NBS CIRCULAR 539

VOLUME V

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

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Standard X-ray Diffraction Powder Patterns

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Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, Nancy T. Gilfrich, and George M. Ugrinic

National Bureau of Standards Circular 539

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ERRATA

Vol. III	Page 45, first column, in "NBS sample", lines 4 and 5, magnesium should read magnesia.
Vol. IV	Page 13, third line in "Lattice constants", D_{6h}^4–Pb_3/mmc should read D_{6h}^4–$P6_3/mmc$. Page 16, column 1, line 10, 210 should read 201; line 15, 201 should read 210. Page 25, sec. 4, col. 2, line 2, 2.158 should read 6.474.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. V—Data for 45 Inorganic Substances

Howard E. Swanson, Nancy T. Gilfrich,[1] and George M. Ugrinic

Forty-five standard X-ray diffraction powder patterns are presented in revision of seventy-four corresponding patterns in the ASTM file. This is a system for the identification of unknown crystalline materials based on the three strongest reflections of each material or structurally distinct phase. Patterns for five compounds not represented in the file are also included. A 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 exceptionally high purity. The *d*-spacings 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 forty-five substances: $(NH_4)_2PtCl_6$, $(NH_4)_2SnCl_6$, $(NH_4)_2SiF_6$ (cryptohalite), Sb_2S_3 (stibnite), $BaZrO_3$, $3CaO \cdot Al_2O_3$, Cs_2PtCl_6, $Cs_2Sn\ Cl_6$.Cs_2GeF_6, Cs_2SiF_6, Cr, Cr_2O_3, CuF_2, GeI_4, In_2O_3, HIO_3, FeS_2 (pyrite), α-PbF_2, β-PbF_2, PbI_2, $Pb(NO_3)_2$, PbSe (clausthalite), $PbTiO_3$, Mg_2Sn, $MgTiO_3$ (geikielite), MnO, MoS_2 (molybdenite), K_2PtCl_6, K_2SiF_6 (hieratite), $KZnF_3$, PrF_3, Rb_2PtCl_6, Se, Ag_3AsO_4, $AgBrO_3$, $AgNO_3$, $AgNO_2$, Ag_3PO_4, $NaHF_2$, $NaBrO_3$, SrF_2, SrO, Tl_2PtCl_6, SnI_4, and $Zn(CN)_2$.

INTRODUCTION

The National Bureau of Standards in its program[2] for revision and evaluation of published X-ray data for the American Society for Testing Materials card file presents in this paper, the fifth in a series[3] of standard powder diffraction patterns, data for 2 elements and 43 inorganic compounds. These patterns are recommended to replace 74 cards now in the file. Five compounds, cesium chloroplatinate, cesium chlorostannate, germanium (IV) iodide, rubidium chloroplatinate, and thallium chloroplatinate, not represented in the file, have been added.

The experimental procedure and general plan of these reports has not been changed from that of the previous volumes of NBS Circular 539. However, the basic technique is included 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 old and new file card numbers, the ASTM index lines, the radiation used, and the literature references for each card. The old card numbers refer to the original ASTM card file (1939) and the first supplement (1944). The new card numbers are from the second editions and include the fifth set of cards.

Additional published patterns. Literature references and radiation data for patterns that had not been published as ASTM cards are listed, and the patterns are included in the tables of *d*-spacings and intensities.

NBS sample. 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 spectroscopic or chemical analysis. The limit of detection for the alkali elements is 0.05 percent in the NBS spectrographic analysis. 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 well within the range of 5 to 10 microns as suggested by Alexander, Klug, and Kummer [1].[4] In the preparation of an intensity pattern a flat piece of glass was held temporarily over the face of an open-faced sample holder while the powdered sample was drifted in from the top. The sample holder was then turned face up, and the piece of glass was removed. This surface was exposed to the X-ray beam. For a few powder samples that did not flow readily or were prone to orient badly, approximately 50 volume percent finely ground

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[1] Fellow at the National Bureau of Standards sponsored by the Joint Committee on Chemical Analysis by X-ray Diffraction Methods.

[2] This project is sponsored by the Joint Committee on Chemical Analysis by X-ray 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. Financial support is being given by the National Bureau of Standards.

[3] The first paper of this Circular is Standard X-ray Diffraction Powder Patterns, Vol. I. Data for 58 Inorganic Substances, by H. E. Swanson and E. Tatge; the second is Standard X-ray Diffraction Powder Patterns, Vol. II. Data for 30 Inorganic Compounds, by H. E. Swanson and R. K. Fuyat; the third is Standard X-ray Diffraction Powder Patterns, Vol. III. Data for 34 Inorganic Compounds, by H. E. Swanson, R. K. Fuyat, and G. M. Ugrinic; and the fourth is Standard X-ray Diffraction Powder Patterns. Vol. IV. Data for 42 Inorganic Substances, by H. E. Swanson, R. K. Fuyat, and G. M. Ugrinic.

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

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 were prepared for *d*-spacing measurement by packing into a shallow holder a sample containing approximately 5 weight percent of tungsten powder as an internal standard. The lattice constant of tungsten at 25° C is 3.1648 A, as determined by Jette and Foote [2]. All of the NBS patterns were made by using copper $K_{\alpha 1}$ radiation, 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 [3]. The conversions were from Bragg angle data, from *d*-spacings in kX units, using the factor 1.00202, or from *d*-spacings based on wavelengths given in other than kX units. In each case the type of conversion made was indicated. The wavelength values in the tables of *d*-spacings and intensities are given in angstrom units. The values listed under the first section of each report are the original values taken from the literature. The table of patterns contains data which is based on the original work rather than that which is found on the ASTM cards.

Intensities, when not numerically evaluated, were given the following abbreviations: strong, s; medium, m; weak, w; very, v; diffuse, D; and doublet, db.

In indexing cubic patterns, the number of possible combinations of *hkl*'s for a specific value of the expression $(h^2+k^2+l^2)$ can be very great, particularly when the value becomes large. It has been customary in this Circular to make $h>k>l$ and to choose the *hkl* with the largest *h* if not limited by the space group. Noncubic patterns were indexed by comparing *d*-spacings of the NBS pattern with calculated values obtained from cell dimensions found in the literature which have been modified by partial indexing of the NBS pattern. The calculations were made with the help of this Bureau's electronic computer, the SEAC, which lists all possible spacing values for given cell dimensions. The noncubic indexing includes all of the probable indices for any given *d*-spacing allowed by the space group of that structure. An attempt was made to reconcile these values with published single crystal work when it was available. However, errors inherent in the indexing of powder data undoubtedly are present in some patterns.

A table comparing the three most intense lines of each pattern is included with the discussion of interplanar spacing and intensity measurements. The strongest lines are listed by Miller indices rather than *d*-spacing values because of the variation in spacing values. The intensities measured for these three lines are of particular importance since the use of the ASTM card-file system for identification of materials is based upon the ability to sort cards by the first, second, and third strongest line.

Lattice constants. The NBS lattice constants of cubic materials were calculated for all *d*-spacings, and the average of the last five lines was assumed to be the best value because of greater accuracy of measurement in the large-angle part of the pattern. The unit-cell values for each noncubic substance were determined from all of the *d*-spacings of its pattern, for which there was only one possible Miller index by means of a least-squares calculation made on the SEAC.

The conversion of published unit-cell data to angstroms is presented in the same manner as that used for the *d*-spacings. The unit-cell values were corrected for temperature comparison with the NBS values if the temperature of measurement and the thermal expansion of the substance were known. The coefficient of linear thermal expansion as used is defined as the change in length per unit length per degree C in the room temperature range, unless otherwise indicated. Thermal expansion data have been given whenever the data were readily available, even though no temperature conversions were made in the unit-cell table. The limits of errors generally published with unit-cell data have not been included in the table as 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 [4] in 1954. The refractive index measurements were made in white light by grain-immersion methods, using oils standardized in sodium light.

References

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

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

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

[4] E. Wichers, Report of the Committee on Atomic Weights of the American Chemical Society, J. Am. Chem. Soc. **76,** 2033 (1954).

Ammonium Chloroplatinate, $(NH_4)_2PtCl_6$ (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
345	0418 1–0176 1–0175	5. 7 4. 93 2. 97	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The ammonium chloroplatinate was prepared at the NBS from ammonium chloride and chloroplatinic acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium; 0.001 to 0.01 percent silicon; and 0.0001 to 0.001 percent each of calcium, iron, and magnesium.

The sample is bright yellow. The index of refraction is 1.835.

Interplanar spacings and intensity measurements. The *d*-spacings for the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	200	311
Swanson, Gilfrich, and Ugrinic	111	200	311

Lattice constant. The structure of ammonium chloroplatinate was determined by Wyckoff and Posnjak [2] in 1921. The cubic lattice has the space group O_h^5-Fm3m with potassium chloroplatinate-type structure and $4((NH_4)_2PtCl_6)$ per unit cell.

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

Lattice constants

		A
1921	Wyckoff and Posnjak [2]	9.863
1928	Ewing and Pauling [3]	9.86
1933	Bødtker-Naess and Hassel [4]	9.866
1935	Engel [5]	9.854
1955	Swanson, Gilfrich, and Ugrinic	9.858 at 25° C

The density of ammonium chloroplatinate calculated from the NBS lattice constant is 3.078 at 25° C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	5. 7	100	9. 9	5. 697	100	9. 87
200	4. 94	60	9. 88	4. 929	68	9. 86
220	3. 49	20	9. 87	3. 485	30	9. 856
311	2. 98	50	9. 88	2. 9731	55	9. 861
222	-----	--	-----	2. 8464	4	9. 860
400	2. 46	30	9. 84	2. 4655	47	9. 862
331	2. 26	10	9. 85	2. 2618	19	9. 859
420	2. 20	20	9. 84	2. 2046	33	9. 859
422	2. 01	8	9. 85	2. 0124	14	9. 859
511	1. 89	16	9. 82	1. 8971	24	9. 858
440	1. 74	14	9. 84	1. 7427	24	9. 858
531	1. 66	16	9. 82	1. 6662	20	9. 857
600	1. 64	8	9. 84	1. 6431	16	9. 860
620	1. 56	3	9. 87	1. 5589	4	9. 859
533	1. 50	3	9. 84	1. 5034	4	9. 858
444	1. 424	3	9. 87	1. 4230	5	9. 859
711	1. 379	6	9. 85	1. 3805	12	9. 859
640	-----	--	-----	1. 3672	8	9. 859
642	1. 318	3	9. 86	1. 3173	4	9. 858
731	1. 285	4	9. 87	1. 2833	8	9. 857
800	-----	--	-----	1. 2325	2	9, 860
733	-----	--	-----	1. 2042	1	9. 857
820	1. 197	3	9. 87	1. 1956	6	9. 859
822	1. 162	2	9. 86	1. 1617	3	9. 857
751	1. 142	2	9. 89	1. 1382	6	9. 857
840	1. 102	3	9. 86	1. 1021	10	9. 858
911	-----	--	-----	1. 0820	4	9. 858
842	-----	--	-----	1. 0755	5	9. 857
664	-----	--	-----	1. 0507	2	9. 856
931	-----	--	-----	1. 0333	5	9. 857
844	-----	--	-----	1. 0060	5	9. 857
933	-----	--	-----	0. 9907	5	9. 857
10·0·0	-----	--	-----	. 9858	3	9. 858
10·2·0	-----	--	-----	. 9666	3	9. 857
951	-----	--	-----	. 9529	5	9. 857
953	-----	--	-----	. 9192	7	9. 857
10·4·0	-----	--	-----	. 9153	5	9. 858
10·4·2	-----	--	-----	. 8999	1	9. 858
11·1·1	-----	--	-----	. 8888	2	9. 857
880	-----	--	-----	. 8713	6	9. 858
11·3·1	-----	--	-----	. 8614	5	9. 859
10·4·4	-----	--	-----	. 8580	3	9. 8577
11·3·3	-----	--	-----	. 8361	3	9. 8575
12·0·0	-----	--	-----	. 8215	4	9. 8580
11·5·1	-----	--	-----	. 8131	2	9. 8583
12·2·0	-----	--	-----	. 8103	1	9. 8577
12·2·2	-----	--	-----	. 7996	2	9. 8581
11·5·3	-----	--	-----	. 7918	6	9. 8578
Average value of last five lines			9. 87	------	--	9. 8580

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 and E. W. Posnjak, The crystal structure of ammonium chloroplatinate, J. Am. Chem. Soc. **43,** 2292–2309 (1921).

