lithium Nitrate, $LiNO_3$ (trigonal)

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_o=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_____	113	012	104
Zachariasen_____	113	012	104
National Bureau of Standards____	012	113	104

Structural data. Zachariasen [2] in 1928 determined that lithium nitrate has calcite-type structure, the space group D_{3d}^6–$R\bar{3}c$, and 2($LiNO_3$) per unit rhombohedral cell or 6($LiNO_3$) 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.

Lattice constants

		a	*c*
		A	*A*
1928	Zachariasen [2]_____	4. 70	15. 3
1957	National Bureau of Standards.	4. 692	15.22 at 25° C.

The density of lithium nitrate calculated from the NBS lattice constants is 2.367 at 25° C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1928 Zachariasen Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
012	3. 59	67	3. 60	80	3. 60	100
104	2. 79	53	2. 75	70	2. 79	83
006	2. 54	20	2. 54	40	2. 54	74
---	---	-	2. 36	20	-----	-
113	2. 13	100	2. 12	100	2. 134	86
202	1. 95	1	1. 965	5	1. 968	2
018 116	1. 72	11	1. 714	25	1. 725	14
211	1. 53	27	1. 523	25	1. 528	9
1·0·10 214	1. 423	1	1. 423	5	1. 425	2
119 125	1. 374	20	1. 365	40	1. 373	14
300	1. 358	13	1. 355	10	1. 355	7
0·0·12	---	-	1. 274	5	1. 269	3
217	1. 258	4	1. 255	15	1. 255	4
128 306	1. 196	4	1. 192	20	1. 195	3
223	1. 142	1	1. 143	5	1. 144	<1
1·1·12 312	1. 119	3	1. 113	10	1. 116	1
2·1·10 134	1. 084	4	1. 080	20	1. 0812	2
315	---	-	----	-	1. 0587	<1
0·1·14	---	-	----	-	1. 0511	<1
1·2·11	1. 027	1	1. 028	10	1. 0279	<1
042	1. 010	3	1. 007	15	1. 0073	1
404	0. 984	3	0. 9832	15	0. 9817	2
318	---	-	. 9703	10	. 9698	1
229 045	--	-	----	-	. 9641	<1
1·1·15 321	. 935	1	----	-	. 9311	3
3·0·12	. 929	1	----	-	. 9260	3
1·3·10	---	-	----	-	. 9058	<1
048	. 897	1	----	-	. 8961	1
235	. 892	1	----	-	. 8915	<1
140	---	---	----	-	. 8867	<1
327	---	---	----	-	. 8569	1

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] W. H. Zachariasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1928**, No. 4, (1928).

Magnesium Carbonate (magnesite), $MgCO_3$ (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
3–0773	2. 75 2. 10 1. 70	Molybdenum	Dow Chemical Co.
2–0871	2. 74 2. 10 1. 70	Copper	Michigan Alkali Co.
2–0905	2. 70 2. 10 1. 70	Copper	British Museum.
3–0788	2. 73 2. 10 1. 70	Molybdenum	New Jersey Zinc Co.
2–0875	2. 74 1. 70 2. 10	Molybdenum	United Steel Companies 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	104	113	116
Michigan Alkali Co	104	113	116
British Museum	104	113	116
New Jersey Zinc Co	104	113	116
United Steel Companies	104	116	113
Boldyrev et al	104	116	113
National Bureau of Standards	104	113	116

Structural data. Wyckoff [2] in 1920 determined that magnesium carbonate has calcite-type structure, the space group D^6_{3d}–$R\bar{3}c$, and $2(MgCO_3)$ per unit rhombohedral cell or $6(MgCO_3)$ 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.

Lattice constants

		a	*c*
		A	*A*
1935	Schoklitsch [3]	4. 596	14. 91
1937	Bragg [4]	4. 58	14. 84
1957	National Bureau of Standards.	4. 6332	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), $MgCO_3$ (trigonal)

hkl	Dow Chemical Co. Mo, ------		Michigan Alkali Co. Cu, ------		British Museum Cu, ------		New Jersey Zinc Co. Mo, ------		United Steel Companies Mo, ------		1938 Boldyrev et al. Fe, ------		1957 National Bureau of Standards Cu, 1.5405, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*		*A*	
---------	-----	---	-----	---	3. 03	60	-----	---	3. 54	20	-----	---	------	----
104	2. 76	100	2. 75	100	2. 71	100	2. 74	100	2. 75	100	2. 742	100	2. 742	100
006	2. 52	17	2. 51	20	2. 51	60	2. 51	5	2. 51	60	2. 505	50	2. 503	17
---------	-----	---	-----	---	-----	---	2. 42	1	-----	---	-----	---	------	----
110	2. 32	8	-----	---	2. 32	60	2. 32	3	2. 31	40	-----	---	2. 318	4
---------	-----	---	2. 14	10	-----	---	-----	---	-----	---	-----	---	------	----
113	2. 10	65	2. 10	80	2. 10	80	2. 10	67	2. 10	80	2. 105	90	2. 102	43
---------	2. 00	5	-----	---	-----	---	-----	---	-----	---	-----	---	------	----
022	1. 93	20	1. 93	40	1. 95	60	1. 94	16	1. 93	60	1. 939	60	1. 939	12
---------	1. 84	3	-----	---	1. 88	40	-----	---	-----	---	-----	---	------	----
024	1. 77	5	1. 77	10	1. 76	40	1. 78	3	1. 77	40	1. 770	20	1. 769	3
116	1. 70	65	1. 70	80	1. 70	80	1. 70	60	1. 70	90	1. 700	100	1. 700	34
---------	-----	---	1. 67	5	-----	---	-----	---	-----	---	-----	---	------	----
---------	-----	---	1. 64	5	1. 65	20	-----	---	-----	---	-----	---	------	----
---------	-----	---	1. 56	10	1. 55	20	-----	---	-----	---	-----	---	------	----

Magnesium Carbonate (magnesite), $MgCO_3$ (trigonal)—Continued

hkl	Dow Chemical Co. Mo, ------		Michigan Alkali Co. Cu, ------		British Museum Cu, ------		New Jersey Zinc Co. Mo, ------		United Steel Companies Mo, ------		1938 Boldyrev et al. Fe, ------		1957 National Bureau of Standards Cu, 1.5405, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*		*A*	
211	1.51	9	1.51	10	1.51	40	1.51	7	1.51	40	1.506	30	1.510	4
122	1.49	11	1.49	30	1.48	60	1.49	8	1.48	50	1.488	50	1.488	5
1·0·10	1.41	13	1.40	20	1.40	50	1.41	8	1.40	60	1.407	50	1.426	4
214														
------	-----	---	1.38	5	-----	---	-----	---	-----	---	-----	---	------	----
208	-----	---	1.37	5	-----	---	1.37	1	1.37	20	1.370	5	1.371	3
119	1.35	17	1.35	20	1.36	40	1.35	5	1.35	60	1.355	60	1.354	7
300	1.34	20	1.34	40	1.33	60	1.34	13	1.34	60	+1.339	70	1.338	8
------	-----	---	-----	---	-----	---	1.30	1	-----	---	-----	---	------	----
0·0·12	1.25	8	1.25	10	1.25	40	1.25	2	1.25	50	1.252	30	1.252	3
217	-----	---	1.24	5	1.24	40	1.23	1	1.24	20	1.239	20	1.2386	<1
0·2·10	1.20	4	-----	---	1.20	20	1.20	1	1.20	40	1.202	50	1.2022	<1
128	1.18	7	1.18	20	1.18	40	1.18	3	1.18	50	1.191	5	1.1798	<1
306														
220	1.16	1	-----	---	1.16	20	1.16	1	1.16	20	1.158	5	1.1583	<1
2·0·11	1.13	1	-----	---	1.13	20	-----	---	1.13	20	-----	---	1.1297	<1
------	1.11	1	-----	---	-----	---	-----	---	-----	---	-----	---	------	----
1·1·12	1.10	3	-----	---	1.10	20	-----	---	1.10	40	1.102	80	1.1011	<1
2·1·10	1.07	13	1.07	20	1.06	60	1.07	11	1.07	70	1.067	50	1.0669	4
134														
226	-----	---	1.05	5	1.05	40	1.05	1	1.05	50	-----	---	1.0510	1
1·2·11	-----	---	1.01	10	1.01	40	-----	---	1.01	40	1.014	20	1.0145	<1
------	-----	---	-----	---	-----	---	-----	---	-----	---	1.007	20	------	----
404	0.973	7	0.970	20	-----	---	-----	---	0.969	70	-----	---	0.9692	2
318	.963	5	959	20	-----	---	-----	---	.957	70	-----	---	.9573	1
------	-----	---	-----	---	-----	---	-----	---	.951	10	-----	---	------	----
2·0·14	-----	---	-----	---	-----	---	-----	---	.946	50	-----	---	.9455	<1
2·1·13														
1·1·15	.919	13	-----	---	-----	---	-----	---	.919	60	-----	---	.9188	3
321														
3·0·12														
1·0·16	-----	---	.915	40	-----	---	-----	---	.914	100	-----	---	.9134	7
324	-----	---	-----	---	-----	---	-----	---	-----	---	-----	---	.8941	<1
048	-----	---	.884	10	-----	---	-----	---	-----	---	-----	---	.8837	1
140	-----	---	.875	10	-----	---	-----	---	-----	---	-----	---	.8758	1
418														
3·1·11	-----	---	-----	---	-----	---	-----	---	-----	---	-----	---	.8626	<1
327	-----	---	-----	---	-----	---	-----	---	-----	---	-----	---	.8460	<1
0·0·18														
4·0·10	-----	---	-----	---	-----	---	-----	---	-----	---	-----	---	.8346	<1
416														
238	-----	---	-----	---	-----	---	-----	---	-----	---	-----	---	.8265	<1
2.1.16														
502	-----	---	-----	---	-----	---	-----	---	-----	---	-----	---	.7981	1

References

[1] A. K. Boldyrev, V. I. Mikheiev, V. N. Dubinina and G. A. Kovalev, X-ray determinative tables for minerals, Ann. Inst. Mines Leningrad, II, liv. 2 (1938).

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[4] W. L. Bragg, Atomic structure of minerals, Cornell University Press, Ithaca, N. Y., p. 116 (1937).

[5] J. Brentano and J. Adamson, Precision measurements of X-ray reflections from crystal powders. The lattice constants of zinc carbonate, manganese carbonate and cadmium oxide, Phil. Mag. **7,** 507–517 (1929).

[6] A. Ferrari and C. Colla, Soluzioni solide fra carbonati neutri romboedrici di metalli bivalente. Nota I. Gazz. chim. ital. **66,** 571–580 (1936).

Magnesium Sulfate Heptahydrate (epsomite), $MgSO_4 \cdot 7H_2O$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0399	4. 22 2. 66 5. 9	Molybdenum.	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 $2V \cong 40°$.

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	121	240, 420	020
National Bureau of Standards.	121	120	240

Structural data. Westenbrink [2] in 1926 determined that magnesium sulfate heptahydrate has the space group D_2^4–$P2_12_12_1$, 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*	*c*
		A	A	A
1926	Westenbrink [2]	11. 91	12. 03	6. 87
1930	Cardoso [3]	11. 93	12. 04	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.

References

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[3] G. M. Cardoso, Los modernos métodos roentgenográfico aplicados en la determinación de la estructura cristalina de la epsomita, Trabjos Museo nac. cienc. nat., Ser. geol., Madrid, no. 37 (1930).

[4] W. H. Barnes and R. G. Hunter, Conformation of the space groups of epsomite, Nature **130**, 96 (1932).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		A	
020	5. 9	20	5. 99	22
011	------	----	5. 95	6
120	5. 3	20	5. 35	26
201	4. 51	8	4. 48	14
121	4. 23	100	4. 21	100
130	3. 77	10	3. 79	13
310			3. 76	7
031	3. 42	12	3. 453	16
301	------	----	3. 424	2
320	------	----	3. 304	3
112	3. 18	2	3. 178	6
040	2. 97	18	3. 000	13
022			2. 977	14
410	2. 88	20	2. 880	20
212				
330	------	----	2. 812	1
041	2. 75	8	2. 748	14
240	2. 67	40	2. 677	24
420			2. 659	22
241	2. 49	2	2. 493	2
421	------	----	2. 482	<1
340	2. 38	5	2. 389	5
150	------	----	2. 352	<1
042	------	----	2. 258	5
431	2. 27	2	2. 253	7
250	------	----	2. 229	4
151				
113	2. 21	7	2. 206	11
412				
251	2. 10	6	2. 115	7
440	------	----	2. 110	4
242				
530	------	----	2 040	1
441	2. 03	2	2. 017	3
052	1. 96	3	1. 964	4
351				
432	------	----	1. 955	3
531				
601	------	----	1. 900	1
260	------	----	1. 894	2
161				
233	1. 88	4	1. 882	1
611	------	----	1. 877	1
540	------	----	1. 861	1
261	------	----	1. 826	<1
451	1. 80	4	1. 799	4
541	------	----	1. 795	2
361	1. 72	4	1. 726	3
062				
601	------	----	1. 712	2
162	------	----	1. 710	2
170	------	----	1. 695	2
114	------	----	1. 679	<1
710				
071	------	----	1. 661	3
262	------	----	1. 658	4
433	------	----	1. 650	3
503	------	----	1. 646	1
270				
171				
124	------	----	1. 632	4

Magnesium Sulfide, MgS (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–1096	2. 60 1. 83 1. 50	Molybdenum	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	200	220	222
Holgersson	200	220	222
National Bureau of Standards	200	220	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.