[3] F. J. Ewing and L. Pauling, The crystal structure of potassium chloroplatinate, Z. Krist. **68,** 223–230 (1928).

[4] G. Bødtker-Naess and O. Hassel, Ionerabstände in Kristallen von Komplexsalzen mit Fluoritstruktur, Avhandl. Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1933,** No. 7 (1933).

[5] G. Engel, Die Kristallstrukturen einiger Hexachlorokomplexsalze, Z. Krist. **90,** 341–373 (1935).

Ammonium Chlorostannate, $(NH_4)_2SnCl_6$ (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
335	0409 1–0172 1–0171	5. 8 2. 50 5. 0	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The ammonium chlorostannate was prepared at the NBS from ammonium chloride and stannic chloride. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent of silicon; 0.001 to 0.01 percent each of aluminum, iron, and magnesium; and 0.0001 to 0.001 percent each of silver, calcium, and copper.

The sample is colorless. The index of refraction is 1.688.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	400	440
Swanson, Gilfrich, and Ugrinic	111	200	400

Lattice constant. The structure of ammonium chlorostannate was determined by Dickinson [2] in 1922. The cubic lattice has the space group O_h^5-Fm3m with potassium chloroplatinate-type structure and 4 ($(NH_4)_2SnCl_6$) per unit cell.

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

Ammonium Chlorostannate, $(NH_4)_2SnCl_6$ (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	5. 8	100	10. 0	5. 813	100	10. 07
200	5. 0	50	10. 0	5. 032	84	10. 06
220	3. 55	20	10. 00	3. 557	20	10. 06
311	3. 03	53	10. 00	3. 033	47	10. 06
222	2. 90	20	10. 04	2. 9033	27	10. 057
400	2. 51	100	10. 04	2. 5153	55	10. 061
331	2. 30	13	10. 03	2. 3081	17	10. 061
420	2. 24	53	10. 02	2. 2499	33	10. 062
422	2. 04	11	9. 99	2. 0535	7	10. 060
511	1. 93	33	10. 03	1. 9367	20	10. 063
440	1. 77	67	10. 01	1. 7787	28	10. 062
531	1. 69	33	10. 00	1. 7004	19	10. 060
600	1. 67	27	10. 02	1. 6765	16	10. 059
620	1. 58	7	9. 99	1. 5908	4	10. 061
533	1. 53	8	10. 03	1. 5340	5	10. 059
622	---	--	---	1. 5165	3	10. 060
444	1. 452	17	10. 06	1. 4519	8	10. 059
711	1. 406	17	10. 04	1. 4087	9	10. 060
640	---	--	---	1. 3950	6	10. 059
642	1. 343	7	10. 05	1. 3442	3	10. 059
731	1. 310	13	10. 06	1. 3092	5	10. 056
800	1. 257	7	10. 06	1. 2570	4	10. 056
733	---	--	---	1. 2290	2	10. 060
820	1. 219	13	10. 05	1. 2197	7	10. 058
822	1. 184	5	10. 05	1. 1855	<1	10. 060
751	1. 160	9	10. 05	1. 1616	3	10. 060
662	---	--	---	1. 1539	1	10. 059
840	1. 112	13	9. 95	1. 1248	7	10. 061
911	---	--	---	1. 1041	4	10. 059
842	1. 101	11	10. 09	1. 0975	5	10. 059
931	---	--	---	1. 0545	3	10. 059
844	---	--	---	1. 0267	5	10. 060
933	---	--	---	1. 0109	2	10. 058
10·0·0	---	--	---	1. 0060	1	10. 060
10·2·0	---	--	---	0. 9865	<1	10. 060
951	---	--	---	. 9726	2	10. 061
953	---	--	---	. 9380	2	10. 059
10·4·0	---	--	---	. 9341	2	10. 061
Average value of last five lines			10. 04	----	--	10. 060

Lattice constants

		A
1922	Dickinson [2]	10.07
1928	Ewing and Pauling [3]	10.07
1935	Engel [4]	10.058
1955	Swanson, Gilfrich, and Ugrinic.	10.060 at 25° C.

The density of ammonium chlorostannate calculated from the NBS lattice constant is 2.371 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. G. Dickinson, The crystal structures of potassium and ammonium chlorostannates, J. Am. Chem. Soc. **44**, 276–288 (1922).

[3] F. J. Ewing and L. Pauling, The crystal structure of potassium chloroplatinate, Z. Krist. **68**, 223–230 (1928).

[4] G. Engel, Die Kristallstrukturen einiger Hexachlorokomplexsalze, Z. Krist. **90**, 341–373 (1935).

Ammonium Fluosilicate (cryptohalite), $(NH_4)_2SiF_6$ (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
577	0624 1–0283 1–0269	4. 85 2. 42 2. 09	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The ammonium fluosilicate was prepared at the NBS from ammonium chloride, silica gel and hydrofluoric acid. Spectrographic analysis of the NBS sample showed the following impurities: 0.01 to 0.1 percent each of sodium and germanium; 0.001 to 0.01 percent each of aluminum and platinum; and 0.0001 to 0.001 percent each of calcium, iron, magnesium and lead. Bararite, the hexagonal form of ammonium fluosilicate, is also known and has been prepared artificially at 5° C [2].

The sample is colorless. The index of refraction is too low to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines for the two patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	222	400
Swanson, Gilfrich, and Ugrinic	111	222	400

Lattice constant. The structure of ammonium fluosilicate was determined by Bozorth [3] in 1922. The cubic lattice has the space group O_h^5-Fm3m with potassium chloroplatinate-type structure and $4((NH_4)_2SiF_6)$ per unit cell.

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

Ammonium Fluosilicate (cryptohalite), $(NH_4)_2SiF_6$ (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	4. 86	100	8. 42	4. 844	100	8. 390
200	4. 20	15	8. 40	4. 195	26	8. 390
220	2. 97	20	8. 40	2. 967	17	8. 393
311	2. 53	8	8. 39	2. 531	8	8. 393
222	2. 42	50	8. 38	2. 422	45	8. 389
400	2. 09	50	8. 36	2. 098	33	8. 394
331	1. 92	2	8. 37	1. 926	3	8. 393
420	1. 88	2	8. 41	1. 877	3	8. 393
511	1. 61	30	8. 37	1. 615	18	8. 392
440	1. 481	15	8. 38	1. 4837	8	8. 393
531	1. 415	10	8. 37	1. 4188	6	8. 394
600	-----	--	-----	1. 3989	2	8. 393
620	1. 328	8	8. 399	1. 3271	4	8. 393
622	-----	--	-----	1. 2653	<1	8. 393
444	1. 212	2	8. 397	1. 2109	2	8. 389
711	1. 176	8	8. 398	1. 1750	5	8. 391
640	-----	--	-----	1. 1638	2	8. 392
642	1. 122	2	8. 396	1. 1216	2	8. 393
731	1. 094	2	8. 403	1. 0927	2	8. 393
800	-----	--	-----	1. 0492	1	8. 394
820	-----	--	-----	1. 0175	<1	8. 390
822	-----	--	-----	0. 9888	1	8. 390
751	0. 970	1	8. 400	. 9688	2	8. 390
840	-----	--	-----	. 9384	<1	8. 393
911	-----	--	-----	. 9210	<1	8. 391
664	-----	--	-----	. 8946	1	8. 392
844	-----	--	-----	. 8563	<1	8. 390
10·2·0	-----	--	-----	. 8230	2	8. 393
951	-----	--	-----	. 8113	1	8. 392
Average value of last five lines			8. 399	------	--	8. 392

Lattice constants

		A
1922	Bozorth [3]	8.40
1934	Gossner and Kraus [4]	8.40
1935	Ketelaar [5]	8.355
1955	Swanson, Gilfrich, and Ugrinic	8.395 at 25° C

The density of ammonium fluosilicate calculated from the NBS lattice constant is 2.000 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] B. Gossner, Untersuchung polymorpher Körper, Z. Krist. **38,** 110–168 (1903).

[3] R. M. Bozorth, The crystal structure of ammonium fluosilicate, J. Am. Chem. Soc. **44,** 1066–1070 (1922).

[4] E. Gossner and O. Kraus, Das Kristallgitter von Ammonium-hexafluosilicat, Z. Krist. **88,** 223–225 (1934).

[5] J. A. A. Ketelaar, Die Kristallstruktur von K-, Rb-, Cs- und Tl- Silicofluorid und von $LiMnO_4{\cdot}3H_2O$, Z. Krist. **92,** 155–156 (1935).

Antimony (III) Sulfide (stibnite), Sb_2S_3 (orthorhombic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
1356	1322	3. 57	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
	1–0571	1. 92		
	1–0538	3. 02		
II–849	1321	3. 55	Copper	Harcourt [2] 1942.
	2–0390	1. 94		
	2–0374	1. 69		
II–903	1389	3. 48	Copper 1.541 A.	British Museum.
	2–0410	1. 91		
	2–0403	1. 67		

The Harcourt pattern was made using copper radiation rather than molybdenum radiation as indicated on the ASTM card.

Additional published patterns. None.

NBS sample. The antimony sulfide was prepared at the NBS. It was precipitated from a solution of antimony oxide in hydrochloric acid by hydrogen sulfide. The precipitate was annealed in a closed tube at 350° C. for 12 hours. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent each of arsenic, copper, lead, and silicon; 0.001 to 0.01 percent each of silver, aluminum, calcium, magnesium, and tin; and 0.0001 to 0.001 percent of iron.

The sample is a lead gray color and is opaque.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel, of the Harcourt, and of the British Museum patterns were converted from kX to angstrom units.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	130, 310	431	211
Harcourt	130, 310	431	132
British Museum	130, 310	431	132
Swanson, Gilfrich, and Ugrinic	221	211	310

Lattice constants. The structure of antimony sulfide was determined by Ôe [3] in 1926. The orthorhombic lattice has the space group D_{2h}^{16}-Pbnm with $4(Sb_2S_3)$ per unit cell. Stibnite has been 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
1927	Gottfried [4]	11. 41	11. 50	3. 90
1928	Ôe [3]	11. 18	11. 27	3. 82
1933	Hoffmann [5]	11. 22	11. 30	3. 84
1955	Swanson, Gilfrich, and Ugrinic.	11. 229	11. 310	3. 8389 at 25°C.

The density of antimony sulfide calculated from the NBS lattice constants is 4.625 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] G. A. Harcourt, Tables for the identification of ore minerals by X-ray powder patterns, Am. Min. **27,** 63–113 (1942).

[3] J. Ôe, Crystal structure of stibnite, J. Geol. Soc. Japan **33,** 187–204 (1926).

[4] C. Gottfried, Über die Struktur des Antimonits, Z. Krist. **65,** 428–434 (1927).

[5] W. Hoffmann, Die Struktur der Minerale der Antimonitgruppe, Z. Krist. **86,** 225–245 (1933).