Magnesium Sulfide, MgS (cubic)

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	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	3. 00	5	5. 20	-------	----	-------	3. 004	8	5. 203
200	2. 60	100	5. 20	2. 53	s	5. 06	2. 601	100	5. 202
220	1. 83	83	5. 18	1. 79	s	5. 06	1. 8388	60	5. 201
222	1. 499	40	5. 19	1. 47	s	5. 09	1. 5010	15	5. 200
400	1. 299	20	5. 196	1. 27	m	5. 08	1. 3001	7	5. 200
420	1. 160	40	5. 188	1. 14	s	5. 10	1. 1630	13	5. 201
422	1. 060	33	5. 193	1. 05	s	5. 14	1. 0617	10	5. 201
440	0. 920	8	5. 204	-------	----	-------	0. 9194	<1	5. 201
600	. 867	13	5. 202	-------	----	-------	. 8667	6	5. 200
620	. 823	8	5. 205	-------	----	-------	. 8222	6	5. 200
622	. 784 [a]	8	5. 200	-------	----	-------	. 7840	5	5. 200
Average of last five lines			5. 200	-------	----	5. 09	-------	----	5. 200

[a] Four additional lines are omitted.

Lattice constants

		A
1923	Holgersson [2]	5.08
1927	Goldschmidt [3]	5.20
1948	Primak, Kaufman, and Ward [4].	5.20
1956	Güntert and Faessler [5]	5.2034 at 21° C
1957	National Bureau of Standards.	5.200 at 25° C

The density of magnesium sulfide calculated from the NBS lattice constant is 2.663 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).

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Manganese(II) Carbonate (rhodochrosite), $MnCO_3$ (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
2–0785	2. 85 1. 76 1. 99	Molybdenum.	Krieger [1] 1930.
1–0981	2. 84 1. 76 3. 65	Molybdenum.	Hanawalt, Rinn, and and Frevel [2] 1938.
2–0798	2. 84 1. 78 2. 18	Iron	British Museum.
3–1280	[a]	[a]	Brentano and Adamson [3] 1929.

[a] 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 each 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 fine-grained.

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

Pattern	1	2	3
Krieger	104	018, 116	202
Hanawalt, Rinn, and Frevel.	104	018, 116	012
British Museum	104	018, 116	113
National Bureau of Standards.	104	012	116

Structural data. Wyckoff [4] in 1920 determined that manganous carbonate has calcite-type structure, the space group D^6_{3d}–$R\bar{3}c$, and $2(MnCO_3)$ per unit rhombohedral cell or $6(MnCO_3)$ per unit hexagonal cell.

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 pseudocubic cell values, they were not included in the lattice constants table.

Lattice constants

		a	*c*
		A	A
1920	Wyckoff [4]	4. 74	15. 52
1947	Oftedahl [5]	4. 914	15. 92
1957	National Bureau of Standards.	4. 777	15.67 at 25° C.

The density of manganous carbonate calculated from the NBS lattice constants is 3.697 at 25° C.

Manganese(II) Carbonate (rhodochrosite), $MnCO_3$ (trigonal)

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	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A	
012	------	----	3. 66	30	3. 66	60	3. 66	35
------	------	----	------	----	3. 14	40	------	----
104	2. 856	100	2. 85	100	2. 85	100	2. 84	100
------	------	----	------	----	2. 64	20	------	----
110	2. 394	40	2. 36	14	2. 41	60	2. 39	20
113	2. 184	40	2. 16	12	2. 18	70	2. 172	27
202	1. 994	50	2. 00	12	2. 01	60	2. 000	23
024	1. 813	30	1. 82	2	1. 84	40	1. 829	12
018	1. 766	80	1. 76	50	1. 78	80	1. 770	30
116							1. 763	33
211	------	----	------	----	1. 56	40	1. 556	1
122	1. 543	40	1. 53	6	1. 54	50	1. 533	13
214	1. 460	40	1. 455	4	1. 46	50	1. 452	1
------	------	----	------	----	1. 44	20	------	----
208	------	----	------	----	1. 42	20	1. 423	<1
------	------	----	------	----	1. 41	20	------	--
030	1. 381	30	1. 368	4	1. 39	60	1. 379	10
0·0·12	1. 312	5	1. 301	2	1. 32	40	1. 306	<1
0·2·10	1. 261	10	------	----	1. 23	40	1. 248	<1
128	1. 224	20	------	----	1. 22	20	1. 221	3
------	1. 199	5	------	----	1. 20	20	------	----
1·1·12	1. 130	20	------	----	------	----	1. 146	1
134	1. 102 [a]	20	------	----	------	----	1. 1014	1

[a] Seven additional lines are omitted.

References

[1] P. Krieger, Notes on an X-ray diffraction study of the series calcite-rhodochrosite, Am. Mineralogist **15**, 23–29 (1930).

[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).

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[4] R. W. G. Wyckoff, The crystal structures of some carbonates of the calcite group, Am. J. Sci. **50**, 317–360 (1920).

[5] A. Oftedahl, Mixed crystals of carbonates of the calcite group, in L. Vegard, Investigation into the structure and properties of solid matter with the help of X-rays, Skrifter Norske Videnskaps-Akad. Oslo. I. Mat.-Naturv. Kl. **1947**, No. 2 (1947).

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Mercury(I) Bromide, Hg_2Br_2 (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0675	3. 29 4. 30 2. 12	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Havighurst [2] 1925	Molybdenum.	0.710 A
Hylleraas [3] 1925	Iron.	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 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	110	101	114
Havighurst	110	114	101
Hylleraas	110	219, 228	114
National Bureau of Standards.	110	101	114

Mercury(I) Bromide, Hg_2Br_2 (tetragonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1925 Havighurst Mo, 0.7107 A		1925 Hylleraas Fe, 1.9323 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A	
101	4. 31	50	4. 31	40	4. 32	40	4. 30	48
110	3. 30	100	3. 287	100	3. 316	100	3. 30	100
103	------	----	------	----	------	----	2. 906	1
004	2. 78	20	2. 776	40	2. 794	30	2. 785	30
200	2. 32	24	2. 340	30	2. 347	70	2. 3339	24
114	2. 12	40	2. 123	60	2. 138	80	2. 1281	44
211	2. 05	4	2. 054	15	2. 062	20	2. 0512	10
105	2. 00	16	2. 008	35	2. 016	40	2. 0106	24
204	1. 78	12	1. 793	25	1. 796	60	1. 7885	17
220	1. 64	4	1. 647	15	1. 655	30	1. 6496	8
215	1. 52	8	1. 521	25	1. 529	50	1. 5228	12
310	1. 473	4	1. 474	10	1. 480	40	1. 4752	7
224	1. 423	8	1. 421	20	1. 423	40	1. 4192	8
008	------	----	1. 391	4	------	----	1. 3919	1
314	1. 307	4	1. 305	20	1. 310	50	1. 3039	6
118 305	1. 277	4	1. 281	15	1. 288	w	1. 2828 1. 2750	4 2
109 208	1. 200	4	1. 201	20	1. 199	70	1. 1961	6
400	------	----	------	----	1. 169	10	1. 1668	1
325	------	----	1. 121	5	1. 121	30	1. 1193	1
330	------	----	------	----	1. 102	15	1. 1000	<1
404	------	----	------	----	1. 079	15	1. 0761	<1
219 228	1. 066	4	1. 066	15	1. 066	100	1. 0644	6
420	------	----	------	----	------	----	1. 0440	1
334	------	----	------	----	------	----	1. 0233	1
318	------	----	1. 016	4	------	----	1. 0131	<1
415	------	----	------	----	------	----	1. 0095	2
424	------	----	0. 972	4	------	----	0. 9767	1
309	------	----	------	----	------	----	. 9687	1
329 408	------	----	------	----	------	----	. 8945	2
435	------	----	------	----	------	----	. 8609	<1
1 0·13	------	----	------	----	------	----	. 8427	<1
419 428	------	----	------	----	------	----	. 8352	<1
532	------	----	------	----	------	----	. 7925	<1

Structural data. Hylleraas [3] in 1925 determined that mercurous bromide has mercurous chloride-type structure, the space group D_{4h}^{17}–I4/mmm, and 2(Hg_2Br_2) 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

		a	*c*
1925	Havighurst [2]	4. 66	11.12
1925	Hylleraas [3]	4. 68	11.18
1927	Vegard [4]	4. 666	11.142
1957	National Bureau of Standards.	4. 667	11.138 at 25° C.

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).

[3] E. Hylleraas, Die Anordnung der Atome in den tetragonalen Kristallen der einwertigen Quecksilberhalogenide Hg_2Cl_2, Hg_2Br_2, Hg_2J_2. Berechnung der optischen Doppelbrechung von Hg_2Cl_2, Z. Physik **36**, 859–96 (1925).

[4] L. Vegard, Gitterschwankungen bei Mischkristallbildung durch Fällung von Lösungen, Z. Physik **43**, 299 (1927).

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

ASTM cards

Card numbers	Index lines	Radiation	Source
2–0402	3. 48 2. 13 1. 82	Copper	DeJong [1] 1926. Harcourt [2] 1942.
3–0408	3. 38 2. 10 1. 79	Copper	Harcourt [2] 1942.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [3] 1926	Copper	K_α
Earley [4] 1950	Copper	$K_{\alpha 1}$

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	220	311	111
Harcourt	111	220	311
Zachariasen	111	220	311
Earley	111	220	311
National Bureau of Standards	111	220	311

Structural data. DeJong [1] in 1926 determined that mercuric selenide has sphalerite-type structure, the space group T_d^2–F$\bar{4}$3m, 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

		A
1926	DeJong [1]	6. 05
1926	Goldschmidt [5]	6. 08
1926	Hartwig [6]	6. 081
1926	Zachariasen [3]	6. 080
1950	Earley [4]	6. 084
1957	National Bureau of Standards.	6. 085 at 25° C

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

References

[1] W. F. DeJong, Die Struktur des Tiemannit und Koloradoit, Z. Krist. **63**, 466–472 (1926).

[2] G. A. Harcourt, Tables for the identification of ore minerals by X-ray powder patterns, Am. Mineralogist **27**, 63–113 (1942).

[3] W. H. Zachariasen, Über die Kristallstrukturen der Selenide von Beryllium, Zink, Cadmium und Quecksilber, Z. phys. Chem. **124**, 436–448 (1926).

[4] J. W. Earley, Description and synthesis of the selenide minerals, Am. Mineralogist **35**, 338–364 (1950).

[5] 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).

[6] W. Hartwig, Die Kristallstruktur einiger Mineralien der regulären HgS-Reihe, Sitzb. preuss. Akad. Wiss. Berlin, Phys.-Math. Klasse **XI**, 79–80 (1926).

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

hkl	1926 DeJong Cu, 1.5418 A			1942 Harcourt Cu, 1.5418 A			1926 Zachariasen 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*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	3. 4	80	5. 9	3. 39	100	5. 87	3. 51	100	6. 08	3. 51	100	6. 08	3. 51	100	6. 08
200	3. 0	20	6. 0	2. 96	20	5. 92	3. 04	20	6. 08	3. 05	20	6. 10	3. 041	15	6. 082
220	2. 13	100	6. 02	2. 10	80	5. 94	2. 15	100	6. 08	2. 14	80	6. 05	2. 151	51	6. 084
311	1. 82	90	6. 04	1. 79	80	5. 94	1. 833	80	6. 08	1. 833	80	6. 08	1. 835	32	6. 086
222	1. 74	10	6. 03	1. 72	10	5. 96	1. 755	10	6. 08	1. 758	5	6. 09	1. 757	3	6. 086
400	1. 51	40	6. 04	1. 49	20	5. 96	1. 522	20	6. 09	1. 518	10	6. 07	1. 521	6	6. 084
331	1. 39	60	6. 06	1. 36	40	5. 96	1. 396	40	6. 08	1. 397	20	6. 09	1. 396	9	6. 085
420	1. 36	10	6. 08	---	--	--	1. 355	10	6. 06	1. 358	5	6. 07	1. 361	2	6. 087
422	1. 23	80	6. 03	1. 22	40	5. 98	1. 241	50	6. 08	1. 241	20	6. 080	1. 2424	8	6. 086
511	1. 16	60	6. 03	1. 15	30	5. 98	1. 170	30	6. 08	1. 171	10	6. 085	1. 1707	4	6. 083
440	1. 07	10	6. 05	1. 06	20	6. 00	1. 074	20	6. 08	1. 076	10	6. 087	1. 0757	2	6. 085
531	1. 02	20	6. 03	1. 017	20	6. 02	1. 028	40	6. 08	1. 027	20	6. 076	1. 0286	3	6. 085
600	---	--	--	---	--	--	---	-	--	---	-	---	1. 0141	<1	6. 085
620	0. 955	10	6. 04	0. 952	30	6. 02	0. 961	30	6. 08	0. 961	5	6. 078	0. 9622	2	6. 086
533	---	--	--	. 919	20	6. 03	. 927	20	6. 08	. 928	5	6. 085	. 9282	1	6. 087
444	---	--	--	---	--	--	---	-	--	. 877	5	6. 076	. 8784	2	6. 086
711	---	--	--	. 844	20	6. 03	---	-	--	. 851	5	6. 077	. 8519	1	6. 084
642	---	--	--	. 806	30	6. 03	---	-	--	. 813	10	6. 084	. 8130	2	6. 084
731	---	--	--	. 787	20	6. 04	---	-	---	. 792	10	6. 083	. 7921	1	6. 084
Average of last five lines			6. 04	---	--	6. 03	---	-	6. 08	---	-	6. 081	----	-	6. 085

Nickel Sulfate Hexahydrate (retgersite), $NiSO_4 \cdot 6H_2O$ (tetragonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–0388	4. 26 4. 6 2. 72	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
1–0389	--	--------	This is a continuation of the previous card.