Antimony Sulfide (stibnite), Sb_2S_3 (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1942 Harcourt Cu, 1.5405 A		---- British Museum Cu, 1.5405 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C	
	d	I	d	I	d	I	d	I
	A		A		A		A	
110	8. 2	6	-----	-----	-----	-----	7. 99	16
020	5. 6	23	5. 61	33	5. 5	70	5. 654	36
120	5. 0	46	5. 01	33	4. 9	70	5. 052	57
220	3. 98	23	3. 96	17	3. 85	50	3. 987	28
101	-----	-----	-----	-----	-----	-----	3. 632	29
130	3. 57	100	3. 56	100	3. 49	100	3. 573	67
310							3. 556	72
111	-----	-----	-----	-----	-----	-----	3. 458	25
021	-----	-----	-----	-----	-----	-----	3. 178	18
230	-----	-----	3. 12	33	3. 05	50	3. 128	37
211	3. 02	86	3. 06	50	3. 00	70	3. 053	95
221	2. 75	86	2. 78	50	2. 70	70	2. 764	100
301	2. 67	34	2. 67	8	2. 63	50	2. 680	52
311	2. 60	6	-----	-----	2. 58	20	2. 609	25
240	2. 50	34	2. 52	50	2. 50	70	2. 525	46
231	2. 42	23	2. 42	17	2. 37	50	2. 426	22
041	-----	-----	2. 28	17	2. 29	50	2. 277	24
430	-----	-----	2. 23	33	2. 24	50	2. 252	14
141	2. 23	29	-----	-----	2. 18	50	2. 233	25
510	-----	-----	-----	-----	-----	-----	2. 202	7
331	-----	-----	-----	-----	-----	-----	2. 185	6
421	2. 09	40	2. 10	50	2. 07	70	2. 101	21
520							2. 088	12
440	-----	-----	1. 994	5	-----	-----	1. 992	10
431	1. 92	100	1. 944	67	1. 91	100	1. 940	46
002	-----	-----	-----	-----	1. 89	70	1. 920	36
151								
060	-----	-----	1. 889	5	1. 84	50 D	1. 885	9
600	-----	-----	-----	-----	-----	-----	1. 871	9
160	-----	-----	-----	-----	-----	-----	1. 858	5
610	-----	-----	1. 789	5	-----	-----	1. 846	9
351	1. 72	57	1. 728	33	1. 71	70	1. 729	19
531							1. 725	20
132	-----	-----	1. 693	67	1. 67	100	1. 6906	34
232	1. 63	6	-----	-----	1. 62	20	1. 6358	8
322								
720	-----	-----	1. 543	17	1. 57	20	1. 5431	10
242	1. 53	17	1. 528	17	1. 51	50	1. 5280	16
370	1. 478	6	1. 488	8	1. 47	20	1. 4837	5
432	-----	-----	-----	-----	-----	-----	1. 4617	5
342								
560	-------	-----	1. 445	8	1. 43	20	1. 4441	7
271	-------	-----	-----	-----	-----	-----	1. 4397	5
721	-------	-----	-----	-----	-----	-----	1. 4320	7
252	-----	-----	-----	-----	-----	-----	1. 4163	7
080	-----	-----	-----	-----	-----	-----	1. 4131	6
522								
470	1. 403	6	1. 403	8	1. 39	20	1. 4003	6
532	-----	-----	-----	-----	1. 35	20	1. 3604	8
561	1. 353	6	-----	-----	-----	-----	1. 3513	6
570	1. 308	11	1. 315	8	1. 30	60	1. 3114	10
741								
			(a)		(b)			

[a] Twelve additional lines are omitted.

[b] Five additional lines are omitted.

Barium Zirconate, $BaZrO_3$ (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
-----	2257 3–0644 3–0641	2.96 1.71 1.21	Copper	Hoffmann [1] 1935.
2174	2255 1–0903 1–0890	2.97 1.71 2.09	Molybdenum.	New Jersey Zinc Co.
-----	2270 3–0648 3–0632	2.97 0.82 1.71	-----------	Megaw, Philips Lamps, Ltd.

In the fifth supplement of the ASTM card file, the Hoffmann card 3–0641 has been corrected to agree with the literature and is replaced by a new card of the same number.

Additional published patterns. None.

NBS sample. The barium zirconate used for the NBS pattern was prepared at the NBS by George R. Shelton by heating barium carbonate and zirconium dioxide for 1 hour at 1,550° C on a button of previously prepared barium zirconate. Spectrographic analysis at the NBS showed the following impurities: 0.1 to 1.0 percent each of hafnium and tin; 0.01 to 0.1 percent each of aluminum, calcium, iron, magnesium and silicon and; 0.0001 to 0.001 percent each of manganese and strontium.

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

Interplanar spacings and intensity measurements. The *d*-spacings of the New Jersey Zinc Co. and the Megaw patterns were converted from kX to angstrom units and the *d*-spacings of the Hoffmann pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hoffmann	110	211	321
New Jersey Zinc Co.	110	211	321
Megaw	110	510	211
Swanson, Gilfrich, and Ugrinic	110	211	200

Lattice constant. The structure of barium zirconate was determined by Hoffmann [2] in 1934. The cubic lattice has the space group O_h^1-Pm3m with perovskite-type structure and 1($BaZrO_3$) per unit cell. Several unit-cell determinations have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1935	Hoffmann [1]	4.185
1943	Náray-Szabó [3]	4.20
1946	Megaw [4]	4.190
1955	Swanson, Gilfrich, and Ugrinic.	4.1929 at 26° C

The density of the barium zirconate calculated from the NBS lattice constant is 6.229 at 26° C.

Barium Zirconate, $BaZrO_3$ (cubic)

hkl	1934 Hoffmann Cu, 1.5405 A			New Jersey Zinc Co. Mo, 0.7093 A			Megaw			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C.		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
100--	------	-----	------	-----	-----	------	------	-----	-----	4. 194	10	4. 194
110--	2. 963	100	4. 187	2. 98	100	4. 21	2. 98	100	4. 21	2. 965	100	4. 194
111--	------	-----	------	2. 41	9	4. 17	2. 42	40	4. 19	2. 421	9	4. 193
200--	2. 091	90	4. 182	2. 09	34	4. 18	2. 09	70	4. 18	2. 097	34	4. 193
----	------	-----	------	1. 92	1	------	------	-----	-----	------	-----	------
210--	------	-----	------	1. 87	2	4. 18	------	-----	-----	1. 8750	2	4. 1926
211--	1. 707	100	4. 181	1. 71	57	4. 19	1. 71	80	4. 19	1. 7116	37	4. 1925
220--	1. 480	80	4. 186	1. 48	29	4. 19	1. 48	70	4. 19	1. 4824	19	4. 1929
310--	1. 323	90	4. 184	1. 33	26	4. 20	1. 33	70	4. 20	1. 3258	17	4. 1925
311--	------	-----	------	1. 26	4	4. 18	1. 26	20	4. 18	1. 2641	2	4. 1926
222--	------	-----	------	1. 21	6	4. 19	1. 21	60	4. 19	1. 2104	5	4. 1930
321--	1. 118	100	4. 183	1. 12	32	4. 19	1. 12	80	4. 19	1. 1206	16	4. 1929
400--	1. 046	20	4. 182	1. 05	4	4. 20	1. 05	50	4. 20	1. 0482	3	4. 1928
411--	------	-----	------	0. 99	14	4. 20	0. 992	70	4. 21	0. 9883	9	4. 1926
420--	------	-----	------	-----	-----	------	. 940	70	4. 20	. 9376	7	4. 1931
332--	------	-----	------	-----	-----	------	. 896	70	4. 20	. 8939	5	4. 1928
422--	------	-----	------	-----	-----	------	. 857	70	4. 20	. 8559	6	4. 1930
510--	------	-----	------	-----	-----	------	. 824	100	4. 20	. 8223	12	4. 1929
Average value of last five lines----------			4. 184	-----	-----	4. 19	------	-----	4. 20	------	-----	4. 1929

References

[1] A. Hoffmann, Untersuchungen über Verbindungen mit Perowskitstruktur, Z. phys. Chem. **28B**, 65–77 (1935).

[2] A. Hoffmann, Sauerstoffsäuren des vierwertigen Cerium und Thorium, Naturwissenschaften **22**, 206 (1934).

[3] S. Náray-Szabó, Der Strukturtyp des Perowskits ($CaTiO_3$), Naturwissenschaften **31**, 202–203 (1943).

[4] H. D. Megaw, Crystal structure of double oxides for the perovskite type, Proc. Phys. Soc. London **58**, 133–152 (1946).

tri-Calcium Aluminate, $3CaO \cdot Al_2O_3$ (cubic)

Card numbers		New index lines	Radiation	Source
Old	New			
II-1930	2842	2.69	Molybdenum.	Harrington [1] 1927.
	2-0945	1.56	Molybdenum.	Brownmiller and Bogue [2] 1932.
	2-0920	1.90	Chromium	Lagerquist, Wallmark, and Westgren [3] 1937.
			Copper	McMurdie [4] 1941.
2624	2820 1-1065 1-1060	2.68 1.90 1.55	Molybdenum.	Hanawalt, Rinn, and Frevel [5] 1938.
2603	2733 1-1047 1-1051	2.70 1.91 1.56	Molybdenum.	Brady and Davey [6] 1941.
II-1901	2731 3-0795 3-0807	2.70 1.91 1.56	Copper	McMurdie [4] 1941.

The Hanawalt, Rinn, and Frevel and the Brady and Davey patterns were marked for deletion in the fifth supplement to the ASTM card file. The data of Brady and Davey were not found in the reference given on the ASTM card.

Additional published patterns

Pattern	Radiation	Wave-length
Koyanagi, Katoh, and Sudoh [7] 1938.	Iron	
Yannaquis [8] 1952	Copper	1.5418

NBS sample. The tricalcium aluminate was prepared by A. C. Bonanno of the Portland Cement Association Fellowship at the NBS. Spectrographic analysis of the sample showed the following impurities: 0.1 to 1.0 percent of sodium; 0.01 to 0.1 percent each of iron and manganese; 0.001 to 0.01 percent each of copper, magnesium, silicon, silver, and strontium; and 0.0001 to 0.001 percent each of chromium and tin.

The sample is colorless. The index of refraction is 1.701.

Interplanar spacings and intensity measurements. The *d*-spacings of the Harrington, the Brownmiller and Bogue, the McMurdie, the Hanawalt, Rinn, and Frevel, the Brady and Davey and the Koyanagi, Katoh and Sudoh patterns were converted from kX to angstrom units and the *d*-spacings of the Lagerquist, Wallmark, and Westgren pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Harrington	440	844	800
Brownmiller and Bogue	440	844	800
Lagerquist, Wallmark, and Westgren	440	800	844
McMurdie	440	800	844
Hanawalt, Rinn, and Frevel	440	800	844
Brady and Davey	440	800	844
Koyanagi, Katoh, and Sudoh	440	844	800
Yannaquis	440	800	844
Swanson, Gilfrich, and Ugrinic	440	800	844

Lattice constant. The latest work on the structure of tricalcium aluminate was described by Ordway [9] in 1952. The cubic lattice has the space group T_h^6-Pa3 with 24 ($3CaO \cdot Al_2O_3$) per unit cell. The indexing of the NBS pattern was checked with the unpublished calculated single crystal intensity data of Ordway referred to in his 1952 report.

A group of unit-cell values have been converted from kX to angstrom units. The values of Harrington, and of Davey and Steele have been doubled for comparison with the NBS measurement.

Lattice constants

		A
1927	Harrington [1]	15.276
1929	Davey and Steele [10]	15.278
1937	Lagerquist, Wallmark, and Westgren [3].	15.25
1941	Brady and Davey [6]	15.266
1941	McMurdie [4]	15.27
1952	Ordway [9]	15.22
1952	Yannaquis [8]	15.27
1955	Swanson, Gilfrich, and Ugrinic.	15.262 at 25° C.