Additional published patterns

Source	Radiation	Wavelength
Borghijs [2] 1937----------	Copper	Kα

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 optically negative with the indices of refraction $N_o=1.513$ 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	112	004, 111	204
National Bureau of Standards.	112	004	203

Structural data. Beevers and Lipson [3] in 1932 determined that nickel sulfate hexahydrate has the space group D_4^4–$P4_12_12$ (or its enantiomorph D_4^8–$P4_32_1$) with $4(NiSO_4{\cdot}6H_2O)$ per unit cell. Nickel sulfate hexahydrate is used as a structure-type.

Several unit-cell 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

		a	c
		A	A
1932	Beevers and Lipson [3]	6.80	18.3
1937	Borghijs [2]	6.790	18.249
1949	Frondel and Palache [4]	6.779	18.24
1957	National Bureau of Standards.	6.782	18.28 at 25°C

The density of nickel sulfate hexahydrate calculated from the NBS lattice constants is 2.075 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] L. Borghijs, Over het tetragonale, enantiomorfe nickkelsulfaat met 6 aq., Natuurw. Tijdschr. Belg. **19**, 115–148 (1937).

[3] C. A. Beevers and H. Lipson, The crystal structure of nickel sulphate hexahydrate, $NiSO_4{\cdot}6H_2O$, Z. Krist. **83**, 123–135 (1932).

[4] C. Frondel and C. Palache, Retgersite, $NiSO_4{\cdot}6H_2O$, a new mineral, Am. Mineralogist **34**, 188–194 (1949).

Nickel Sulfate Hexahydrate (retgersite), $NiSO_4{\cdot}6H_2O$ (tetragonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1937 Borghijs Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
101	6.4	4	---	-	6.36	8
111	4.6	25	4.86	-	4.64	18
004					4.57	42
112	4.27	100	4.24	-	4.25	100
104	3.97	2	4.11	-	3.789	5
113	3.78	2	3.60	-	3.768	5
200	3.39	12	---	-	3.392	11
201	3.23	2	---	-	3.336	7
202	3.19	2	---	-	3.179	4
210	--	-	---	-	3.033	3
203	2.97	18	2.96	-	2.964	19
115	--	-	2.90	-	2.908	6
212	--	-	---	-	2.880	3
106	--	-	---	-	2.778	2
204	2.73	20	2.72	-	2.721	18
116	2.58	20	---	-	2.571	13
214	--	-	2.52	-	2.526	8
215	2.35	16	2.33	-	2.334	12
224	2.13	20	2.12	-	2.125	11
312	2.07	2	2.088	-	2.088	4
118	--	-	---	-	2.062	<1
313	2.02	4	2.022	-	2.023	7
225	--	-	---	-	2.006	<1
217	1.98	2	1.984	-	1.978	4
314	--	-	1.942	-	1.941	2
208	1.89	10	1.895	-	1.895	6
320	--	-	---	-	1.880	3
315	1.85	4	1.850	-	1.849	5
218	1.83	2	1.824	-	1.825	3
323	1.80	2	---	-	1.799	1
227	--	-	---	-	1.766	1
1·0·10						
316	1.75	10	1.751		1.755	6
324	--	-	---		1.740	1
1·1·10	1.70	8	1.721		1.708	5
401	--	-	1.687	-	1.688	4
219						
317	--	-	---	-	1.6559	2
228	1.65	8	1.653	-	1.6535	2
411	--	-	---	-	1.6372	3
403	--	-	1.616	-	1.6329	2
404	1.59	4	1.614	-	1.5888	<1
413						
229	-- [a]	-	1.540 [b]	-	1.5496	1

[a] Sixteen additional lines are omitted.
[b] Eight additional lines are omitted.

Potassium Bromate, $KBrO_3$ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0743	3. 21 3. 01 4. 39	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_o=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	012	110	101
Zachariasen	012	202	104
National Bureau of Standards	012	110	101

Structural data. Zachariasen [2] in 1928 determined that potassium bromate has the space group C_{3v}^5–R3m with 1($KBrO_3$) per unit rhombohedral cell or 3($KBrO_3$) 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	*c*
		A	*A*
1928	Zachariasen [2]	6. 018	8.157
1957	National Bureau of Standards.	6. 014	8.156 at 25° C

The density of potassium bromate calculated from the NBS lattice constants is 3.256 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] W. H. Zachairasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1928**, No. 4 (1928).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1928 Zachariasen Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
101	4. 39	50	4. 42	35	4. 39	60
012	3. 21	100	3. 23	100	3. 21	100
110	3. 01	63	3. 03	50	3. 008	70
003	2. 73	5	2. 75	10	2. 718	10
021	---	--	2. 46	15	2. 482	2
202	2. 18	50	2. 20	70	2. 196	49
113	2. 01	8	2. 02	10	2. 017	7
211	1. 89	25	1. 93	50	1. 914	10
104			1. 91	60	1. 899	16
122	1. 77	25	1. 78	20	1. 773	21
300	1. 73	10	1. 74	5	1. 737	11
024	1. 60	10	1. 61	10	1. 606	7
220	1. 50	10	1. 51	40	1. 504	11
303	1. 463	8	1. 47	5	1. 463	2
131	---	--	1. 42	50	1. 422	3
214	1. 415	25	1. 39	5	1. 416	11
205	1. 383	5	1. 37	40	1. 383	2
312	1. 361	15			1. 362	10
223	1. 238	15	1. 32	10	1. 3158	3
125	---	--	1. 26	10	1. 2561	1
116	---	--	1. 24	50	1. 2393	6
321	1. 180	10	1. 18	40	1. 1822	3
134					1. 1788	4
232	1. 142	10	1. 15	25	1. 1467	4
140		5	1. 14	25	1. 1367	4
404	1. 102	5	1. 10	10	1. 0973	1
306	1. 076	--	1. 09	5	1. 0701	2
027	---	--	1. 06	25	1. 0635	1
413	---	5	1. 05	10	1. 0488	2
324	1. 027		1. 03	20	1. 0310	3
045	---	--	1. 02	2. 5	1. 0174	<1
226	1. 006	5	1. 01	25	1. 0086	3
330	---	--	1. 00	25	1. 0022	3
018	---	--	---	---	1. 0006	4
241	---	--	---	---	0. 9774	<1
235	---	--	---	---	. 9638	<1
422	---	--	---	---	. 9568	1
208	---	--	---	---	. 9494	<1
333	---	--	---	---	. 9405	<1
511	---	--	---	---	. 9298	<1
054	---	--	---	---	. 9276	2
152	---	--	---	---	. 9119	3
137	---	--	---	---	. 9068	2
009						
244	---	--	---	---	. 8865	1
505	---	--	---	---	. 8780	<1
416	---	--	---	---	. 8720	4
600	---	--	---	---	. 8680	3
119						
514	---	--	---	---	. 8503	3
342	---	--	---	---	. 8380	3
250	---	--	---	---	. 8341	3
318	---	--	---	---	. 8329	2
063	---	--	---	---	. 8270	<1
155	---	--	---	--	. 8115	<1
336	---	--	---	---	. 8067	1
1·0·10	---	--	---	---	. 8058	<1
048	---	--	---	---	. 8030	<1
253	---	--	---	---	. 7975	<1
434	---	--	---	---	. 7895	2

Potassium Cyanate, KCNO (tetragonal)

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	112	200	211
National Bureau of Standards	112	200	211

Structural data. Hendricks and Pauling [2] in 1925 determined that potassium cyanate has potassium trinitride-type structure, the space group D_{4h}^{18}–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

		a	*c*
		A	*A*
1925	Hendricks and Pauling [2]	6. 082	7. 044
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)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25°C	
	d	*I*	*d*	*I*
	A		*A*	
110	4. 30	14	4. 31	16
002	------	----	3. 52	1
200	3. 05	50	3. 05	43
112	2. 74	100	2. 724	100
211	2. 54	30	2. 538	26
202	2. 30	30	2. 302	23
220	2. 14	20	2. 152	16
310	1. 92	25	1. 925	16
222	1. 84	12	1. 835	6
213	1. 77	10	1. 777	5
004	1. 75	10	1. 759	9
312	1. 68	20	1. 6885	11
321	------	----	1. 6414	2
114	1. 63	4	1. 6284	2
204	1. 52	12	1. 5232	7
402	1. 39	12	1. 3968	5
224	1. 36	20	1. 3616	8
332	1. 33	12	1. 3279	7
314	1. 30	8	1. 2983	4
422	1. 27	2	1. 2690	2
215	------	----	1. 2499	1
510	1. 19	2	1. 1931	<1
404	1. 15	2	1. 1503	<1
116	1. 13	8	1. 1311	4
206	------	----	1. 0939	1
424	1. 07	6	1. 0761	4
226	------	----	1. 0294	<1
600	------	----	1. 0140	<1
316	1. 00	4	1. 0010	3
514	------	----	0. 9876	<1
620	------	----	. 9622	<1
217	------	----	. 9427	<1
406	------	----	. 9288	<1
444	------	----	. 9178	<1

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] 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, K_2TiF_6 (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–1218	2. 18 3. 39 2. 85	Molybde-num.	Hanawalt, Rinn, and Frevel [1] 1938.

Card number 1–1218 is listed as $K_2TiF_6 \cdot H_2O$. The *d*-values of the pattern can be indexed according to the structure data given for anhydrous K_2TiF_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_o=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	201	101	110
National Bureau of Standards	101	201	110

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

Lattice constants

		a	*c*
		A	*A*
1952	Siegel [2]	5. 715	4.656
1957	National Bureau of Standards.	5. 7271	4.6619 at 25° C.

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

References

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

[2] S. Siegel, The crystal structure of K_2TiF_6, Acta Cryst. **5**, 683–684 (1952).

Potassium Metaperiodate, KIO_4 (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0618	3. 41 5. 2 2. 11	Molybdenum	Hanawalt, Rinn, and 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_o=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	112	101	204
Hylleraas	112	312	411, 208
National Bureau of Standards.	112	101	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 Hylleraas has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

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

The density of the potassium metaperiodate calculated from the NBS lattice constant is 3.690 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] E. Hylleraas, The atomic arrangement in the tetragonal crystals of $K_2I_2O_8$ potassium metaperiodate, Z. Physik. **39**, 308–321 (1926).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1926 Hylleraas Fe, 1.9360 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
101	5. 2	40	5. 21	20	5. 22	59
112	3. 40	100	3. 42	100	3. 41	100
004	3. 14	16	3. 17	20	3. 15	15
200	2. 86	16	2. 88	30	2. 867	20
202	----	---	------	---	2. 608	2
211	2. 51	10	2. 52	25	2. 512	10
114	----	---	------	---	2. 487	4
105	2. 31	1	------	---	2. 306	3
213	2. 17	3	2. 19	10	2. 187	6
204	2. 11	24	2. 13	50	2. 121	25
220	2. 02	8	2. 04	25	2. 027	9
301	----	---	1. 871	35	1. 890	14
116	1. 86	16	------	---	1. 8660	10
215	1. 79	6	1. 806	15	1. 7977	7
312	1. 74	24	1. 750	60	1. 7409	24
224	1. 70	8	1. 713	35	1. 7042	18
321 008	1. 57	5	1. 580	15	1. 5783	6
305	1. 52	1	------	---	1. 5230	3
323	----	---	1. 493	5	1. 4869	4
217	1. 470	1	1. 468	10	1. 4733	3
400	1. 427	1	1. 439	10	1. 4328	5
411 208	----	---	1. 381	60	1. 3812	7
316	1. 371	16	------	---	1. 3720	11
413 332	1. 317	3	1. 328	25	1. 3209	7
404	1. 301	1	1. 3096	20	1. 3044	3
420	1. 276	2	1. 2871	25	1. 2816	4
228	1. 240	2	1. 2480	15	1. 2433	3
415	----	---	------	---	1. 2174	1
1·1·10	----	---	1. 2075	15	1. 2030	4
424	----	---	1. 1918	35	1. 1875	22
501	----	---	------	---	1. 1416	2
336	----	---	------	---	1. 1361	2
512 503	----	---	------	---	1. 1065	3
521 408	----	---	------	---	1. 0604	<1
0·0·12	----	---	------	---	1. 0506	1
505	----	---	------	---	1. 0430	2
3·1·10	----	---	------	---	1. 0348	2
440	----	---	------	---	1. 0132	1
428	----	---	------	---	0. 9944	2
516	----	---	------	---	. 9908	1
532	----	---	------	---	. 9711	3
507	----	---	------	---	. 9670	1
444	----	---	------	---	. 9643	<1
600	----	---	------	---	. 9551	1
3·3·10	----	---	------	---	. 9214	1
613	----	---	------	---	. 9192	1
604	----	---	------	---	. 9138	1
620	----	---	------	---	. 9062	<1
536	----	---	------	---	. 8898	3
615	----	---	------	---	. 8826	1
624	----	---	------	---	. 8705	2
448 631	----	---	------	---	. 8520	2

Potassium Permanganate, $KMnO_4$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0725	3. 22 2. 95 3. 57	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 measurements. The *d*-values reported by Hanawalt, 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	211	112	210
McCrone	211	210	112
National Bureau of Standards	211	210	112

Structural data. Basche and Mark [3] in 1926 determined that potassium permanganate has barium sulfate-type structure, the space group D_{2h}^{16}–Pnma, and $4(KMnO_4)$ per unit cell.