The density of tricalcium aluminate calculated from the NBS lattice constant is 3.028 at 25° C.

tri-Calcium Aluminate, $3CaO \cdot Al_2O_3$ (cubic)

hkl	1927			1932			1937			1938			1941			1941			1938			1952			1955		
	Harrington			Brownmiller and Bogue			Lagerquist, Wallmark, and Westgren			Hanawalt, Rinn, and Frevel			McMurdie			Brady and Davey			Koyanagi, Katoh, and Sudoh			Yannaquis			Swanson, Gilfrich, and Ugrinic		
	Mo, 0.710 A			Mo, 0.7107 A			Cr, 2.2909 A			Mo, 0.7107 A			Cu, 1.5405 A			Mo, 0.7107 A			Fe, 1.9373 A			Cu, 1.5418 A			Cu, 1.5405A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*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*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
																						6.831	4				
																						6.241	3				
																						5.401	3				
221																4.86	7	15				5.091	3	15.27	5.09	5	15.27
113																						4.605	4	15.27	4.604	4	15.27
023																4.15	2	15				4.235	12	15.27	4.235	10	15.27
321	4.11	20	15.4	4.08	m	15.3	4.07	w	15.2	4.09	20	15.3	4.09	w	15.3							4.083	15	15.28	4.080	16	15.26
004							3.79	vw	15.2							3.79	10	15.2				3.822	3	15.29	3.816	1	15.27
223																						3.708	2	15.29	3.705	2	15.28
331							3.49	vw	15.2													3.504	2	15.27	3.501	2	15.26
421	3.31	10	15.2	3.33	w	15.3	3.33	w	15.3	3.31	4	15.2	3.35	vw	15.4							3.333	6	15.28	3.332	5	15.27
332																									3.252	1	15.25
422							3.10	vw	15.2							3.13	2	15.3							3.120	<1	15.28
430	3.05	5	15.2	3.04	w	15.2	3.049	w	15.25							3.05	15	15.2				3.055	4	15.28	3.052	3	15.26
431							2.988	vw	15.24							3.00	6	15.3	2.979	mw	15.19	2.998	2	15.29	2.993	3	15.26
432				2.84	w	15.3	2.829	w	15.23													2.837	8	15.28	2.834	6	15.26
521				2.78	w	15.2	2.780	w	15.23													2.789	14	15.28	2.787	14	15.26
400	2.71	100	15.3	2.70	vs	15.3	2.695	vs	15.25	2.69	100	15.2	2.71	vs	15.3	2.71	100	15.3	2.701	vs	15.28	2.700	100	15.27	2.700	100	15.27
531				2.58	vw	15.3	2.579	vw	15.26													2.584	3	15.29	2.581	3	15.27
610																									2.512	<1	15.28
611				2.46	vw	15.2	2.476	vw	15.26													2.480	2	15.29	2.477	1	15.27
620	2.42	10	15.3	2.405	w	15.21	2.405	m	15.21	2.39	4	15.1	2.40	w	15.2	2.40	4	15.2	2.410	w	15.24	2.415	7	15.27	2.413	7	15.26
621				2.380	w	15.24	2.383	w	15.26																2.384	6	15.26
541							2.357	vw	15.28													2.359	4	15.29	2.355	2	15.26
							2.301	vw								2.30	6										
630				2.275	w	15.26	2.279	vw	15.29				2.263	vw	15.2										2.277	3	15.27
444	2.20	40	15.2	2.204	m	15.27	2.201	m	15.25	2.19	8	15.17	2.204	m	15.27	2.19	5	15.2	2.199	mw	15.24	2.205	16	15.28	2.204	11	15.27
632							2.181	vw	15.27													2.184	2	15.29	2.181	2	15.26
711				2.138	vw	15.27																			2.138	<1	15.27
641				2.089	w	15.21													2.102	w	15.30	2.098	4	15.27	2.097	3	15.27
721							2.079	vw	15.28															15.27	3.078	2	15.27
642	2.04	5	15.3	2.037	w	15.24	2.041	w	15.27	2.03	4	15.19	2.043	vw	15.27				2.037	w	15.24	2.041	8	15.27	2.040	5	15.26
722							2.022	vw	15.27																2.021	<1	15.26
							2.005	vw																			
731				1.985	w	15.25	1.988	vw	15.27				1.988	vw	15.27							1.989	4	15.28	1.988	4	15.27
650				1.951	w	15.24	1.955	w	15.27				1.954	vw	15.26							1.955	4	15.27	1.955	4	15.27

tri-Calcium Aluminate, $3CaO\cdot Al_2O_3$ (cubic)—Continued

hkl	1927			1932			1937			1938			1941			1941			1938			1952			1955		
	Harrington			Brownmiller and Bogue			Lagerquist, Wallmark, and Westgren			Hanawalt, Rinn, and Frevel			McMurdie			Brady and Davey			Koyanagi, Katoh, and Sudoh			Yannaquis			Swanson, Gilfrich, and Ugrinic		
	Mo, 0.710 A			Mo, 0.7107 A			Cr, 2.2909 A			Mo, 0.7107 A			Cu, 1.5405 A			Mo, 0.7107 A			Fe, 1.9373 A			Cu, 1.5418 A			Cu, 1.5405A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*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*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
732							1.939	vw	15.27							1.93	6	15.2							1.940	<1	15.28
008	1.909	70	15.27	1.909	s	15.27	1.908	s	15.26	1.90	24	15.20	1.911	s	15.29	1.91	37	15.28	1.909	s	15.27	1.909	37	15.27	1.908	36	15.26
810							1.893	w	15.26													1.895	6	15.28	1.893	4	15.27
733																						1.868	2	15.29	1.865	1	15.27
821							1.838	vw	15.27													1.840	3	15.28	1.838	3	15.27
653	1.834	5	15.34	1.825	w	15.27	1.824	w	15.26				1.830	vw	15.31				1.821	w	15.24	1.825	5	15.27	1.824	3	15.27
822							1.799	vw	15.26													1.802	2	15.29	1.799	<1	15.27
830				1.789	vw	15.28	1.788	vw	15.28																1.785	<1	15.25
751																									1.763	<1	15.26
832	1.736	2	15.23	1.734	m	15.22	1.740	vw	15.27													1.740	2	15.27	1.740	2	15.27
752							1.729	vw	15.27										1.719	mw	15.18	1.731	2	15.29	1.727	2	15.25
840																									1.706	<1	15.26
841				1.696	vw	15.26	1.702	m	15.32													1.688			1.695	2	15.26
911				1.672	vw	15.23	1.675	vw	15.26																1.675	<1	15.26
																1.66	6					1.668					
921				1.643	w	15.24	1.646	w	15.26													1.648	3	15.28	1.646	2	15.26
664							1.626	vw	15.25													1.629	3	15.28	1.627	2	15.26
922				1.614	w	15.23	1.618	w	15.26													1.620	3	15.28	1.618	<1	15.26
851							1.608	vw	15.25																1.610	1	15.28
802																									1.583	1	15.27
932							1.571	vw	15.23																1.574	1	15.26
844	1.558	80	15.26	1.557	vs	15.26	1.559	s	15.28	1.55	24	15.19	1.559	s	15.28	1.56	24	15.28	1.558	vs	15.26	1.559	37	15.28	1.558	27	15.26
							1.525	vw														1.529	3				
10·1·0				1.515	vw	15.23	1.519	vw	15.26							1.52	3	15.28							1.519	2	15.26
																						1.514	3				
10·2·0																									1.497	2	15.26
10·2·1				1.489	w	15.26	1.488	vw	15.25										1.489	w	15.26				1.490	2	15.26
							1.482	w														1.483	3				
9·5·1							1.475	vw	15.26													1.476	3	15.27	1.476	2	15.26
10·3·0							1.462	vw	15.26																1.462	3	15.26
10·3·1				1.450	w	15.21	1.453	vw	15.24													1.456	<1	15.27	1.455	2	15.26
							1.448	vw																			
10·3·2				1.429	vw	15.26	1.435	vw	15.32																1.436	1	15.27
871							1.422	vw	15.25																1.429	<1	15.26

10·4·1				1. 407	w	15. 22	1. 410	vw	15. 25										1. 410	w	15. 25	1. 412	3	15. 27	1. 411	1	15. 26
10·3·3							1. 393	vw	15. 26										1. 391	w	15. 24				1. 405	2	15. 26
962							1. 388	vw	15. 27																1. 390	1	15. 28
10·5·0				1. 363	w	15. 24	1. 365	vw	15. 26																1. 3649	2	15. 260
11·2·1							1. 358	vw	15. 24							1. 36	5	15. 27				1. 360	3	15. 27	1. 3596	2	15. 261
880	1. 348	50	15. 25	1. 348	s	15. 25	1. 348	s	15. 25	1.345	12	15. 22	1. 349	m	15. 26	1. 35	20	15. 27	1. 349	s	15. 26	1. 350	11	15. 27	1. 3491	9	15. 263
11·3·1																									1. 3336	<1	15. 264
11·3·2	1. 314	2	15. 21	1. 318	vw	15. 26	1. 325	vw	15. 34																1. 3190	1	15. 269
10·6·0																			1. 308	w	15. 25				1. 3087	<1	15. 262
11·3·3																			1. 293	w	15. 24				1. 2948	<1	15. 265
11·4·2																									1. 2852	<1	15. 261
																						1. 272	3				
12·1·0				1. 265	vw	15. 23																			1. 2676	2	15. 264
																						1. 264	2				
12·2·1																									1. 2506	<1	15. 266
11·5·2																									1. 2461	<1	15. 262
12·2·2	1. 237	20	15. 25				1. 238	w	15. 26																1. 2379	2	15. 262
12·3·0				1. 233	w	15. 25	1. 234	w	15. 26										1. 234	w	15. 26				1. 2342	3	15. 266
12·3·2																									1. 2179	<1	15. 260
12·4·0	1. 206 (a)	50	15. 25	1. 206 (b)	s	15. 25	1. 202 (c)	m	15. 20	1. 205 (d)	8	15. 24	1. 208 (d)	m	15. 28	1. 21 (e)	3	15. 30	1. 206 (f)	s	15. 25				1. 2064	9	15. 260
Average value of last five lines			15. 25			15. 25			15. 26			15. 21			15. 28			15. 28			15. 25			15. 27			15. 262

[a] Nine additional lines were omitted.
[b] Eleven additional lines were omitted.
[c] Two additional lines were omitted.
[d] One additional line was omitted.
[e] Four additional lines were omitted.
[f] Seven additional lines were omitted.

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Cesium Chloroplatinate, Cs_2PtCl_6 (cubic)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wave-length
Natta and Pirani [1] 1932	Iron	K_α.
Bødtker-Naess and Hassel [2] 1933.	Iron	

NBS sample. The cesium chloroplatinate was prepared at the NBS from cesium chloride, and chloroplatinic acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium; 0.001 to 0.01 percent each of aluminum, iron, silicon, and zirconium; and 0.0001 to 0.001 percent each of calcium and copper.

The sample is pale yellow. The index of refraction is 1.757.

Interplanar spacings and intensity measurements. The *d*-spacings of the Natta and Pirani and the Bødtker-Naess and Hassel patterns were calculated from Bragg angle data. The Bødtker-Naess and Hassel pattern did not include intensity measurements.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Natta and Pirani	400	422	440
Swanson, Gilfrich, and Ugrinic	220	111	400

Lattice constant. The structure of cesium chloroplatinate was determined by Natta and Pirani [1] in 1932. The cubic lattice has the space group O_h^5–Fm3m with potassium chloroplatinate-type structure and 4 (Cs_2PtCl_6) per unit cell.

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

Lattice constants

		A
1932	Natta and Pirani [1]	10.17
1933	Bødtker-Naess and Hassel [2]	10.140
1935	Engel [3]	10.218
1955	Swanson, Gilfrich, and Ugrinic	10.215 at 26°C

The density of cesium chloroplatinate calculated from the NBS lattice constant is 4.198 at 26° C.

References

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Cesium Chloroplatinate, Cs_2PtCl_6 (cubic)