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] W. C. McCrone, Potassium permanganate, $KMnO_4$, Anal. Chem. **22**, 1459 (1950).

[3] W. Basche and H. Mark, Über die Struktur von Verbindungen des Typus $MeXO_4$, Z. Krist. **64**, 1–70 (1926).

[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: $KMnO_4$–$KClO_4$–H_2O and NH_4Cl–$MnCl$–H_2O, J. Chem. Phys. **8**, 645 (1940).

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

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1926	Basche and Mark [3]	8. 86	5. 66	7. 24
1931	Mooney [4]	9. 11	5. 73	7. 42
1940	Greenberg and Walden [5].	9. 117	5. 7191	7. 426 at 23 to 29° C.
1950	McCrone [2]	9. 098	5. 730	7. 394
1957	National Bureau of Standards.	9. 122	5. 715	7. 430 at 25° C.

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

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1950 McCrone ----		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
101	5. 7	8	5. 72	21	5. 79	13
200 011	4. 56	50	4. 54	50	4. 57 4. 53	11 47
201	3. 90	8	3. 85	21	3. 89	22
002	3. 72	30	3. 70	35	3. 718	44
210	3. 58	60	3. 54	90	3. 567	93
102	3. 44	4	3. 42	35	3. 437	21
211	3. 23	100	3. 21	100	3. 217	100
112	2. 96	80	2. 94	82	2. 948	73
202	2. 87	40	2. 87	54	2. 879	34
020	--	--	--	--	2. 861	36
212	2. 57	30	2. 56	37	2. 574	28
---	--	--	2. 43	vw	---	--
302	--	--	2. 34	vw	2. 353	1
221	--	--	2. 28	9	2. 305	1
113 203	2. 19	60	2. 18	65	2. 202 2. 177	31 44
213	2. 03	2	1. 98	vw	2. 034	1
303	1. 93	4	1. 91	12	1. 920	10
004 412	1. 84	20	1. 84	22	1. 857 1. 839	14 14
123	--	--	--	--	1. 835	12
104	--	--	1. 81	22	1. 820	20
230	1. 74	10	1. 75	7	1. 755	7
223	--	--	1. 73	18	1. 731	21
511	--	--	1. 71	15	1. 693	1
403	1. 68	8	1. 66	15	1. 676	9
---	--	--	1. 63	vw	---	--
323	1. 60	6	1. 59	12	1. 595	7
124	1. 54	2	1. 53	vw	1. 535	2

Rubidium Bromide, RbBr (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–0616	3. 41 2. 41 1. 97	----------	Davey [1] 1923.
1–0609	3. 43 2. 42 1. 53	Molybdenum	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	200	220	222
Hanawalt, Rinn, and Frevel	200	220	420
National Bureau of Standards	200	220	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

		A
1921	Davey [3]	6. 944
1922	Posnjak and Wyckoff [4]	6. 94
1923	Davey [1]	6. 840
1924	Havighurst, Mack, and and Blake [5].	6. 882
1926	Ott [6]	6. 868
1948	Mehmel [7]	6. 86
1957	National Bureau of Standards.	6. 889 at 25° C

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	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
200	3. 42	100	6. 84	3. 44	100	6. 88	3. 44	100	6. 88
220	2. 41	67	6. 82	2. 42	57	6. 84	2. 436	73	6. 891
222	1. 974	20	6. 838	1. 97	17	6. 82	1. 989	25	6. 890
400	1. 706	7	6. 824	1. 71	11	6. 84	1. 722	11	6. 887
420	1. 530	20	6. 887	1. 53	34	6. 84	1. 541	23	6. 892
422	1. 399	13	6. 854	1. 40	23	6. 86	1. 406	15	6. 890
440	1. 213	3	6. 862	----	---	----	1. 218	4	6. 888
600	1. 142	7	6. 852	1. 14	11	6. 84	1. 148	7	6. 889
620	1. 085	3	6. 862	----	---	----	1. 0892	5	6. 889
622	1. 032	3	6. 846	----	---	----	1. 0384	4	6. 888
444	-----	---	-----	----	---	----	0. 9946	2	6. 891
640	-----	---	-----	----	---	----	. 9554	3	6. 889
642	-----	---	-----	----	---	----	. 9207	4	6. 890
800	-----	---	-----	----	---	----	. 8611	<1	6. 889
820	-----	---	-----	----	---	----	. 8353	2	6. 888
822	-----	---	-----	----	---	----	. 8111	<1	6. 888
662	-----	---	-----	----	---	----	. 7902	<1	6. 889
Average of last five lines			6. 855	----	---	6. 84	------	---	6. 889

References

[1] W. P. Davey, Precision measurements of crystals of the alkali halides, Phys. Rev. **21,** 143–161 (1923).
[2] J. W. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. **10,** 457–512 (1938).
[3] W. P. Davey, The cubic shapes of certain ions as confirmed by X-ray crystal analysis, Phys. Rev. **17,** 402–403 (1921).
[4] E. Posnjak and R. W. G. Wyckoff, The crystal structures of the alkali halides, J. Wash. Acad. Sci. **12,** 248–251 (1922).
[5] R. J. Havighurst, E. Mack, and F. C. Blake, Precision crystal measurements on some alkali and ammonium halides, J. Am. Chem. Soc. **46,** 2368–2374 (1924).
[6] H. Ott, Die Strukturen von MnO, MnS, AgF, NiS, SnJ_4, $SrCl_2$, BaF_2; Präzisionsmessungen einiger Alkalihalogenide, Z. Krist. **63,** 222–230 (1926).
[7] M. Mehmel, Kristallchemische Betrachtungen zur I. und VII. Gruppe des periodischen Systems der Elemente, Optik **3,** 41–46 (1948).

Silver Chlorate, $AgClO_3$ (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	202	422	622
National Bureau of Standards	202	220	200

Structural data. Náray-Szabó and Pócza [2] in 1942 determined that silver chlorate has the space group C_{4h}^5–I4/m with 8($AgClO_3$) 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 Harang Cr, 2.2909 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		A	
101	------	--	5. 81	6
200	4. 27	m	4. 25	38
002	3. 95	w	3. 973	15
211	3. 44	m	3. 429	31
220	3. 01	s	3. 006	46
202	2. 90	vs	2. 900	100
310	2. 70	vw	2. 688	5
301	2. 65	vw	2. 668	4
103	------	--	2. 527	4
222	2. 39	m	2. 395	22
321	2. 25	w	2. 260	6
213	2. 17	m	2. 171	15
400	2. 12	s	2. 124	25
004	------	--	1. 9844	4
420	1. 90	s	1. 9012	20
402	1. 87	m	1. 8739	10
204	------	--	1. 7984	3
323	1. 76	w	1. 7593	7
422	1. 71	vs	1. 7146	22
510	------	--	1. 6665	2
501	------	--	1. 6620	5
224	1. 66	m	1. 6556	9
413	------	--	1. 6263	2
314	------	--	1. 5973	1
105	------	--	1. 5603	3
521	------	--	1. 5485	2
440	1. 50	w	1. 5027	3
215	------	--	1. 4646	3
404	1. 45	w	1. 4505	3
503	1. 43	w	1. 4302	3
600	------	--	1. 4165	1
442	1. 40	w	1. 4054	4
305	------	--	1. 3844	1
611	------	--	1. 3759	2
424	------	--	1. 3727	1
532	------	--	1. 3686	1
620	1. 34	s	1. 3438	3
602	1. 33	s	1. 3338	4
325	------	--	1. 3170	2
622	1. 27	vs	1. 2728	4
206	------	--	1. 2635	1
415	------	--	1. 2576	1
613	------	--	1. 2353	2
444	------	--	1. 1983	2
316 543	------	--	1. 1870	2
640	------	--	1. 1787	2
505	------	--	1. 1599	1
604	------	--	1. 1528	1
633	------	--	1. 1423	<1
642	------	--	1. 1298	2
525	------	--	1. 1194	1
624	------	--	1. 1125	1
336 703	------	--	1. 1038	<1

Lattice constants

		a	*c*
		A	*A*
1927	Ferrari and Fontana [3]	8. 50	7. 93
1928	Zachariasen [4]	8. 492	7.92
1942	Náray-Szabó and Pócza [2].	8. 503	7.91
1957	National Bureau of Standards.	8. 498	7.938 at 25° C

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

References

[1] L. Harang, Über die Kristallstruktur der tetragonalen Verbindungen $AgClO_3$ und $AgBrO_3$, Z. Krist. **66,** 399–407 (1927).

[2] St. Náray-Szabó and J. Pócza, Die Struktur des Silberchlorats $AgClO_3$, Z. Krist. **104,** 28–38 (1942).

[3] A. Ferrari and C. G. Fontana, La struttura del clorato d'argento, Rend. accad. Lincei **6,** 312–314 (1927).

[4] W. H. Zachariasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat-Naturv. Kl. **1928,** No. 4 (1928).

Silver Molybdate, Ag_2MoO_4 (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–1002	2. 81 1. 78 1. 64	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
3–1317	[a]	[a]	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	311	511	440
National Bureau of Standards	311	440	511

Structural data. Wyckoff [2] in 1922 determined that silver molybdate has magnesium aluminate-type structure, the space group O_h^7–Fd3m, and $8(Ag_2MoO_4)$ 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

		A
1922	Wyckoff [2]	9.28
1957	National Bureau of Standards.	9.3127 at 25° C

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	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	5. 3	6	9. 18	5. 38	7	9. 31
220	3. 29	17	9. 31	3. 292	28	9. 31
311	2. 81	100	9. 32	2. 808	100	9. 31
222	2. 69	17	9. 28	2. 689	26	9. 32
400	2. 32	14	9. 28	2. 329	17	9. 32
331	2. 12	5	9. 24	2. 138	5	9. 32
422	1. 89	6	9. 26	1. 900	9	9. 31
511	1. 78	42	9. 25	1. 792	30	9. 312
440	1. 64	43	9. 28	1. 6461	32	9. 313
531	---	--	--	1. 5754	2	9. 320
620	1. 478	1	9. 35	1. 4725	3	9. 313
533	1. 425	11	9. 34	1. 4201	8	9. 312
622	1. 409	11	9. 35	1. 4037	8	9. 311
444	1. 358	1	9. 41	1. 3444	3	9. 313
642	1. 248	5	9. 34	1. 2444	4	9. 312
731	1. 213	17	9. 32	1. 2125	14	9. 313
800	1. 166	3	9. 33	1. 1638	3	9. 310
822	1. 099	1	9. 33	1. 0975	3	9. 313
751	1. 077	9	9. 33	1. 0753	6	9. 312
662	---	--	--	1. 0683	2	9. 313
840	1. 045	1	9. 35	1. 0412	1	9. 313
664	---	--	--	0. 9928	1	9. 314
931	0. 980	2	9. 35	. 9761	3	9. 312
844	. 953	5	9. 34	. 9503	5	9. 311
10·2·0	. 917	1	9. 35	. 9134	2	9. 3147
951	---	--	--	. 9003	5	9. 3128
10·2·2	---	--	--	. 8961	3	9. 3127
10·4·2	---	--	--	. 8501	2	9. 3125
11·1·1	---	--	--	. 8397	2	9. 3129
880	---	--	--	. 8231	2	9. 3127
10·6·0	---	--	--	. 7985	2	9. 3121
11·3·3	---	--	--	. 7899	4	9. 3129
10·6·2	---	--	--	. 7871	4	9. 3130
Average of last five lines			9. 34	----	---	9. 3127

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. W. G. Wyckoff, The crystal structure of silver molybdate, J. Am. Chem. Soc. **44,** 1994–1998 (1922).

Silver Sulfate, Ag_2SO_4 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0961	2. 86 3. 17 2. 64	Molybdenum.	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 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	113	040	220
National Bureau of Standards	113	220	040

Structural data. Herrmann and Ilge [1] in 1931 determined that silver sulfate has sodium sulfate-type 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

		a	*b*	*c*
		A	*A*	*A*
1931	Herrmann and Ilge [1].	5. 859	12. 684	10. 271
1957	National Bureau of Standards.	5. 8167	12. 704	10. 269 at 25°C

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

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
111	4. 71	7	4. 71	12
022	3. 98	27	3. 994	27
040	3. 17	53	3. 173	73
113	2. 86	100	2. 873	100
220	2. 64	53	2. 644	86
202	2. 52	11	2. 529	20
133	2. 41	33	2. 420	34
222	2. 35	1	2. 350	4
151	2. 27	8	2. 271	9
242	1. 97	11	1. 979	11
062	------	----	1. 957	8
153	1. 91	40	1. 925	36
311	------	----	1. 883	5
135	1. 75	3	1. 761	6
331	-------	----	1. 7375	3
260	1. 70	13	1. 7113	19
313	1. 66	9	1. 6726	11
026	1. 64	7	1. 6513	6
------	1. 58	1	------	----
333	1. 56	9	1. 5666	11
173	1. 53	9	1. 5459	10
206	1. 465	5	1. 4746	4
400	1. 447	1	1. 4545	4
353	1. 400	7	1. 4059	7
422	1. 361	1	1. 3665	4
335 246	1. 330	11	1. 3372	6
066	------	----	1. 3310	1
440	------	----	1. 3224	7
193	1. 270	4	1. 2736	6
373	1. 230	5	1. 2362	6
048	1. 187	1	1. 1883	2
444	------	----	1. 1775	3
317	1. 161	4	1. 1651	3
228	------	----	1. 1557	3
------	1. 112	3	------	----
513	1. 091	4	1. 0979	2
426	------	----	1. 0925	2
139 393	------	----	1. 0825	3
286	------	----	1. 0807	3
480	1. 075	3	1. 0724	4
533	------	----	1. 0661	4
553	------	----	1. 0101	3
484	------	----	0. 9895	2
466	------	----	. 9817	3
620	------	----	. 9583	2
3·11·3 179	------	----	. 9531	2
622	------	----	. 9416	3

References

[1] K. Herrmann and W. Ilge, The structure of silver sulfate, Z. Krist. **80**, 402–415 (1931).

[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).

Sodium Iodate, $NaIO_3$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0916	2. 93 4. 25 3. 19	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [2] 1928------	Copper	K_α

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.	021, 112	110	020
Zachariasen----------	021, 112	312,204	132
National Bureau of Standards.	021	110	020

Structural data. MacGillavry and Panthaleon [3] in 1943 determined that sodium iodate has the space group D_{2h}^{16}–Pbnm and 4($NaIO_3$) 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, Rinn, and Frevel Mo, 0.7107 A		1928 Zachariasen Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
110	4. 27	50	4. 28	50	4. 28	83
002	4. 06	20	4. 05	20	4. 07	29
111	---	-	---	-	3. 784	5
020	3. 21	30	3. 23	20	3. 202	34
021	2. 95	100	2. 98	100	2. 978	100
112					2. 947	22
200	2. 88	9	2. 89	20	2. 875	1
210	---	-	---	-	2. 623	3
022	2. 52	25	2. 52	40	2. 516	20
103	---	-	---	-	2. 4525	2
202	2. 33	9	2. 36	40	2. 3486	11
122	---	-	---	-	2. 3041	<1
220	2. 12	20	2. 13	50	2. 1391	22
004	2. 02	7	2. 03	30	2. 0342	9
130	1. 98	5	1. 993	10	1. 9993	6
131	---	-	---	-	1. 9414	3
222	1. 88	10	1. 893	20	1. 8926	14
301	---	-	---	-	1. 8664	1
114	1. 82	13	1. 839	30	1. 8360	17
132	1. 78	25	1. 794	60	1. 7948	26
024	1. 70	10	1. 714	20	1. 7163	12
312	1. 66	30	1. 669	70	1. 6732	21
204					1. 6606	7
040	1. 60	1	1. 602	5	1. 5999	4
042	---	-	---	-	1. 4886	3
224	1. 470	10	1. 476	30	1. 4731	9
400	1. 431	8	1. 428	30	1. 4373	2
330					1. 4257	8
331	-----	-	---	-	1. 4037	3
240	1. 393	4	1. 400	10	1. 3977	5
043	-----	-	---	-	1. 3787	3
314	-----	-	1. 361	30	1. 3627	4
006	-----	-	---	-	1. 3558	4
332	1. 351	8	1. 346	30	1. 3454	6
242	-----	-	1. 323	20	1. 3222	3
420	1. 314	4	1. 315	10	1. 3114	7
116	1. 287	6	1. 291	30	1. 2923	5
044	1. 251	6	---	-	1. 2576	3
026	-----	-	1. 249	30	1. 2481	10
152	1. 191	3	---	-	1. 1937	3
404	1. 171	2	---	-	1. 1739	2
334	-----	-	---	-	1. 1675	2
244	1. 149	3	---	-	1. 1519	2
226	-----	-	---	-	1. 1449	<1
510	-----	-	---	-	1. 1318	<1
117	1. 122	2	---	-	1. 1218	4
424	1. 103	1	---	-	1. 1018	4
316	1. 091	2	---	-	1. 0903	7
512						
440	---	-	---	-	1. 0692	4
060	---	-	---	-	1. 0666	<1

Sodium Iodate, $NaIO_3$ (orthorhombic)—Con.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1928 Zachariasen Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
154	--	-	---	-	1. 0645	<1
350						
442	---	-	---	-	1. 0339	3
352	---	-	---	-	1. 0295	4
530	---	-	---	-	1. 0121	3
260	--	-	---	-	1. 0001	<1
261	--	-	---	-	0. 9922	<1
063						
118	--	-	---	-	. 9890	1
514						
336	--	-	---	-	. 9824	4
532						
246	--	-	---	-	. 9727	2
262	--	-	---	-	. 9710	2
208	--	-	---	-	. 9587	2
600						
444	---	-	---	-	. 9464	1
354	---	-	---	-	. 9432	2

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1928	Zachariasen [2]	5. 76	6. 38	8. 12
1943	MacGillavry and Panthaleon [3].	5. 75	6. 38	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

[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] W. H. Zachariasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1928,** No. 4, (1928).

[3] C. H. MacGillavry and C. L. Van Eck Panthaleon, The crystal structure of sodium and ammonium iodate, Recueil des Travaux Chim. des Pays-Bas, **62,** 729–735 (1943).

[4] I. Naráy-Szabó and J. Neugebauer, The crystal structure of sodium iodate, J. Am. Chem. Soc. **69,** 1280–1283 (1947).

Sodium Metaperiodate, $NaIO_4$ (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 $N_o=1.705$ 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^6_{4h}–$I4_1/a$, 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	*c*
		A	*A*
1926	Kirkpatrick and Dickinson [1].	5. 333	11. 95
1938	Hazlewood [2]	5. 3330	11. 95
1957	National Bureau of Standards.	5. 3372	11. 952 at 25° C

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

References

[1] 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 $NaIO_4$, a determination of the oxygen parameters for $NaIO_4$, Z. Krist. [A] **98,** 439–446 (1938).

Sodium Metaperiodate, $NaIO_4$ (tetragonal)

hkl	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		*hkl*	1957 National Bureau of Standards Cu, 1.5405 A, 25° C		*kkl*	1957 National Bureau of Standards Cu, 1.5402 A, 25° C	
	d	*I*		*d*	*I*		*d*	*I*
	A			*A*			*A*	
101	4. 87	89	404	1. 2184	3	444	. 8997	2
112	3. 191	100	420	1. 1936	3			
004	2. 988	12	228	1. 1716	2	600	. 8896	<1
200	2. 669	17	219	1. 1608	1	2·2·12	. 8809	2
202	2. 437	2				3·2·11	. 8758	2
			1·1·10	1. 1396	2	3·3·10	. 8665	2
114	2. 343	21	318	1. 1184	1	2·1·13	. 8579	2
105	2. 182	4	327					
213	2. 048	9	406	1. 1081	9	3·1·12	. 8577	2
204	1. 991	38	424			518	. 8571	6
220	1. 887	12				527		
			309	1. 0638	4	446	. 8526	1
116	1. 761	19	336			604		
215	1. 689	10	417	1. 0319	4			
303	1. 624	26	503	1. 0311	6	620	. 8438	2
312			512			1·1·14	. 8326	4
206	1. 595	13				4·1·11	. 8320	6
224			0·0·12	0. 9954	2	509		
			408			615	. 8237	3
008	1. 494	2	2·1·11	. 9886	3			
314	1. 469	5	329			543	. 8159	3
321			3·1·10	. 9751	4	606	. 8122	4
305	1. 426	5				624		
118	1. 3882	8	338	. 9619	1	4·0·12	. 7982	3
217			523			448	. 7978	5
			440	. 9435	1			
400	1. 3341	6	2·0·12	. 9332	4	631	. 7938	12
208	1. 3033	15	3·0·11	. 9269	5	1·0·15	. 7879	3
109	1. 2884	12	419			5·1·10	. 7874	8
325	1. 2584	3						
307			525	. 9154	2			
413	1. 2312	7	1·0·13	. 9061	2			
			507					
332			532	. 9048	4			

Sodium Perchlorate, $NaClO_4$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0552	3. 53 3. 97 2. 95	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 $2V\cong10°$.

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	020	111	102
Zachariasen	020	022	111
National Bureau of Standards	020	111	102

Structural data. Zachariasen [3] in 1930 determined that sodium perchlorate has barium sulfate-type structure, the space group D_{2h}^{17}–Amma, and 4($NaClO_4$) 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

		a	*b*	*c*
		A	*A*	*A*
1930	Zachariasen [3]	7. 07	7. 09	6. 49
1957	National Bureau of Standards.	7. 055	7. 088	6. 519 at 25° C.

The density of sodium perchlorate calculated from the NBS lattice constan ts is 2.494 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] 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, $NaClO_4$, Z. Krist. **73,** 141–146 (1930).

Sodium Perchlorate, $NaClO_4$ (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1930 Zachariasen Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
011	4. 80	8	4. 80	w	4. 80	8
111	3. 98	53	3. 97	s	3. 97	63
020	3. 54	100	3. 55	vs	3. 54	100
002	3. 26	7	3. 25	w	3. 260	7
102	2. 96	53	2. 95	s	2. 960	38
211	2. 86	17	2. 85	m	2. 839	13
220	2. 51	4	2. 51	m	2. 498	4
022	2. 40	40	2. 396	vs	2. 400	26
-----	--	-	2. 390	vw	----	--
122	2. 27	17	2. 267	m	2. 271	11
031	--	-	2. 220	mw	2. 222	5
131	2. 12	5	2. 117	w	2. 118	2
311			2. 113	w	2. 112	3
013	2. 07	4	2. 069	w	2. 077	2
222	1. 98	7	1. 982	w	1. 983	3
302	1. 90	33	1. 909	s	1. 907	15
231			1. 881	w	1. 879	<1
040	1. 77	13	1. 774	m	1. 772	4
400			1. 768	m	1. 763	3
322	1. 68	20	---	-	1. 680	9
411	--	-	---	-	1. 655	3
331	1. 62	1	---	-	1. 616	<1
240	1. 58	3	---	-	1. 584	2
420	1. 56	11	---	-	1. 580	4
142	1. 52	5	---	-	1. 521	2
024	--	-	---	-	1. 480	<1
233	--	-	---	-	1. 457	1
124	--	-	---	-	1. 450	2
242	--	-	---	-	1. 424	3
422	--	-	---	-	1. 4211	2
224	--	-	---	-	1. 3651	1
151	--	-	---	-	1. 3590	<1
511	--	-	---	-	1. 3536	<1
304	--	-	---	-	1. 3395.	<1

Strontium Molybdate, $SrMoO_4$ (tetragonal)

ASTM cards. None.