hkl	1932 Natta and Pirani Fe, 1.937 A			1933 Bødtker-Naess and Hassel Fe, 1.937 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	5. 6	D	9. 7	-------	--	-------	5. 901	73	10. 22
220	3. 5	90	9. 8	-------	--	-------	3. 613	100	10. 219
311	3. 0	29	9. 9	-------	--	-------	3. 085	34	10. 217
222	2. 8	33	9. 8	-------	--	-------	2. 950	27	10. 219
400	2. 5	100	9. 9	-------	--	-------	2. 554	59	10. 218
331	2. 29	43	10. 0	-------	--	-------	2. 344	9	10. 219
422	2. 05	100	10. 1	-------	--	-------	2. 086	39	10. 217
511	1. 94	48	10. 1	1. 947	--	10. 12	1. 966	16	10. 216
440	1. 78	95	10. 0	1. 792	--	10. 14	1. 806	29	10. 217
531	1. 696	52	10. 03	1. 714	--	10. 14	1. 726	14	10. 212
620	1. 591	81	10. 06	1. 598	--	10. 11	1. 615	17	10. 215
533	--------	--	--------	-------	--	-------	1. 558	5	10. 215
622	1. 517	29	10. 06	-------	--	-------	1. 5400	6	10. 215
444	1. 457	71	10. 09	1. 462	--	10. 13	1. 4746	9	10. 216
711	1. 413	48	10. 09	1. 426	--	10. 18	1. 4304	7	10. 215
-------	1. 395	24	--------	-------	--	-------	--------	--	--------
642	1. 345	71	10. 07	1. 354	--	10. 13	1. 3653	15	10. 217
731	1. 317	48	10. 12	1. 319	--	10. 13	1. 3300	5	10. 216
800	1. 265	43	10. 12	-------	--	-------	1. 2772	5	10. 218
733	1. 228	29	--------	-------	--	-------	1. 2483	<1	10. 217
822	1. 196	62	10. 15	1. 194	--	10. 13	1. 2040	6	10. 216
751	1. 170	29	10. 13	-------	--	-------	1. 1797	3	10. 216
662	--------	--	--------	-------	--	-------	1. 1718	1	10. 216
840	1. 134	71	10. 14	-------	--	-------	1. 1422	8	10. 215
911	1. 115	29	10. 16	-------	--	-------	1. 1212	2	10. 216
664	1. 083	52	10. 16	-------	--	-------	1. 0890	3	10. 216
931	1. 066	43	10. 17	-------	--	-------	1. 0709	3	10. 216
844	1. 038	62	10. 17	-------	--	-------	1. 0426	5	10. 217
933	1. 023	38	10. 18	-------	--	-------	1. 0266	3	10. 216
10·2·0	--------	--	--------	-------	--	-------	1. 0017	6	10. 215
951	--------	--	--------	-------	--	-------	0. 9875	3	10. 215
10·2·2	--------	--	--------	-------	--	-------	. 9829	1	10. 215
953	--------	--	--------	-------	--	-------	. 9525	3	10. 214
10·4·2	--------	--	--------	-------	--	-------	. 9324	5	10. 214
11·1·1	--------	--	--------	-------	--	-------	. 9210	1	10. 214
880	--------	--	--------	-------	--	-------	. 9028	2	10. 214
11·3·1	--------	--	--------	-------	--	-------	. 8925	3	10. 215
10·6·0	--------	--	--------	-------	--	-------	. 8759	4	10. 215
11·3·3	--------	--	--------	-------	--	-------	. 8665	1	10. 216
10·6·2	--------	--	--------	-------	--	-------	. 8633	<1	10. 215
12·0·0	--------	--	--------	-------	--	-------	. 8512	5	10. 214
11·5·1	--------	--	--------	-------	--	-------	. 8425	2	10. 215
12·2·2	--------	--	--------	-------	--	-------	. 8285	6	10. 214
11·5·3	--------	--	--------	-------	--	-------	. 8205	1	10. 215
12·4·0	--------	--	--------	-------	--	-------	. 8075	3	10. 214
Average value of last five lines			10. 17	-------	--	10. 14	--------	--	10. 215

Cesium Chlorostannate, Cs_2SnCl_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS pattern. The cesium chlorostannate was prepared at the NBS from cesium chloride and stannic chloride. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent of sodium; 0.001 to 0.01 percent each of aluminum, calcium, magnesium, lead, and silicon; and 0.0001 to 0.001 percent each of silver, barium, chromium, cesium, iron, and magnesium.

The sample is colorless. The index of refraction is 1.672.

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

Pattern	1	2	3
Swanson, Gilfrich, and Ugrinic	220	400	222

Lattice constant. The structure of cesium chlorostannate was determined by Engel [1] in 1933. The cubic lattice has the space group O_h^5-Fm3m with potassium chloroplatinate-type structure and $4(Cs_2SnCl_6)$ per unit cell.

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

Lattice constants

		A
1935	Engel [1]	10.369
1955	Swanson, Gilfrich, and Ugrinic.	10.381 at 25° C.

The density of cesium chlorostannate calculated from the NBS lattice constant is 3.545 at 25° C.

Cesium Chlorostannate, Cs_2SnCl_6 (cubic)

hkl	1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	5. 991	48	10. 38
200	5. 187	7	10. 37
220	3. 670	100	10. 38
311	3. 131	20	10. 38
222	2. 997	52	10. 38
400	2. 596	58	10. 38
331	2. 383	6	10. 39
420	2. 322	4	10. 39
422	2. 120	35	10. 39
511	1. 999	10	10. 39
440	1. 835	31	10. 38
531	1. 7543	7	10. 379
600	1. 7299	2	10. 379
620	1. 6410	12	10. 379
533	1. 5828	3	10. 379
622	1. 5647	10	10. 379
444	1. 4981	9	10. 379
711	1. 4531	5	10. 377
642	1. 3870	10	10. 381
731	1. 3513	2	10. 380
800	1. 2973	1	10. 378
820	1. 2587	<1	10. 380
822	1. 2233	3	10. 380
751	1. 1987	1	10. 381
662	1. 1905	1	10. 378
840	1. 1604	4	10. 379
911	1. 1392	1	10. 379
842	1. 1325	1	10. 380
664	1. 1064	3	10. 379
931	1. 0882	<1	10. 381
844	1. 0594	3	10. 380
933	1. 0431	1	10. 379
10·2·0	1. 0178	3	10. 380
951	1. 0034	2	10. 379
10·2·2	0. 9988	2	10. 380
953	. 9680	1	10. 381
10·4·2	. 9477	2	10. 382
880	. 9175	1	10. 380
11·3·1	. 9069	<1	10. 380
10·6·0	. 8901	1	10. 380
10·6·2	. 8773	1	10. 380
12·0·0	. 8651	2	10. 381
12·2·2	. 8420	2	10. 381
11·5·3	. 8338	1	10. 381
12·4·0	. 8207	2	10. 381
991	. 8131	<1	10. 381
10·8·2	. 8009	1	10. 381
Average value of last five lines			10. 381

References

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Cesium Fluogermanate Cs_2GeF_6 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
1817	1849 1-0778 1-0753	3. 19 1. 84 2. 25	Molybdenum.	Wyckoff and Müller [1] 1927.
II-1169	1850 2-0548 2-0540	3. 18 1. 84 2. 25	Molybdenum.	Wyckoff and Müller [1] 1927.
-------	1851 3-0525 3-0507	3. 19 1. 84 1. 20	Copper----	Schütz [2] 1936.

The two ASTM cards for Wyckoff and Müller give data from the same powder pattern.

Additional published patterns. None.

NBS sample. The cesium fluogermanate was prepared at the NBS from cesium chloride, germanium oxide and hydrofluoric acid. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent each of aluminum, sodium, platinum, and silicon; 0.001 to 0.01 percent each of calcium and tin; and 0.0001 to 0.001 percent each of silver, iron, magnesium, lead, and strontium.

The sample is colorless. The index of refraction is too low to be determined by the liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-spacings of the Wyckoff and Müller and the Schütz patterns were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Wyckoff and Müller	220	422	400
Schütz	220	422	642
Swanson, Gilfrich, and Ugrinic	220	111	222

Lattice constant. The structure of cesium fluogermanate was determined by Wyckoff and Müller [1] in 1927. The cubic lattice has the space group O_h^5–Fm3m with potassium chloroplatinate-type structure and 4(Cs_2GeF_6) per unit cell.

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

Lattice constants

		A
1927--	Wyckoff and Müller [1]------	9.009
1936--	Schütz [2]------------------	9.09
1955--	Swanson, Gilfrich, and Ugrinic.	9.021 at 26°C

The density of cesium fluogermanate calculated from the NBS lattice constant is 4.093 at 26°C.

References

[1] R. W. G. Wyckoff and J. H. Müller, The crystal structure of cesium fluogermanate, Am. J. Sci. 13, 347–352 (1927).

[2] W. Schütz, Die kristallchemische Verwandtschaft zwischen Germanium und Silicium, Z. physik. Chem. **31**, 292–308 (1936).

Cesium Fluogermanate, Cs_2GeF_6 (cubic)

hkl	1927 Wyckoff and Müller Mo, 0.7107 A			1936 Schütz Cu, 1.5418 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	5.25	30	9.09	--------	----	--------	5.21	40	9.03
200	4.53	20	9.06	--------	----	--------	4.52	30	9.04
220	3.19	100	9.02	3.18	100	8.99	3.192	100	9.02
311	2.72	5	9.02	--------	----	--------	2.723	8	9.032
222	2.64	40	9.15	2.60	60	9.01	2.606	34	9.028
400	2.24	50	8.96	2.25	80	9.00	2.256	30	9.026
420	2.01	10	9.00	2.01	60	8.99	2.019	13	9.028
422	1.84	60	9.00	1.84	100	9.01	1.8419	26	9.023
511	1.73	5	8.99	1.73	20	9.00	1.7363	5	9.022
440	1.59	40	9.01	1.59	60	9.00	1.5950	12	9.023
531	--------	----	--------	--------	----	--------	1.5250	2	9.022
600	1.503	10	9.02	1.501	40	9.01	1.5038	5	9.023
620	1.423	40	9.00	1.422	80	8.99	1.4265	12	9.022
533	--------	----	--------	--------	----	--------	1.3772	1	9.030
622	1.358	10	9.01	1.362	20	9.03	1.3604	4	9.024
444	1.298	10	8.99	1.300	20	9.01	1.3024	3	9.023
711	1.257	5	8.98	--------	----	--------	1.2633	2	9.022
640	--------	----	--------	--------	----	--------	1.2510	1	9.021
642	1.202	40	8.99	1.203	100	9.00	1.2056	8	9.022
731	--------	----	--------	--------	----	--------	1.1752	<1	9.027
800	1.120	5	8.96	1.125	10	9.00	1.1277	1	9.022
820	1.091	5	9.01	1.093	10	9.01	1.0944	2	9.025
822	1.059	20	8.99	1.062	60	9.01	1.0636	3	9.025
751	--------	----	--------	1.040	10	9.01	1.0424	<1	9.027
662	--------	----	--------	--------	----	--------	1.0351	<1	9.023
840	0.9907	10	8.86	1.008	40	9.02	1.0090	1	9.024
911	--------	----	--------	--------	----	--------	0.9906	<1	9.025
842	.9805	5	8.99	0.9828	20	9.01	.9843	1	9.021
664	.9585	10	8.99	.9609	40	9.01	.9618	2	9.022
844	.9182	5	9.00	.9197	20	9.01	.9208	1	9.022
10·0·0	--------	----	--------	--------	----	--------	.9024	<1	9.024
10·2·0	.8813	10	8.99	.8832	80	9.01	.8847	2	9.022
10·2·2	--------	----	--------	--------	----	--------	.8680	<1	9.020
10·4·0	--------	----	--------	.8359	10	9.01	.8376	<1	9.021
10·4·2	--------	----	--------	.8223	40	9.01	.8235	1	9.021
880	--------	----	--------	--------	----	--------	.7975	<1	9.023
10·4·4	--------	----	--------	--------	----	--------	.7852	<1	9.021
Average value of last five lines			8.99	--------	----	9.01	--------	----	9.021

Cesium Fluosilicate, Cs_2SiF_6 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
----	1826 3–0516 3–0526	3. 15 2. 58 1. 19	Copper K_α--	Schütz [1] 1936.

Additional published patterns. None.

NBS sample. The cesium fluosilicate was prepared at the NBS from cesium chloride, silica gel and hydrofluoric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum and sodium; 0.001 to 0.01 percent each of calcium, iron, and titanium; and 0.0001 to 0.001 percent each of barium, lead, and magnesium.

The sample is colorless. The index of refraction is too low to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-spacings of the Schütz pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Schütz	220	222	642
Swanson, Gilfrich, and Ugrinic	220	200	222

Lattice constant. The structure of cesium fluosilicate was determined by Ketelaar [2] in 1935. The cubic lattice has the space group O_h^5–Fm3m with potassium chloroplatinate-type structure and $4(Cs_2SiF_6)$ per unit cell.

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

Lattice constants

		A
1935	Ketelaar [2]	8.885
1936	Schütz [1]	8.91
1955	Swanson, Gilfrich, and Ugrinic.	8.919 at 25° C.

The density of cesium fluosilicate calculated from the NBS lattice constant is 3.818 at 25° C.

Cesium Fluosilicate, Cs_2SiF_6 (cubic)

hkl	1936 Schütz Cu, 1.5418 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	----	--	--	5. 16	26	8. 93
200	4. 46	40	8. 92	4. 47	62	8. 93
220	3. 15	100	8. 91	3. 15	100	8. 92
311	----	--	--	2. 69	<1	8. 93
222	2. 57	100	8. 90	2. 576	48	8. 92
400	2. 22	60	8. 88	2. 231	26	8. 92
420	1. 99	80	8. 90	1. 996	25	8. 92
422	1. 817	80	8. 90	1. 821	19	8. 92
511	1. 715	10	8. 91	1. 717	4	8. 92
440	1. 575	60	8. 90	1. 577	9	8. 92
600	1. 486	60	8. 92	1. 487	9	8. 92
620	1. 408	80	8. 91	1. 4099	10	8. 917
622	1. 342	60	8. 90	1. 3442	6	8. 916
444	1. 287	20	8. 92	1. 2872	3	8. 918
711	----	--	--	1. 2486	1	8. 917
640	1. 236	20	8. 91	1. 2364	2	8. 916
642	1. 191	100	8. 91	1. 1918	9	8. 919
731	----	--	--	1. 1610	<1	8. 918
800	----	--	--	1. 1147	1	8. 918
820	1. 081	40	8. 91	1. 0814	4	8. 918
822	1. 050	40	8. 91	1. 0509	4	8. 917
751	1. 029	10	8. 91	1. 0294	<1	8. 915
662	----	--	--	1. 0228	2	8. 917
840	0. 995	20	8. 90	0. 9968	4	8. 916
842	. 971	40	8. 90	. 9731	2	8. 919
664	. 948	20	8. 90	. 9506	4	8. 917
844	. 908	10	8. 90	. 9102	1	8. 918
10·0·0	. 894	10	8. 94	. 8918	1	8. 918
10·2·0	. 873	40	8. 90	. 8746	6	8. 919
10·2·2	----	--	--	. 8582	1	8. 919
10·4·0	----	--	--	. 8281	1	8. 919
10·4·2	----	--	--	. 8141	2	8. 918
Average value of last five lines			8. 898	----	--	8. 919

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Chromium, Cr (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
3348	3537 1–1250 1–1250	2.05 1.18 0.92	Molybdenum 0.712 A.	Hull [1] 1921.
3339	3538 1–1251 1–1251	2.05 1.17 0.77	Molybdenum 0.7121 A.	Patterson [2] 1925.
3380	3588 1–1267 1–1261	2.03 1.17 1.44	Molybdenum	Hanawalt, Rinn, and Frevel [3] 1938.

Additional published patterns

Source	Radiation	Wave-length
Sillers [4] 1927	Molybdenum	

NBS sample. The chromium was electrodeposited from highly purified salts at the NBS by James T. Sterling. It was crushed, acid washed for 10 days in nitric acid, annealed in hydrogen at 1,200° C for 1 hour, then in helium at 1,200° C for 1 hour, and cooled 100° C per hour to room temperature in a dry helium atmosphere.

The same sample had been previously annealed and cooled in a hydrogen atmosphere. It was found that the hydrogen cooled chromium gave a unit cell of 2.8855 A and the helium cooled chromium a cell of 2.8839 A. The helium cooled sample is believed to contain less gas than the hydrogen cooled sample. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of silicon; 0.001 to 0.01 percent each of copper, manganese, and tin; and 0.0001 to 0.001 percent each of silver and iron.

The sample is opaque with a very bright surface.

Interplanar spacings and intensity measurements. The Siller pattern does not include intensity values. The *d*-spacings of the Hull, the Patterson, the Hanawalt, Rinn, and Frevel and the Siller patterns were converted from kX to angstrom units.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hull	110	211	310
Patterson	110	211	321
Hanawalt, Rinn, and Frevel	110	211	200
Swanson, Gilfrich, and Ugrinic	110	211	200

Lattice constant. Hull [5] determined the crystal structure of cubic chromium in 1919. The cubic lattice has the space group O_h^9-Im3m with 2 (Cr) per unit cell.

The following group of unit-cell measurements have been converted from kX to angstrom units, and the measurements of Wood [6] and of Fricke [7] have been temperature corrected to 25° C for comparison with the NBS value. The linear coefficient of expansion of chromium is 6.6×10^{-6} between 0° and 100° C according to Hidnert [8].

Lattice constants

		A
1919	Hull [5]	2.92
1921	Hull [1]	2.901
1925	Goldschmidt, Ulrich, and Barth [9].	2.900
1925	Phebus and Blake [10]	2.881
1925	Patterson [2]	2.878
1926	Smith [11]	2.866
1927	Sillers [4]	2.878
1930	Sasaki and Sekito [12]	2.883
1931	Adcock [13]	2.8844
1932	Preston [14]	2.8844
1934	Jette, Nordstrom, Queneau, and Foote [15].	2.8844
1935	Wright, Hirst, and Riley [16]	2.8839
1936	Brück [17]	2.89
1936	Glocker [18]	2.884
1937	Wood [6]	2.8855 at 25° C
1939	van Arkel [19]	2.8856 at 25° C
1941	Fricke [7]	2.884 at 25° C
1947	Vegard [20]	2.885
1951	Fine, Greiner, and Ellis [21]	2.8849 at 25° C
1952	Taylor and Floyd [22]	2.8843 at 25° C
1953	Pearson and Hime-Rothery [23].	2.8846 at 25° C
1955	Straumanis and Weng [24]	2.88502 at 25° C
1955	Swanson, Gilfrich, and Ugrinic	2.8839 at 25° C

The density of alpha chromium calculated from the NBS lattice constant is 7.200 at 25° C

Chromium, Cr (cubic)

hkl	1921 Hull Mo, 0.7107 A			1925 Patterson Mo, 0.7107 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1927 Sillers Mo, 0.7107 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° 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*
110	2.052	100	2.901	2.056	100	2.908	2.03	100	2.871	-----	--	-----	2.0390	100	2.8836
200	1.451	20	2.902	1.439	40	2.878	1.440	17	2.880	1.437	--	2.874	1.4419	16	2.8838
211	1.185	50	2.903	1.174	80	2.876	1.176	30	2.881	1.179	--	2.888	1.1774	29	2.8840
220	1.027	10	2.905	1.016	50	2.874	1.020	3	2.885	1.020	--	2.885	1.0195	17	2.8836
310	0.917	30	2.900	0.911	60	2.881	0.910	3	2.878	0.910	--	2.878	0.9120	21	2.8840
222	.839	5	2.906	.831	20	2.879	-----	--	-----	.832	--	2.882	.8325	6	2.8839
321	.776	30	2.903	.770	70	2.881	.770	3	2.881	.769	--	2.877	-----	--	-----
400	.724	5	2.896	.719	10	2.876	-----	--	-----	-----	--	-----	-----	--	-----
411	.683	20	2.898	.6789	40	2.880	-----	--	-----	-----	--	-----	-----	--	-----
420	.649	5	2.902	.6433	30	2.877	-----	--	-----	-----	--	-----	-----	--	-----
332	.618	2	2.899	.6132	30	2.876	-----	--	-----	-----	--	-----	-----	--	-----
422	.592	1	2.900	.5877	30	2.879	-----	--	-----	-----	--	-----	-----	--	-----
510	.568	15	2.896	.5641	40	2.876	-----	--	-----	-----	--	-----	-----	--	-----
Average value of last five lines			2.899	-----	--	2.878	-----	--	2.881	-----	--	2.882	-----	--	2.8839

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Chromium (III) Oxide, Cr_2O_3 (hexagonal)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
II–3492	3786	1.67	Chromium	Wretblad [1] 1930.
	2–1365	1.43	Iron	Passerini [2] 1930.
	2–1362	2.66		
3667	3781	1.67	Molybdenum.	Hanawalt, Rinn, and Frevel [3] 1938.
	1–1294	2.67		
	1–1294	2.47		
-------	3783	1.67	Chromium	United Steel Companies, England.
	3–1126	2.67		
	3–1124	1.47		
-------	4–0764	2.48	Electron Diffraction.	Hickman and Gulbransen [4] 1949.
	4–0765	2.66		
		2.17		

The Wretblad and Passerini patterns have been combined on one ASTM card, No. 2–1362. The old and new ASTM cards of Wretblad and Passerini state that molybdenum radiation was used. However, in both cases the patterns were made with chromium radiation.

The reference on the ASTM card for Hickman and Gulbransen erroneously gives the page numbers 534–546, whereas they should be 519–533.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [5] 1928	Copper	----------

NBS sample. The chromic oxide was obtained from Johnson, Matthey and Co., Ltd. Their spectrographic analysis showed less than 0.001 percent each of calcium and magnesium, and less than 0.0001 percent each of silicon and copper. The sample was annealed at 1,250° C for 2 hours in an open chromium tube.

The refractive indices were too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-spacings of the Wretblad, the Passerini and the Zachariasen patterns were calculated from their Bragg angle data and the *d*-spacings of the Hanawalt, Rinn, and Frevel, the United Steel Companies and the Hickman and Gulbransen patterns were converted from kX to angstrom units.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Wretblad	116	012	104
Passerini	116	104	110
Hanawalt, Rinn, and Frevel	116	104	214
United Steel Companies	116	104	214
Hickman and Gulbransen	110	104	113
Zachariasen	116	104	110
Swanson, Gilfrich, and Ugrinic	104	110	116

Lattice constants. The structure of chromic oxide was determined by Wretblad [1] in 1930. The hexagonal lattice has the space group D_{3d}^{6}–$R\bar{3}c$ with ferric oxide-type structure and $6(Cr_2O_3)$ per unit cell.

A group of unit-cell measurements have been converted from kX to angstrom units and the United Steel Companies' rhombohedral cell has been referred to hexagonal axes for comparison with the NBS values. The cell values given by Passerini have been doubled in the *c*-direction to conform with the accepted cell size.

Lattice constants

		a	*c*
		A	*A*
1923	Davey [6]	4.942	13.609
1928	Zachariasen [5]	4.94	13.60
1930	Wretblad [1]	4.959	13.60
1930	Passerini [2]	4.960	13.639
------	United Steel Companies	4.959	13.597
1955	Swanson, Gilfrich, and Ugrinic.	4.954	13.584 at 26° C

The density of the chromic oxide calculated from the NBS lattice constants is 5.245 at 26° C.

Chromium (III) Oxide, Cr_2O_3 (hexagonal)

hkl	1930		1930		1938		----		1949		1928		1955	
	Wretblad		Passerini		Hanawalt, Rinn, and Frevel		United Steel Companies		Hickman and Gulbransen		Zachariasen		Swanson, Gilfrich, and Ugrinic	
	Cr, 2.2897 A		Fe, 1.9360 A		Mo, 0.7107 A		Cr, 2.2897 A		Electron diff.		Cu, 1.5405 A		Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*		*A*	
012	3. 62	s	3. 58	w	3. 63	45	3. 64	50	3. 60	20	3. 64	20	3. 633	74
104	2. 66	s	2. 64	s	2. 68	70	2. 68	70	2. 67	60	2. 66	60	2. 666	100
110	2. 48	s	2. 46	s	2. 47	70	2. 49	60	2. 49	100	2. 47	60	2. 480	96
006	------	--	------	---	------	-----	2. 27	30	------	--	------	--	2. 264	12
113	2. 17	s	2. 17	s	2. 17	30	2. 18	60	2. 17	60	2. 18	30	2. 176	38
202	2. 04	w	2. 00	w	2. 03	4	------	--	2. 05	10	------	--	2. 048	9
024	1. 81	s	1. 80	m	1. 81	45	1. 82	60	1..83	40	1. 81	40	1. 816	39
116	1. 67	vs	1. 664	vs	1. 67	100	1. 67	100	1. 68	40	1. 67	100	1. 672	90
------	------	--	1. 616	mw	------	-----	------	--	------	--	------	--	------	---
122	1. 58	w	1. 579	mw	1. 58	6	1. 58	50	1. 58	10	1. 579	20	1. 579	13
214	1. 46	s	1. 464	ms	1. 468	30	1. 47	70	1. 478	50	1. 461	40	1. 465	25
300	1. 43	s	1. 434	vs	1. 435	45	1. 43	70	1. 436	50	1. 426	70	1. 4314	40
1·0·10	1. 297	m	1. 301	ms	1. 297	16	1. 30	70	1. 311	50	1. 295	40	1. 2961	20
------	1. 294	w	------	---	------	-----	1. 29	50	------	--	------	--	------	---
220	1. 240	m	1. 240	mw	1. 238	6	1. 24	60	1. 241	20	1. 237	30	1. 2398	17
306	1. 210	w	------	---	1. 211	6	1. 21	60	1. 196	20	1. 205	20	1. 2101	7
------	1. 197	vw	------	---	------	-----	1. 20	50	------	--	------	--	------	---
128 312	1. 174	w	------	---	1. 174	5	1. 17	60	------	--	------	--	1. 1731	14
0·2·10	------	--	------	---	1. 150	6	------	--	------	--	1. 147	30	1. 1488	10
134	------	--	------	---	1. 125	6	------	--	1. 116	10	1. 123	30	1. 1239	10
226	------	--	------	---	1. 089	12	------	--	1. 096	30	1. 087	50	1. 0874	17
2·1·10	------	--	------	---	1. 049	10	------	--	1. 055	10	1. 042	40	1. 0422	16
------	------	--	------	---	1. 027	2	------	--	------	--	------	--	------	---
324	------	--	------	---	0. 948	6(α_1)	------	--	0. 9479	30	------	--	0. 9462	13
410	------	--	------	---	------	-----	------	--	------	--	------	--	. 9370	12
1·3·10	------	--	------	---	------	-----	------	--	------	--	------	--	. 8957	14
3·0·12	------	--	------	---	------	-----	------	--	------	--	------	--	. 8883	7
416	------	--	------	---	------	-----	------	--	------	--	------	--	. 8658	23
4·0·10	------	--	------	---	------	-----	------	--	------	--	------	--	. 8425	8
1·0·16	------	--	------	---	------	-----	------	--	------	--	------	--	. 8331	11
330	------	--	------	---	------	-----	------	--	------	--	------	--	. 8263	9
3·2·10	------	--	------	---	------	-----	------	--	------	--	------	--	. 7977	15

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Copper (II) Fluoride, CuF_2 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The cupric fluoride was prepared at the NBS by the action of hydrofluoric acid on cuprous chloride. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, magnesium, and tungsten; 0.001 to 0.01 percent each of silver, boron, barium, chromium, iron, molybdenum, nickel, lead, platinum, antimony, tin, strontium, and titanium; and 0.0001 to 0.001 percent of manganese.