Additional published patterns

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

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	112	312, 303	204
Broch	112	204	312, 303
National Bureau of Standards.	112	204	312, 303

Structural data. Broch [2] in 1925 determined that strontium molybdate has calcium tungstate-type structure, the space group C_{4h}^6–$I4_1/a$, and 4($SrMoO_4$) 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	*c*
		A	*A*
1925	Zambonini and Levi [1]	5. 37	11. 96
1929	Broch [2]	5. 39	11. 99
1957	National Bureau of Standards.	5. 3944	12. 020 at 25° C

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

Strontium Molybdate, $SrMoO_4$ (tetragonal)

hkl	1925 Zambonini and Levi Cu, 1.5418 A		1930 Broch Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
101	---	-	----	-	4. 92	3
112	3. 08	vs	3. 21	vvs	3. 222	100
004	2. 91	m	3. 01	m	3. 006	16
200	2. 61	mw	2. 70	s	2. 698	21
202	---	-	----	-	2. 461	1
114	---	-	2. 37	vvw	2. 362	6
213	---	-	----	-	2. 067	<1
204	1. 95	s	2. 010	vvs	2. 008	30
220	1. 86	m	1. 911	s	1. 907	12
116	1. 74	s	1. 774	vs	1. 774	17
312	1. 61	vs	1. 642	vvs	1. 642	25
303						
224	1. 58	ms	1. 611	vs	1. 611	11
008	---	-	----	-	1. 503	2
---	---	-	1. 444	vw	------	---
217	--	-	----	-	1. 399	1
118						
400	---	-	1. 350	vw	1. 3486	4
208	1. 29	s	1. 312	s	1. 3129	7
316	1. 28	s	1. 298	s	1. 2994	11
332	1. 23	mw	1. 244	s	1. 2441	7
413						
404	1. 21	w	1. 231	s	1. 2308	6
420	1. 19	mw	1. 206	s	1. 2064	6
228	1. 17	mw	1. 1810	m	1. 1807	3
1·1·10	1. 14	mw	1. 1464	m	1. 1467	4
424	1. 11	m	1. 1198	vs	1. 1193	7
406						
336	1. 06	w	1. 0737	m	1. 0736	3
512	--	-	1. 0426	vs	1. 0420	6
503						
408	1. 03	mw	1. 0039	m	1. 0036	3
0·0·12	0. 999	mw	----	-	1. 0011	2
3·1·10	. 977	m	0. 9830	s	0. 9826	4
440	---	-	----	-	. 9536	<1
428	---	-	. 9413	vs	. 9406	5
2·0·12	---	-	----	-	. 9389	2
516	. 937	mw	----	-	. 9355	4
532	---	-	----	-	. 9143	5
444	. 911	m	----	-	. 9089	3
600	---	-	----	-	. 8990	<1
2·2·12	---	-	----	-	. 8868	3
3·3·10	. 871	w	----	-	. 8735	2
604	. 860	w	----	-	. 8614	2
446						
620	. 853	mw	----	-	. 8529	2
536	. 840	ms	----	-	. 8399	5
1·1·14	---	-	----	-	. 8376	4
606	. 820	ms	----	-	. 8205	5
624						
448	---	-	----	-	. 8051	3
4·0·12	. 806	ms	----	-	. 8041	3
545	. 795	m	----	-	. 7950	5

References

[1] 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 Sulfide, SrS (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
2–0659	3. 00 2. 12 3. 47	Molybdenum	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	200	220	111
Holgersson	200	220	420
National Bureau of Standards	200	220	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.

Strontium Sulfide, SrS (cubic)

hkl	---- General Electric Co. Mo, 0.7107 A			1923 Holgersson Cu, 1.5418 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
111	3. 48	70	6. 03	-------	----	-------	3. 479	29	6. 03
200	3. 01	100	6. 02	2. 91	vs	5. 81	3. 007	100	6. 02
220	2. 12	100	6. 00	2. 06	vs	5. 83	2. 129	51	6. 02
311	1. 816	50	6. 023	1. 759	m	5. 83	1. 814	14	6. 02
222	1. 738	60	6. 021	1. 689	s	5. 85	1. 7378	16	6. 020
400	1. 506	40	6. 024	1. 460	s	5. 84	1. 5045	11	6. 018
331	1. 381	20	6. 020	1. 343	m	5. 85	1. 3814	6	6. 021
420	1. 347	70	6. 024	1. 310	vs	5. 85	1. 3464	14	6. 021
422	1. 229	60	6. 021	1. 199	s	5. 87	1. 2290	12	6. 021
511	1. 158	20	6. 017	1. 125	w	5. 85	1. 1584	4	6. 019
440	1. 064	20	6. 019	1. 039	w	5. 88	1. 0641	4	6. 020
531	1. 019	20	6. 028	-------	----	-------	1. 0174	4	6. 019
600	1. 005	50	6. 030	0. 985	s	5. 91	1. 0034	8	6. 020
620	-------	----	-------	. 935	m	5. 91	0. 9519	6	6. 020
533	-------	----	-------	. 893	s	5. 86	. 9182	<1	6. 021
622	-------	----	-------	-------	----	-------	. 9075	5	6. 020
444	-------	----	-------	. 858	w	5. 94	. 8691	<1	6. 020
711	-------	----	-------	. 826	w	5. 90	. 8430	<1	6. 020
640	-------	----	-------	-------	----	-------	. 8346	2	6. 018
642	-------	----	-------	-------	----	-------	. 8044	8	6. 020
731	-------	----	-------	-------	----	-------	. 7837	2	6. 020
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

		A
1923	Holgersson [1]	5.88
1926	Goldschmidt [2]	6.02
1927	Rumpf [3]	6.02
1948	Primak, Kaufman, and Ward [4].	6.020
1956	Güntert and Faessler [5]	6.0199 at 20° C
1957	National Bureau of Standards.	6.020 at 25° C

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

References

[1] 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, $SrWO_4$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
2-0507	3. 23 2. 71 2. 01	Molybdenum	General Electric Co., Wembley, England.

Additional published patterns

Source	Radiation	Wavelength
Broch [1] 1929	Chromium	Kα

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	112	200	204
Broch	112	204	312
National Bureau of Standards	112	204	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 $4(SrWO_4)$ per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1929	Broch [1]	5. 405	11. 90
1957	National Bureau of Standards.	5. 4168	11. 951 at 25° C

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

References

[1] 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, $SrWO_4$ (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	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
101	4. 93	60	---	-	4. 93	19
112	3. 23	100	3. 22	vvs	3. 223	100
004	2. 99	50	2. 99	m	2. 987	16
200	2. 71	70	2. 72	s	2. 707	24
211	2. 37	30	2. 38	vw	2. 373	7
114	--	-	---	-	2. 355	1
105	--	-	---	-	2. 187	<1
213	2. 07	10	---	-	2. 069	3
204	2. 01	70	2. 01	vvs	2. 007	30
220	1. 92	50	1. 916	s	1. 915	14
301	--	-	1. 790	vw	1. 786	1
116	1. 77	60	1. 767	vs	1. 768	19
215	1. 70	20	1. 700	vw	1. 702	4
312	1. 64	70	1. 649	vvs	1. 646	27
224	1. 61	50	1. 612	s	1. 612	14
008	1. 49	20	1. 490	w	1. 493	4
321					1. 490	4
305	1. 44	10	---	-	1. 4411	2
323	1. 40	10	---	-	1. 4059	2
217	1. 39	10	---	-	1. 3953	2
400	1. 35	10	1. 356	w	1. 3542	4
208	1. 31	20	1. 307	s	1. 3077	10
316	1. 28	30	1. 299	vs	1. 2989	16
332	1. 25	10	1. 248	s	1. 2488	7
404	1. 23	10	1. 234	m	1. 2335	6
420	--	-	1. 212	s	1. 2112	7
228	--	-	1. 178	s	1. 1781	4
1·1·10	--	-	1. 140	w	1. 1411	4
424	--	-	1. 123	vs	1. 1226	7
431	--	-	---	-	1. 0790	1
336	--	-	1. 076	w	1. 0749	3
512	--	-	1. 047	vs	1. 0462	7
408	--	-	1. 005	m	1. 0033	3
0·0·12	--	-	---	-	0. 9959	<1
505	--	-	---	-	. 9868	<1
3·1·10	--	-	0. 982	s	. 9801	6
440	--	-	---	-	. 9576	2
428	--	-	. 941	s	. 9408	5
516	--	-	---	-	. 9374	5
2·0·12	--	-	---	-	. 9349	5
525	--	-	---	-	. 9275	<1
532	--	-	---	-	. 9180	6
444	--	-	---	-	. 9118	3
600	--	-	---	-	. 9028	2
2·2·12	--	-	---	-	. 8835	3
3·3·10	--	-	---	-	. 8724	3
604	--	-	---	-	. 8642	2
620	--	-	---	-	. 8564	4
536	--	-	---	-	. 8419	6
4·1·11	--	-	---	-	. 8371	3
615	--	-	---	-	. 8345	2
528						
1·1·14	--	-	---	-	. 8331	3
624	--	-	---	-	. 8233	7
448	--	-	---	-	. 8061	3
529	--	-	---	-	. 8023	3
4·0·12						
545	--	-	---	-	. 7974	1
5·1·10	--	-	---	-	. 7939	5
633	--	-	---	-	. 7913	2

Sulfamic Acid, NH_3SO_3 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
3-0268	4. 06 3. 70 2. 73	Molybdenum.	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 $2V\cong60°$.

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	200, 120	012	212, 313
National Bureau of Standards.	112	012	120

Structural data. Brunt [1] in 1945 reported that sulfamic acid has the space group D_{2h}^{9}–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}^{15}–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	*b*	*c*
		A	*A*	*A*
1940	Brown [2]	8. 08	9. 24	8. 07
1945	Brunt [1]	8. 04	9. 08	7. 96
1955	Osaki, Tadokoro, and Nitta [3].	8. 115	9. 255	8. 066
1957	National Bureau of Standards.	8. 109	9. 240	8.068 at 25° C

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

Sulfamic Acid, NH_3SO_3 (orthorhombic)

hkl	Michigan Alkali Co. Mo, ------		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
111	------	----	4. 86	18
020	4. 62	20	4. 62	25
200	4. 07	100	4. 05	79
120			4. 01	84
012	3. 71	100	3. 699	86
201	------	----	3. 627	38
121	------	----	3. 594	20
112	3. 37	80	3. 366	100
220	3. 13	20	3. 048	9
022	------	----	3. 038	7
122	2. 88	20	2. 848	33
212	2. 74	100	2. 735	59
131			2. 712	37
222	2. 45	5	2. 4325	13
231	2. 35	5	2. 3486	12
320	------	----	2. 3363	11
040	------	----	2. 3109	8
321	------	----	2. 2418	4
203				
123	------	----	2. 2354	2
312	------	----	2. 1831	3
141	------	----	2. 1425	1
004	2. 01	10	2. 0158	6
223				
331	------	----	1. 9705	4
133	------	----	1. 9664	7
401				
241	1. 94	10	1. 9481	6
142			1. 9465	5
411	------	----	1. 9224	2
114	------	----	1. 9152	8
420	------	----	1. 8578	1
421	1. 82	25	1. 8094	14
204			1. 8057	12
412	------	----	1. 7765	1
323	------	----	1. 7615	9
151	------	----	1. 7583	10
341	------	----	1. 7157	4
143	------	----	1. 7128	6
034	------	----	1. 6871	1
431	------	----	1. 6570	1
134	1. 66	10	1. 6515	5
251			1. 6461	7
403	------	----	1. 6198	1
342	------	----	1. 6096	<1
413	1. 58 [a]	5	1. 5943	4

[a] Seven additional lines are omitted.

References

[1] 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).

Tellurium(IV) Oxide, TeO_2 (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0870	2. 99 3. 40 1. 87	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 TeO_2. 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., London. Their spectrographic analysis showed 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 measurements. 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	102	110	212
National Bureau of Standards	102	110	212

Structural data. Stehlik and Balak [2] in 1948 determined that tetragonal tellurium oxide has either the space group D_4^4–$P4_12_1$ or the space group D_4^8–$P4_32_1$. 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.

Lattice constants

		a	*c*
		A	*A*
1926	Goldschmidt [3]	4. 80	7.56
1949	Stehlik and Balak [2]	4. 805	7.609
1957	National Bureau of Standards.	4. 809	7.614 at 25° C

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

hkl	New Jersey Zinc Co. Mo, ------		1957 National Bureau of Standards Cu, 1.5405 A, 25°C	
	d	*I*	*d*	*I*
	A		*A*	
101	------	----	4. 07	9
110	3. 40	80	3. 40	88
111	------	----	3. 10	13
102	2. 99	100	2. 98	100
112	------	----	2. 536	1
200	2. 41	16	2. 407	20
201	------	----	2. 293	2
210	------	----	2. 151	2
211	------	----	2. 071	6
113, 202	------	----	2. 034	1
004	------	----	1. 903	8
212	1. 87	56	1. 872	65
203	------	----	1. 745	<1
220	1. 70	8	1. 700	12
114, 221	1. 66	32	1. 660	22
213	------	----	1. 6401	4
301	------	----	1. 5684	3
310	1. 52	8	1. 5210	12
204	1. 49	25	1. 4923	15
302	------	----	1. 4775	9
223, 312	------	----	1. 4127	2
303	------	----	1. 3554	1
321	------	----	1. 3139	2
313	------	----	1. 3048	<1
224	------	----	1. 2681	4
322	1. 26	14	1. 2590	4
215	------	----	1. 2433	1
106, 304	1. 22	10	1. 2270	5
400	------	----	1. 2020	<1
116, 314	1. 18	14	1. 1881	6
323	------	----	1. 1806	<1
411	------	----	1. 1531	<1
225	------	----	1. 1341	<1
331	------	----	1. 1212	<1
412	1. 11	4	1. 1158	2
216, 324	1. 09	6	1. 0928	4
403, 332	------	----	1. 0866	<1
315, 240	------	----	1. 0753	<1
421	------	----	1. 0647	<1
107, 413	------	----	1. 0601	<1
226, 404	------	----	1. 0164	1

References

[1] H. Inuzuka, The crystal structure of Tellurite, TeO_2, J. Geol. Soc. Tokyo **41**, 131–138 (1934).

[2] B. Stehlik and L. Balak, The crystal structure of tellurium dioxide, Coll. Czech Chem. Commun. **14**, 595–607 (1949).

[3] V. M. Goldschmidt, Geochemische Verteilungsgesetze der Elemente VI. Über die Kristallstrukturen vom 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]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----------	110	211	321
Lunde----------	110	211	321
National Bureau of Standards----	110	211	100

Structural data. Van Arkel [1] in 1924 determined that thallium bromide has cesium chloride-type 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, TlBr (cubic)

hkl	1924 Van Arkel Cu, 1.5418 A			1925 Lunde Cu, 1.5418 A			1957 National Bureau of Standards Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
100	-------	----	-------	4. 0	vw	4. 0	3. 98	25	3. 98
110	2. 83	vs	4. 00	2. 81	vvs	3. 97	2. 818	100	3. 986
111	2. 31	vw	4. 00	2. 29	vw	3. 97	2. 300	7	3. 983
200	1. 99	m	3. 98	1. 99	s	3. 98	1. 9926	18	3. 9852
210	1. 78	w	3. 98	1. 78	s	3. 98	1. 7820	7	3. 9847
211	1. 63	vs	3. 99	1. 62	vvs	3. 97	1. 6268	27	3. 9848
220	1. 41	m	3. 99	1. 40	s	3. 96	1. 4091	7	3. 9855
300	1. 33	w	3. 99	1. 32	w	3. 96	1. 3287	2	3. 9861
310	1. 26	s	3. 98	1. 26	vs	3. 98	1. 2604	8	3. 9857
311	1. 20	vw	3. 98	1. 20	vw	3. 98	1. 2015	1	3. 9849
222	1. 15	w	3. 98	1. 15	w	3. 98	1. 1509	2	3. 9868
320	1. 11	vw	4. 00	1. 10	vw	3. 97	1. 1058	<1	3. 9870
321	1. 07	vs	4. 00	1. 06	vvs	3. 97	1. 0653	6	3. 9860
400	0. 999	vvw	3. 996	0. 996	vw	3. 984	0. 9965	<1	3. 9860
410	. 969	vvw	3. 995	. 965	vw	3. 979	. 9667	<1	3. 9858
411	. 942	s	3. 997	. 937	vvs	3. 975	. 9395	3	3. 9860
420	. 893	m	3. 994	. 890	vs	3. 980	. 8911	1	3. 9851
421	. 872	vw	3. 996	-------	----	-------	. 8696	<1	3. 9850
332	. 853	m	4. 001	-------	----	-------	. 8495	2	3. 9845
422	. 816	m	3. 998	-------	----	-------	. 8135	1	3. 9853
510	. 784	s	3. 998	-------	----	-------	. 7815	3	3. 9849
Average of last five lines------			3. 997	-------	----	3. 978	-------	----	3. 9850

Lattice constants

		A
1924	Van Arkel [1]	3.99
1925	Lunde [3]	3.976
1939	Straumanis, Ievinš, and Karlsons [4].	3.98582 at 25° C
1957	National Bureau of Standards.	3.9850 at 25° C

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, Physica **4**, 33–41 (1924).

[2] G. Wagner and L. Lippert, Über polymorphe Umwandlung bei einfachen Ionengittern. I. Versuche zur Umwandlung von CsCl- in NaCl-Gitter durch 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? Präzionsbestimmungen von Gitterkonstanten des LiF, NaF, As_2O_3, TlCl, 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 Standards.	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: C_6^6–$P6_3$ with $2(Tl_3PO_4)$ per unit hexagonal cell.

Lattice constants

		a	*c*
		A	*A*
1949	Borie	8.35	5.12
1957	National Bureau of Standards.	8.355	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 Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*
	A	
100	7.24	7
110, 101	4.18	44
200	3.62	25
111	3.236	100
201	2.954	88
210	2.735	47
002	2.557	25
300, 211	2.412	14
301, 112	2.181	12
220, 202	2.089	9
310	2.006	24
221	1.9336	6
311, 212	1.8681	54
400	1.8093	4
302	1.7533	7
401	1.7060	3
320	1.6606	6
410, 321, 312, 113	1.5786	40
203	1.5421	9
411	1.5091	5
500, 213	1.4471	3
330, 501, 322, 303	1.3926	13
420	1.3673	6

Thallium(I) Phosphate, Tl_3PO_4 (hexagonal)—Con.

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	*I*		*d*	*I*
	A			*A*	
331, 412	1. 3436	7	701, 612	1. 0132	3
421, 223	1. 3209	4	620	1. 0043	2
510, 313	1. 2995	7	414, 115	0. 9934	4
502, 104	1. 2588	4	621, 603, 205	. 9846	6
332	1. 2231	1	433	. 9751	4
600, 422, 204	1. 2058	5	710, 702, 523, 504, 215	. 9583	4
430, 323	1. 1896	4	711, 334, 305	. 9419	4
601	1. 1739	4	622, 424	. 9338	4
520, 431, 512, 413, 214	1. 1586	10	540, 613	. 9266	4
521, 304	1. 1298	3	630, 541, 514, 315	. 9115	5
610, 503	1. 1033	3	800	. 9045	1
602, 224	1. 0905	2	631, 712	. 8975	5
611, 432, 333, 314	1. 0781	5	801, 443, 405	. 8905	2
522	1. 0551	5			
[a]	1. 0411	2			
700, 513	1. 0336	3	720, 703	. 8839	5
441	1. 0230	4	721, 542, 434, 325	. 8709	4

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

Thallium(III) Phosphate, $TlPO_4$ (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	112	110	020
National Bureau of Standards	112	110	020

Structural data. Mooney [1] in 1956 determined that thallium phosphate has the space group D_{2h}^{17}–Cmcm, and 4($TlPO_4$) per unit cell.

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

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1956	Mooney [1]	5. 406	8. 026	7.085
1957	National Bureau of Standards.	5. 408	8. 027	7.087 at 25° C

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

References

[1] 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, $TlPO_4$ (orthorhombic)

hkl	1956 Mooney Cu, 1.5405 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
110	4. 48	99	4. 48	96
020	4. 01	55	4. 01	51
111	3. 786	8	3. 789	12
002	3. 545	22	3. 542	28
021	3. 493	3	3. 491	9
112	2. 779	100	2. 780	100
200	2. 702	28	2. 703	28
022	2. 656	23	2. 656	24
130	2. 399	38	2. 398	40
220	2. 238	10	2. 242	11
202	2. 149	27	2. 149	27
023	2. 036	<1	2. 036	<1
040	2. 007	11	2. 006	11
132	1. 985	25	1. 986	26
222	1. 8937	33	1. 8949	33
004	1. 7717	11	1. 7720	11
310	1. 7583	9	1. 7593	11
042	1. 7458	14	1. 7461	14
311	1. 7072	<1	1. 7072	<1
133	1. 6817	<1	1. 6822	<1
114	1. 6477	16	1. 6480	15
024	1. 6205	10	1. 6207	12
240	1. 6111	6	1. 6114	7
312	1. 5744	18	1. 5754	17
150	1. 5381	7	1. 5391	8
330	1. 4946	9	1. 4949	10
204	1. 4813	6	1. 4822	8
242	1. 4666	20	1. 4671	15
134	1. 4246	12	1. 4250	13
152	1. 4116	8	1. 4116	9
224	1. 3902	6	1. 3902	7
332	1. 3771	6	1. 3771	7
400, 115	1. 3513	4	1. 3520	5
060	1. 3369	2	1. 3381	3
243, 044	1. 3280	3	1. 3284	6
420	1. 2811	2	1. 2811	3
333, 402	1. 2627	<1	1. 2630	3
062	1. 2508	1	1. 2509	<1
314	1. 2478	5	1. 2481	5
422	1. 2074	4	1. 2046	4
260, 350, 225	1. 1988	6	1. 1989	5
244	1. 1919	3	1. 1922	3
006	1. 1814	<1	1. 1814	<1
154	1. 1615	5	1. 1617	4
334, 116	------	----	1. 1423	12
262, 352	------	----	1. 1356	8
026	------	----	1. 1329	6
170, 440	------	----	1. 1214	5
315	------	----	1. 1030	<1
206	------	----	1. 0822	2
404	------	----	1. 0747	3
510	------	----	1. 0718	10
172, 263, 353, 442	------	----	1. 0690	6
064	------	----	1. 0674	6
511, 136	------	----	1. 0597	3
226	------	----	1. 0451	6
424	------	----	1. 0382	4
512	------	----	1. 0260	2
046	------	----	1. 0180	3

Tin(II) Telluride, SnTe (cubic)

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.	220	420	422
National Bureau of Standards	200	220	222

Structural data. Goldschmidt [1] in 1927 determined that tin telluride has sodium chloride-type 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

		A
1927	Goldschmidt [1]	6. 298
1957	National Bureau of Standards.	6. 303 at 25° C

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

hkl	Amer. Smelting and Refining Co. Fe, 1.9373 A			1957 National Bureau of Standards Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
200	3. 13	70	6. 26	3. 15	100	6. 31
220	2. 22	100	6. 28	2. 23	52	6. 309
222	1. 82	60	6. 30	1. 822	15	6. 310
400	1. 58	40	6. 32	1. 577	10	6. 308
420	1. 41	90	6. 31	1. 410	15	6. 306
422	1. 28	80	6. 30	1. 2870	8	6. 305
440	1. 12	30	6. 34	1. 1147	3	6. 306
600	1. 06	70	6. 36	1. 0511	4	6. 307
620	0. 999	60	6. 32	0. 9969	4	6. 305
622	----	-	--	. 9502	2	6. 303
444	----	-	--	. 9098	1	6. 303
640	----	-	--	. 8741	2	6. 303
642	----	-	--	. 8423	4	6. 303
800	----	-	--	. 7878	1	6. 302
Average of last five lines			6. 33	----	-	6. 303

References

[1] 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).

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

ASTM cards

Card number	Index lines	Radiation	Source
1–0444	4. 00 3. 04 3. 61	Molybdenum.	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_o=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:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	110	111	101
National Bureau of Standards	110	111	101

Structural data. Mark and Weissenberg [3] in 1923 determined that urea has the space group D_{2d}^{3}–$P\bar{4}2_1m$ 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	*c*
		A	*A*
1923	Mark and Weissenberg [3]	5. 64	4.71
1928	Hendricks [4]	5. 75	4.78
1957	National Bureau of Standards.	5. 645	4.704 at 25° C

The density of urea calculated from the NBS lattice constants is 1.330 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] K. Becker and W. Jancke, Röntgenspektroskopische Untersuchungen an Verbindungen. I., Z. physik. Chem. **99**, 242–266 (1921).

[3] H. Mark and K. Weissenberg, Röntgenographische 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. **50**, 2455–2464 (1928).

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

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
110	4. 01	100	4. 01	100
101	3. 62	40	3. 62	25
111	3. 05	53	3. 048	29
200	2. 83	11	2. 826	6
210	2. 53	20	2. 528	12
201	2. 41	20	2. 422	10
002	2. 34	3	2. 349	3
211	2. 23	8	2. 229	5
102	2. 17	20	2. 171	5
------	2. 08	1	------	----
112	2. 01	8	2. 025	2
220	------	----	1. 996	2
221	1. 84	13	1. 837	4
310	------	----	1. 786	<1
301	1. 75	1	1. 747	1
212	------	----	1. 721	<1
311	1. 67	13	1. 669	<1
003	------	----	1. 568	<1
222	------	----	1. 5219	<1
103	1. 51	8	1. 5090	1
312	------	----	1. 4209	<1
401	1. 370	3	1. 3518	<1
330	1. 331	7	1. 3304	1
420	1. 261	1	1. 2622	<1
421	1. 232	1	1. 2190	<1
004	1. 179	4	1. 1771	<1
323	------	----	1. 1076	<1
431	------	----	1. 0979	<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.[a]
2–1413	1. 42 2. 63 2. 31	Copper	Schütz [1] 1936.[b]
2–0813	2. 81 2. 61 3. 44	Copper	British Museum.
1–1076	2. 64 3. 49 2. 83	Molybdenum	New Jersey Zinc Co.