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 three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Ugrinic	111	220	311

Lattice constant. The structure of cupric fluoride was determined by Ebert and Woitinek [1] in 1933. The cubic lattice has the space group O_h^5–Fm3m with calcium fluoride-type structure and 4(CuF_2) per unit cell.

The Ebert and Woitinek unit-cell measurement has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1933	Ebert and Woitinek [1]	5.417
1955	Swanson, Gilfrich, and Ugrinic.	5.416 at 26° C

The density of cupric fluoride calculated from the NBS lattice constant is 4.245 at 26° C.

Copper (II) Fluoride, CuF_2 (cubic)

hkl	1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26°C		
	d	*I*	*a*
	A		*A*
111	3. 127	100	5. 416
200	2. 708	6	5. 416
220	1. 915	49	5. 416
311	1. 633	28	5. 416
400	1. 3539	3	5. 416
331	1. 2425	5	5. 416
422	1. 1055	5	4. 416
511	1. 0424	3	5. 416
440	0. 9574	1	5. 416
531	. 9156	2	5. 417
620	. 8564	1	5. 416
Average value of last five lines			5. 416

References

[1] F. Ebert and H. Woitinek, Crystalline structure of fluorides II. HgF, HgF_2, CuF and CuF_2, Z. anorg. Chem. **210,** 269–272 (1933).

Germanium (IV) Iodide, GeI_4 (cubic)

ASTM cards. None.

Additional published patterns.

Source	Radiation	Wave-length
Jaeger, Terpstra, and Westenbrink [1]	Copper	1.573 A

NBS sample. The germanium tetraiodide was prepared at the NBS by heating a mixture of the elements in a closed tube at 400° C. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent of silicon; 0.001 to 0.01 percent each of aluminum, calcium, chromium, copper, iron, magnesium, and lead; 0.0001 to 0.001 percent each of boron, manganese, and tin; and less than 0.0001 percent of silver.

The sample has a bright orange color. The index of refraction could not be determined by the liquid grain immersion method because the sample reacted with the liquids.

Interplanar spacings and intensity measurements. The *d*-spacings spacings of the Jaeger, Terpstra, and Westenbrink pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Jaeger, Terpstra, and Westenbrink	222	440	622
Swanson, Gilfrich, and Ugrinic	222	440	622

Lattice constant. The structure of germanium tetraiodide was determined by Jaeger, Terpstra, and Westenbrink [1] in 1925. The cubic lattice has the space group T_h^6–Pa3 with tin tetraiodide-type structure and 8 (GeI_4) per unit cell.

The unit-cell value of Jaeger, Terpstra, and Westenbrink has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1925	Jaeger, Terpstra, and Westenbrink [1].	12.00
1955	Swanson, Gilfrich, and Ugrinic	12.040 at 26° C

The density of germanium tetraiodide calculated from the NBS lattice constant is 4.416 at 26° C.

Germanium (IV) Iodide, GeI_4 (cubic)

hkl	1925 Jaeger, Terpstra, and Westenbrink Cu, 1.537 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	-----	--	-----	6. 95	4	12. 04
210	-----	--	-----	5. 384	8	12. 04
211	4. 87	vw	11. 93	4. 918	12	12. 05
222	3. 43	100	11. 88	3. 4740	100	12. 034
400	2. 97	70	11. 88	3. 0104	41	12. 042
421	-----	--	-----	2. 6270	4	12. 038
332	-----	--	-----	2. 5679	3	12. 044
431	-----	--	-----	2. 3605	4	12. 036
440	2. 108	90	11. 92	2. 1286	35	12. 041
622	1. 800	80	11. 94	1. 8148	27	12. 038
631	-----	--	-----	1. 7752	3	12. 040
444	1. 722	30	11. 93	1. 7378	7	12. 040
---	-----	--	-----	1. 5047	4	12. 038
662	1. 371	30	11. 95	1. 3812	7	12. 041
840	1. 338	30	11. 97	1. 3466	6	12. 044
844	1. 221	20	11. 96	1. 2287	5	12. 039
10·2·2	-----	--	-----	1. 1585	3	12. 040
Average value of last five lines			11. 95	------	--	12. 040

References

[1] F. M. Jaeger, P. Terpstra and H. G. K. Westenbrink, On the crystalstructure of germanium-tetraiodide, Proc. Acad. Sci. Amsterdam **28**, 747–766 (1925).

Indium Oxide, In_2O_3 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
2272	2366	2.91	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
	1-0934	1.78		
	1-0929	1.52		

The new ASTM card for Hanawalt, Rinn, and Frevel erroneously states that indium oxide is hexagonal.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [2] 1928	Copper	

NBS sample. The indium oxide was prepared by Johnson, Matthey and Co. Ltd., London. Their spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium and calcium, and 0.0001 to 0.001 percent of silver, magnesium, iron, lithium, tin, cadmium, and silicon.

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

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units, and the *d*-spacings of the Zachariasen pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Zachariasen	222	440	622
Hanawalt, Rinn, and Frevel	222	440	400
Swanson, Gilfrich, and Ugrinic	222	440	400

Lattice constant. The structure of indium oxide was determined by Pauling and Shappell [3] in 1930. The cubic lattice has the space group T_h^7–Ia3 with thallic oxide-type structure and 16(In_2O_3) per unit cell.

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

Lattice constants

		A
1925	Goldschmidt [4]	10.14
1928	Zachariasen [2]	10.06
1930	Pauling and Shappell [3]	10.14
1946	Moeller and Schnizlein [5]	10.14
1955	Swanson, Gilfrich, and Ugrinic	10.118 at 26° C

The density of indium oxide calculated from the NBS lattice constant is 7.117 at 26° 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] L. Pauling and M. D. Shappell, The crystal structure of bixbyite and the c-modification of the sesquioxides, Z. Krist. **75**, 128–142 (1930).

[4] V. M. Goldschmidt, T. Barth, and G. Lunde, Geochemische Verteilungsgesetze der Elemente. V Isomorphie und polymorphie der Sesquioxyde. Die Lanthaniden-Kontraktion und ihre Konsequenzen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1925** No. 7 (1925).

[5] T. Moeller and J. G. Schnizlein, Jr., Contributions to the chemistry of indium. VIII Observations on the formation of magnesium indate, J. Phys. Chem. **51**, 771–775 (1947).

Indium Oxide, In_2O_3 (cubic)

hkl	1938 Hanawalt Rinn, and Frevel Mo, 0.7107 A			1928 Zachariasen Cu, 1.5418 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
211	4. 13	14	10. 1	4. 156	10	10. 18	4. 130	13	10. 115
222	2. 92	100	10. 1	2. 912	100	10. 09	2. 921	100	10. 118
321	2. 71	3	10. 1	--------	--	-------	2. 704	2	10. 118
400	2. 52	43	10. 1	2. 523	40	10. 09	2. 529	33	10. 117
411	2. 38	10	10. 1	2. 375	8	10. 08	2. 385	8	10. 117
420	2. 26	2	10. 1	2. 258	<2	10. 10	2. 262	2	10. 118
332	2. 15	10	10. 1	2. 151	5	10. 09	2. 157	6	10. 118
422	2. 06	2	10. 1	--------	--	-------	2. 066	1	10. 119
431	1. 98	17	10. 1	1. 973	40	10. 06	1. 984	10	10. 118
521	1. 84	4	10. 1	1. 838	5	10. 07	1. 848	3	10. 119
440	1. 78	71	10. 1	1. 778	100	10. 06	1. 788	36	10. 117
433	1. 73	3	10. 1	1. 723	5	10. 05	1. 735	3	10. 119
600	1. 68	2	10. 1	1. 678	15	10. 07	1. 686	1	10. 117
611	1. 63	10	10. 0	1. 631	10	10. 05	1. 641	6	10. 117
620	1. 60	3	10. 1	1. 593	<2	10. 07	1. 600	2	10. 118
541	1. 55	6	10. 0	1. 551	10	10. 05	1. 561	4	10. 118
622	1. 52	7	10. 1	1. 516	100	10. 06	1. 525	24	10. 118
631	1. 493	7	10. 13	1. 482	15	10. 05	1. 492	6	10. 119
444	1. 461	7	10. 12	1. 451	15	10. 05	1. 460	6	10. 119
543	1. 432	3	10. 13	1. 422	8	10. 06	1. 431	2	10. 117
640	1. 404	2	10. 12	1. 394	5	10. 05	1. 403	2	10. 118
721	1. 378	5	10. 13	1. 369	15	10. 06	1. 377	4	10. 118
642	1. 353	3	10. 12	1. 345	5	10. 06	1. 352	2	10. 117
732	1. 284	4	10. 11	--------	--	-------	1. 285	3	10. 117
800	1. 265	5	10. 12	1. 257	20	10. 06	1. 265	4	10. 118
811	1. 244	5	10. 11	--------	--	-------	1. 246	3	10. 118
820	1. 227	2	10. 12	1. 220	15	10. 06	1. 227	2	10. 119
653	1. 207	3	10. 10	1. 201	20	10. 05	1. 209	3	10. 119
822	1. 192	1	10. 11	1. 186	10	10. 06	1. 192	2	10. 117
831	1. 177	3	10. 12	1. 168	20	10. 05	1. 1762	3	10. 1180
662	1. 161	4	10. 12	1. 153	60	10. 05	1. 1606	6	10. 1179
752	--------	--	-------	--------	--	-------	1. 1456	<1	10. 1176
840	1. 132	9	10. 12	1. 125	35	10. 06	1. 1312	4	10. 1178
833	--------	--	----------	1. 112	5	10. 07	1. 1173	1	10. 1176
842	--------	--	-------	1. 098	5	10. 06	1. 1040	1	10. 1183
921	--------	--	-------	1. 084	20	10. 05	1. 0911	2	10. 1184
664	--------	--	-------	--------	--	-------	1. 0786	<1	10. 1182
851	--------	--	-------	1. 060	20	10. 06	1. 0665	2	10. 1177
932	--------	--	-------	1. 037	15	10. 05	1. 0436	2	10. 1181
844	--------	--	-------	1. 027	50	10. 06	1. 0327	3	10. 1184
941	--------	--	-------	1. 016	20	10. 06	1. 0221	2	10. 1183
10·0·0	--------	--	-------	1. 006	15	10. 06	1. 0118	2	10. 1180
10·1·1	--------	--	-------	0. 9963	5	10. 06	1. 0018	1	10. 1177
10·2·0	--------	--	-------	. 9865	35	10. 06	0. 9922	3	10. 1185
943	--------	--	-------	. 9778	5	10. 07	. 9827	3	10. 1175
10·2·2	--------	--	-------	. 9683	60	10. 06	. 9736	3	10. 1180
10·3·1	--------	--	-------	--------	--	-------	. 9648	2	10. 1189
	--------	--	-------	--------	--	-------	. 9477	2	10. 1187
Average value of last five lines			10. 11	--------	--	10. 06	--------	--	10. 118

Iodic Acid, HIO_3 (orthorhombic)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [1] 1928	Copper	----------

NBS sample. The iodic acid was prepared at the Naval Research Laboratories in Washington, D. C., by Samuel Zerfoss. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of sodium and silicon; and 0.0001 to 0.001 percent each of silver, calcium, chromium, and magnesium.