[a] Natural willemite. [b] Synthetic 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_o=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 *d*-values of the Schütz pattern were calculated from reported Bragg angle data. The three strongest

lines of each pattern are as follows:

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

Structural data. Gottfried [2] in 1927 determined that zinc orthosilicate has phenacite-type structure, the space group C_{3i}^2–$R\bar{3}$, 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	*c*
		A	*A*
1927	Gottfried [2]	14. 17	9.60
1929	Pabst [3]	13. 898	9.337
1930	Bragg and Zachariasen [4].	13. 97	9.36
1936	Schütz [1]	13. 97	9.36
1957	National Bureau of Standards.	13. 94	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 (trignal)

hkl	1936 Schütz (natural) Cu, 1.5418 A		1936 Schütz (synthetic) Cu, 1.5418 A		British Museum Cu, 1.5418 A		New Jersey Zinc Co. Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
110	------	----	------	----	6. 85	60	------	----	6. 98	22
012	4. 40	40	4. 40	40	4. 45	40	------	----	4. 35	4
211	------	----	------	----	------	----	------	----	4. 10	17
300	------	----	------	----	4. 04	60	4. 05	30	4. 026	33
-----	------	----	------	----	3. 82	40	------	----	------	----
220	3. 49	60	3. 48	20	3. 45	80	3. 50	75	3. 486	81
122	------	----	------	----	------	----	------	----	3. 264	4
131	------	----	------	----	3. 12	40	------	----	3. 153	7
-----	------	----	------	----	2. 93	40	------	----	------	----
113	2. 85	80	2. 85	60	2. 82	100	2. 84	75	2. 834	97
312	------	----	------	----	------	----	------	----	2. 720	3
140	2. 63	80	2. 63	80	2. 62	100	2. 65	100	2. 634	100
042	------	----	------	----	------	----	------	----	2. 533	2
232	------	----	------	----	------	----	------	----	2. 381	1
223	2. 32	80	2. 32	80	2. 30	70	2. 32	50	2. 318	47
104	------	----	------	----	2. 23	20	------	----	2. 287	2
241	2. 22	10	2. 22	10	------	----	------	----	2. 215	1
502	2. 18	10	2. 18	10	2. 13	20	------	----	2. 144	4
214	------	----	------	----	2. 07	40	------	----	2. 074	1
422	------	----	------	----	------	----	------	----	2. 049	5
600	2. 01	20	2. 01	20	2. 01	40	2. 01	5	2. 013	7
413									2. 0111	9
152	------	----	------	----	------	----	------	----	1. 9656	2
250	1. 94	40	1. 93	20	1. 93	40	1. 93	15	1. 9332	9
333	1. 85	80	1. 85	80	1. 86	80	1. 86	75	1. 8592	36
342	------	----	------	----	------	----	------	----	1. 8260	<1
161	------	----	------	----	------	----	------	----	1. 8074	1
324	------	----	------	----	------	----	------	----	1. 7817	1
125	1. 74	10	1. 74	10	1. 72	20	------	----	1. 7235	3
603	1. 70	10	1. 70	10	1. 69	40	1. 69	8	1. 6882	7
054	------	----	------	----	------	----	------	----	1. 6752	1
621	------	----	------	----	------	----	------	----	1. 6491	2
523	1. 63	20	1. 63	20	1. 64	40	1. 64	8	1. 6404	7
315	------	----	------	----	------	----	------	----	1. 6273	10
710	1. 60	20	1. 60	20	1. 60	60	1. 60	10	1. 5986	10

Zinc Orthosilicate (willemite), Zn_2SiO_4 (trigonal)—Continued

hkl	1936 Schütz (natural) Cu, 1.5418 A		1936 Schütz (synthetic) Cu, 1.5418 A		---- British Museum Cu, 1.5418 A		---- New Jersey Zinc Co. Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A	
514	------	----	------	----	1. 57	40	------	----	1. 5863	<1
006	1. 56	20	1. 56	20	1. 55	60	1. 55	8	1. 5516	11
630	1. 52	20	1. 52	20	1. 52	60	1. 52	8	1. 5203	9
----	------	----	------	----	1. 49	20	------	----	------	----
271	------	----	------	----	------	----	------	----	1. 4570	<1
306	------	----	------	----	------	----	------	----	1. 4475	<1
713	1. 42	100	1. 42	100	1. 42	80	1. 42	75	1. 4205	30
550	1. 397	20	1. 395	20	1. 39	40	------	----	1. 3937	3
633	1. 357	60	1. 354	60	1. 37	60	1. 36	25	1. 3656	13
900	} 1. 342	60	1. 341	60	1. 34	60	1. 34	25	{ 1. 3411	6
416	}								{ 1. 3369	12
820	------	----	------	----	------	----	------	----	1. 3171	<1
553	------	----	------	----	------	----	------	----	1. 2716	1
740	1. 255	10	------	----	1. 25	20	------	----	1. 2518	1
606	1. 233	10	1. 232	10	1. 23	20	------	----	1. 2284	2
823	------	----	------	----	1. 21	40	------	----	1. 2112	4
526	1. 206	20	1. 201	20	------	----	------	----	1. 2106	4
743	1. 165	20	1. 162	20	1. 16	40	1. 16	5	1. 1610	4
10·1·0	1. 148	20	1. 148	20	1. 15	40	1. 14	5	1. 1458	3
716	------	----	1. 117	40	1. 12	60	1. 11	8	1. 1136	4
636	1. 091	40	1. 090	40	1. 09	40	1. 09	8	1. 0862	1
850	1. 066	10	------	----	------	----	------	----	1. 0629	2
933	1. 056	20	1. 056	20	1. 05	40	------	----	1. 0503	2
556	1. 040	20	1. 040	20	1. 04	40	------	----	1. 0370	2
119	------	----	------	----	1. 02	20	------	----	1. 0232	1
906	------	----	------	----	1. 01	60	1. 02	8	1. 0147	2
853	1. 009 [a]	60	1. 009 [b]	60	------	----	------	----	1. 0056	2

[a] Seven additional lines are omitted. [b] Four additional lines are omitted.

References

[1] W. Schütze, 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 Zink-silicaten, Z. physik. Chem. **142**, 227–232 (1929).

[4] W. L. Bragg and W. H. Zachariasen, The crystalline structure of phenacite, Be_2SiO_4 and willemite, Zn_2SiO_4, Z. Krist. **72**, 518–528 (1930).

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

ASTM cards

Cards numbers	Index lines	Radiation	Source
2–0274	4. 17 3. 54 2. 65	Iron	Schiff [1] 1934.
1–1086	2. 61 4. 16 3. 53	Molybdenum	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 measurements. 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	101	111	220
New Jersey Zinc Co	220, 121	101	111
National Bureau of Standards.	111	101	220

Structural data. Schiff [1] in 1934 determined that zinc sulfate has barium sulfate-type structure, the space group D_{2h}^{16}–Pnma, and $4(ZnSO_4)$ 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	c
		A	A	A
1934	Schiff [1]	8. 60	6. 74	4. 77
1936	Hammel [2]	8. 53	6. 74	4. 72
1957	National Bureau of Standards.	8. 588	6. 740	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 magnésienne, Compt. rend. **202**, 57–59 (1936).

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

hkl	1934 Schiff Fe, ----		---- New Jersey Zinc Co. Mo, ----		1957 National Bureau of Standards Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
200	4. 25	vw	---	-	4. 29	27
101	4. 17	s	4. 17	38	4. 17	82
210	3. 63	w	3. 62	15	3. 616	48
111	3. 55	s	3. 54	33	3. 543	100
020	3. 38	w	3. 38	5	3. 371	6
220	2. 65	s	2. 62	100	2. 650	76
121	2. 62	ms			2. 620	72
301	2. 45	s	2. 44	33	2. 451	59
002	2. 38	m	2. 37	10	2. 383	18
221	2. 30	w	2. 30	10	2. 316	14
102	---	-	---	-	2. 296	13
202	---	-	2. 08	5	2. 084	10
031	---	-	2. 03	5	2. 032	4
321	1. 98	m	1. 98	25	1. 984	25
022	---	-	---	-	1. 947	2
302	---	-	---	-	1. 832	2
420	1. 81	w	1. 80	15	1. 810	16
222	1. 77	w	1. 76	25	1. 773	32
040	1. 69	m	1. 68	13	1. 686	15
501	---	-	1. 61	2	1. 616	3
132	---	-	---	-	1, 606	2
402	1. 59	w	1. 59	5	1. 5958	10
511	---	-	---	-	1. 5713	7
103	1. 56	m	1. 56	23	1. 5632	17
430	---	-	---	-	1. 5520	2

hkl	1934 Schiff Fe, ----		---- New Jersey Zinc Co. Mo, ----		1957 National Bureau of Standards Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
013	---	-	---	-	1. 5482	2
113	---	-	---	-	1. 5228	2
203	1. 49	m	---	-	1. 4916	2
431	---	-	---	-	1. 4761	3
521	---	-	1. 45	15	1. 4572	19
422	---	-	---	-	1. 4421	10
600	---	-	---	-	1. 4312	6
123	---	-	1. 41	10	1. 4182	12
341	---	-	1. 38	15	1. 3899	14
303						
042	---	-	---	-	1. 3767	7
242	---	-	---	-	1. 3109	2
323	---	-	1. 28	2	1. 2852	8
602	---	-	1. 22	1	1. 2274	5
630	---	-	1. 19	1	1. 2078	2
612						
143	---	-	1. 15	1	1. 1458	1
523	---	-	---	-	1. 1027	3
640	---	-	1. 08	5	1. 0908	4
702						
260	---	-	---	-	1. 0872	5
224						
343	---	-	---	-	1. 0728	4
731	---	-	---	-	1. 0502	1
811	---	-	---	-	1. 0349	1
820	---	-	---	-	1. 0229	2

Zirconium Sulfate Tetrahydrate, $Zr(SO_4)_2 \cdot 4H_2O$ (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
	%	%
HfO_2+ZrO_2	35.09	35.0
SO_3	44.76	44.5
H_2O	20.15	20.5
	100.00	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 $2V\cong 70°$.

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	311	331	400
Rinn	311	331	400
National Bureau of Standards	311	331	400

hkl	1953 Rinn Cu, 1.5418 A		1956 Staritzky and Singer Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
400	6.50	50	6.49	45	6.49	44
220	5.30	4	5.30	5	5.30	3
111	4.90	30	4.90	25	4.90	27
311	4.32	100	4.32	100	4.32	100
620	3.46	40	3.47	30	3.466	37
---	3.31	2	---	---	----	---
800	3.23	2	3.24	5	3.238	2
131	3.14	4	3.15	5	3.148	5
331	2.96	80	2.98	75	2.977	88
040	2.89	20	2.91	15	2.902	19
531, 202	2.69	6	2.71	5	2.705	6
911	2.49	6	2.50	10	2.495	5
731	2.40	6	2.408	20	2.410	6
10·2·0	2.36	4	2.373	10	2.368	6
422, 602	2.32	40	2.332	35	2.330	31
622, 12·0·0	2.15	6	2.164	5	2.161	7
151, 931, 11·1·1	2.12	25	2.134	30	2.133	19
351	2.07	6	2.080	5	2.080	3
551, 242	1.97	30	1.980	25	1.979	22
---	---	-	1.916	<5	----	---
11·3·1, 10·0·2	1.88	25	1.894	15	1.893	12
751	1.85	10	1.855	5	1.854	4
642, 113	1.81	14	1.818	10	1.818	8
10·2·2	---	-	---	---	1.798	<1
313	---	-	---	---	1.783	2
660	1.76	30	---	---	1.7666	18
12·4·0	1.73	8	---	---	1.7332	4
951, 513	1.715	8	---	---	1.7190	4
13·3·1	1.682	30	---	---	1.6885	10
133	1.654	2	---	---	1.6612	2
333, 713, 12·2·2	1.637	35	---	---	1.6342	13
16·0·0	---	-	---	---	1.6202	<1
11·5·1, 533, 10·4·2	1.57	-	---	---	1.5848	13
371	---	-	---	---	1.5632	5
10·6·0	---	-	---	---	1.5513	3
462, 913	---	-	---	---	1.5400	2
733	---	-	---	---	1.5185	4
14·2·2	---	-	---	---	1.4875	<1

Zirconium Sulfate Tetrahydrate, $Zr(SO_4)_2 \cdot 4H_2O$ (orthorhombic)—Continued

hkl	1953 Rinn Cu, 1.5418 A		1956 Staritzky and Singer Cu, 1.5418 A		1957 National Bureau of Standards Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
13·5·1 } 17·1·1 }	---	-	---	---	1. 4590	6
933 } 11·1·3 }	---	-	---	---	1. 4411	4
480	---	-	---	---	1. 4160	3
16·4·0	---	-	---	---	1. 4148	2
18·2·0	---	-	---	---	1. 3981	3
971 } 553 }	---	-	---	---	1. 3913	3
004	---	-	---	---	1. 3826	2
17·3·1	---	-	---	---	1. 3748	<1
11·3·3 } 14·4·2 } 16·2·2 }	---	-	---	---	1. 3590	3
753 } 15·5·1 } 13·1·3 }	---	-	---	---	1. 3450	1
14·6·0 } 224 }	---	-	---	---	1. 3379	<1
19·1·1	---	-	---	---	1. 3160	<1
20·0·0	---	-	---	---	1. 2956	<1
624	---	-	---	---	1. 2843	1
15·1·3 } 19·3·1 }	---	-	---	---	1. 2536	1
044	---	-	---	---	1. 2491	6
13·7·1 } 244 }	---	-	---	---	1. 2428	4
591	---	-	---	---	1. 2214	1
12·8·0	---	-	---	---	1. 2052	<1
882 } 10·2·4 }	---	-	---	---	1. 1942	<1
791	---	-	---	---	1. 1940	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 $8[Zr(SO_4)_2 \cdot 4H_2O]$ per unit cell.

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

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1956	Staritzky and Singer [1].	26. 11	11. 62	5.56
1957	National Bureau of Standards.	25. 92	11. 62	5.532 at 25° C

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

References

[1] E. Staritzky and J. Singr, Zirconium disulfate tetrahydrate, $Zr(SO_4)_2 \cdot 4H_2eO$ Anal. Chem. **28**, 553–554 (1956).

[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]

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

U. S. GOVERNMENT PRINTING OFFICE: 1957

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