The sample is colorless. The refractive indices could not be determined by the usual liquid grain immersion method because the acid reacted with the liquids.

Interplanar spacings and intensity measurements. The *d*-spacings of the Zachariasen pattern were calculated from Bragg angle data.

The three strongest lines for the two patterns are as follows:

Pattern	1	2	3
Zachariasen	110	112, 200, 021	210
Swanson, Gilfrich, and Ugrinic	110	102	012

Lattice constants. The structure of iodic acid was determined by Rogers and Helmholz [2] in 1941. The orthorhombic lattice has the space group $D_2^4\text{-}P2_12_12_1$ with 4(HIO_3) per unit cell.

Two 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	Zachariasen [1]	5. 54	5. 93	7. 77
1941	Rogers and Helmholz [2].	5. 556	5. 867	7. 731
1955	Swanson, Gilfrich, and Ugrinic.	5. 5379	5. 8878	7. 733 at 26° C.

The density of iodic acid calculated from the NBS lattice constants is 4.633 at 26° C.

hkl	1928 Zachariasen Cu, 1.542 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*
	A		*A*	
011	-------	----	4. 69	15
101	4. 538	w	4. 51	31
110	4. 058	s	4. 035	100
002	-------	----	3. 868	9
111	3. 627	w	3. 577	38
012	3. 239	vw	3. 233	43
102	3. 182	w	3. 172	53
020	-------	----	2. 941	7
112	2. 770	s	2. 790	31
200			2. 768	16
021			2. 746	26
201	-------	----	2. 608	19
120	-------	----	2, 596	32
210	2. 507	s	2. 506	11
121	2. 460	m	2. 462	23
211	2. 379	vw	2. 385	9
013			2. 362	7
022	2. 337	w	2. 340	8
202	-------	----	2. 252	2
113	2. 156	w	2. 173	2
122			2. 157	11
212	2. 104	s	2. 104	22
220	2. 023	w	2. 017	3
221	-------	----	1. 950	17
004	-------	----	1. 934	3
031	-------	----	1. 900	7
203	-------	----	1. 888	5
014	-------	----	1. 838	6
123	-------	----	1. 830	30
131	-------	----	1. 798	26
222	-------	----	1. 788	9
310	-------	----	1. 762	14
114	-------	----	1. 744	14
311	-------	----	1. 718	9
132	-------	----	1. 669	5
302	-------	----	1. 665	7
312	-------	----	1. 603	10
204	-------	----	1. 586	4
231	-------	----	1. 567	5
320	-------	----	1. 563	10
033	-------	----	1. 561	18
124	-------	----	1. 551	4
214	-------	----	1. 531	9
105	-------	----	1. 490	2
232	-------	----	1. 478	3
313	-------	----	1. 454	5
041	-------	----	1. 450	9
115	-------	----	1. 444	10
224	-------	----	1. 396	5
025	-------	----	1. 369	6
233	-------	----	1. 359	8
410	-------	----	1. 3476	4
323	-------	----	1. 3368	6
134				
411	-------	----	1. 3280	6
215	-------	----	1. 3161	2
402	-------	----	1. 3037	1

References

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

[2] M. T. Rogers and L. Helmholz, The crystal structure of iodic acid, J. Am. Chem. Soc. **63**, 278–284 (1941).

Iron Sulfide (pyrite), FeS_2 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
II-3552	3808 2-1375 2-1370	1.63 1.04 2.70	---------- ---------- Molybdenum. Iron----------	United Steel Companies, England. British Museum. Anderson and Chesley [1] 1933. Boldyrev [2] 1938.
3706	3794 1-1295 1-1295	1.63 2.70 2.42	Molybdenum.	Hanawalt, Rinn, and Frevel [3] 1938.
II-3528	3779 2-1363 2-1366	1.65 2.76 2.46	Copper-----	Harcourt [4] 1942.
	2786 3-0815 3-0822	2.67 3.08 2.39	Iron--------	Kerr [5] 1945.

The Harcourt pattern was made using copper radiation rather than molybdenum as indicated on the ASTM card.

Additional published patterns

Pattern	Radiation	Wavelength
Aminoff and Parsons [6] 1928-----	Iron-----	1.934 A

NBS sample. The iron sulfide was prepared at the NBS as a fine precipitate and was heated in a closed tube in a sulfur atmosphere at 700° C for 4 hours. Spectrographic analysis of the sample shows the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, magnesium, and silicon; 0.001 to 0.01 percent each of cobalt, copper, molybdenum, nickel, and lead; and 0.0001 to 0.001 percent each of chromium, germanium, and manganese.

The sample is an opaque black powder.

Interplanar spacings and intensity measurements. The *d*-spacings of the Boldyrev, the Hanawalt, Rinn, and Frevel, the Harcourt, and the Kerr patterns were converted from kX to angstrom units and the *d*-spacings of the Anderson and Chesley and the Aminoff and Parsons patterns were calculated from Bragg angle data. The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Anderson and Chesley----------------	311	200	210
Boldyrev----------------------------	311	200	210
Hanawalt, Rinn, and Frevel----------	311	200	210
Harcourt----------------------------	311	200	210
Kerr--------------------------------	200	111	210
Aminoff and Parsons-----------------	200	210	311
Swanson, Gilfrich, and Ugrinic------	311	200	210

Lattice constant. This structure of iron sulfide was determined by Bragg [7] in 1920. The cubic lattice has the space group T_h^6–Pa3, with 4(FeS_2) per unit cell. Iron sulfide is used as a structure type.

A group of unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value. The value of Gordon was given in angstrom units.

Lattice constants

		A
1920----	Bragg [7]----------------------	5.39
1925----	Ramsdell [8]-------------------	5.39
1927----	de Jong [9]--------------------	5.415
1928----	Oftedal [10]-------------------	5.425
1928----	Aminoff and Parsons [6]--------	5.41
1932----	Parker and Whitehouse [11]-----	5.416
1932–34-	Bannister [12]-----------------	5.41
1933----	Anderson and Chesley [1]-------	5.41
1941----	Peacock and Smith [13]---------	5.421
1945----	Kerr [5]-----------------------	5.41759
1947----	Lundquist [14]-----------------	5.416
1951----	Gordon [15]--------------------	5.4179 at 29° C
1955----	Swanson, Gilfrich, and Ugrinic-----	5.417 at 26° C

The density of iron sulfide calculated from the NBS lattice constant is 5.012 at 26° C.

Iron Sulfide (pyrite), FeS_2 (cubic)

hkl	1933 Anderson and Chesley Mo, 0.7107 A			1938 Boldyrev Fe, 1.9360 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1942 Harcourt Cu, 1.5405 A			1945 Kerr Fe, 1.9360 A			1928 Aminoff and Parsons Fe, 1.7393 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*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*	*A*		*A*	*A*		*A*
111	3.13	w	5.42	3.108	20	5.383	3.13	27	5.42	3.11	12	5.38	3.086	84	5.345	3.16	w	5.47	3.1280	36	5.4179
200	2.71	s	5.42	2.701	80	5.402	2.71	75	5.42	2.77	75	5.54	2.678	100	5.356	2.70	s	5.39	2.7088	84	5.4176
210	2.42	m	5.41	2.422	80	5.416	2.42	45	5.41	2.46	75	5.50	2.399	60	5.364	2.42	s	5.40	2.4281	66	5.4182
211	2.20	m	5.39	2.210	70	5.413	2.21	35	5.41	2.24	25	5.49	2.190	48	5.364	2.22	m	5.44	2.2118	52	5.4178
220	1.91	m	5.40	1.914	60	5.414	1.91	45	5.40	1.93	50	5.46	1.900	34	5.374	1.91	m	5.40	1.9155	40	5.4179
---	-----	--	----	-----	--	-----	-----	--	-----	1.82	12	-----	-----	--	-----	-----	--	----	-----	--	------
311	1.627	vs	5.40	1.632	100	5.413	1.63	100	5.41	1.648	100	5.47	1.621	55	5.376	1.64	s	5.44	1.6332	100	5.4167
222	1.557	w	5.394	1.560	30	5.404	1.56	15	5.40	1.588	8	5.501	1.553	17	5.380	1.56	w	5.40	1.5640	14	5.4179
230	1.497	w	5.398	1.501	40	5.412	1.50	17	5.41	1.525	12	5.498	1.493	17	5.383	1.50	w	5.41	1.5025	20	5.4173
321	1.443	w	5.399	1.447	60	5.414	1.453	25	5.437	1.463	12	5.474	1.439	22	5.384	1.45	m	5.44	1.1448	24	5.4176
331	1.238	w	5.396	1.242	30	5.414	1.243	10	5.418	-----	--	-----	1.240	14	5.405	1.24	w	5.42	1.2427	12	5.4168
420	1.208	w	5.402	1.210	40	5.411	1.212	15	5.420	1.226	8	5.483	1.204	6	5.383	1.21	w	5.42	1.2113	14	4.4171
421	1.181	w	5.412	1.181	40	5.412	1.182	10	5.417	1.195	8	5.476	1.175	5	5.384	1.18	w	5.42	1.1823	7	5.4175
332	1.150	vw	5.394	-----	--	-----	1.155	5	5.417	1.162	8	5.450	1.148	3	5.385	1.15	w	5.39	1.1548	6	5.4165
422	1.100	w	5.389	1.105	50	5.413	1.107	12	5.423	1.122	8	5.497	1.102	17	5.399	1.10	w	5.39	1.1057	6	5.4168
511	1.039	m	5.399	1.042	60	5.414	1.043	25	5.420	1.053	25	5.466	1.040	55	5.404	1.04	s	5.40	1.0427	27	5.4180
---	-----	--	----	-----	--	-----	-----	--	-----	1.030	8	-----	-----	--	-----	-----	--	----	-----	--	------
432	1.003	w	5.401	-----	--	-----	1.007	3	5.423	1.015	8	5.466	-----	--	-----	1.01	s	5.44	1.0060	8	5.4175
521	0.9862	vw	5.402	-----	--	-----	0.989	2	5.417	0.992	8	5.433	-----	--	-----	0.987	s	5.41	0.9892	6	5.4181
440	.9547	w	5.401	-----	--	-----	.959	10	5.425	.963	12	5.448	-----	--	-----	-----	--	-----	.9577	12	5.4176
---	.9138	vw	5.406	-----	--	-----	-----	--	-----	-----	--	-----	-----	--	-----	-----	--	----	-----	--	------
600	.8998	vw	5.418	-----	--	-----	.905	3	5.430	.909	12	5.454	-----	--	-----	-----	--	-----	.9030	15	5.4180
611	.8870	vw	5.468	-----	--	-----	.880	2	5.425	.882	12	5.437	-----	--	-----	-----	--	-----	.8788	8	5.4173
620	.8547	vw	5.406	-----	--	-----	.857	2	5.420	-----	--	-----	-----	--	-----	-----	--	----	.8565	7	5.4170
533	.8239	vw	5.403	-----	--	-----	-----	--	-----	.827	12	5.423	-----	--	-----	-----	--	----	.8261	4	5.4171
622	-----	--	----	-----	--	-----	-----	--	-----	.819	8	5.433	-----	--	-----	-----	--	-----	.8166	4	5.4167
631	-----	--	----	-----	--	-----	-----	--	-----	.809	8	5.487	-----	--	-----	-----	--	----	.7981	5	5.4170
	(a)												(a)								
Average value of last five lines			5.406	-----	--	5.413	-----	--	5.423	-----	--	5.447	-----	--	5.391	-----	--	5.41	-----	--	5.4170

[a] Five additional lines are omitted.

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alpha-Lead Fluoride, α-PbF_2 (orthorhombic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
----	3404 3–0982 3–0994	2. 10 1. 79 2. 43	Chromium----	Ketelaar [1] 1932.

The Ketelaar pattern on ASTM card 3–0994 was obtained from a mixture of orthorhombic and cubic lead fluoride. According to Ketelaar, several lines of the pattern, including the two strongest lines, are values for the cubic form; therefore they should not be included with a pattern for the orthorhombic form.

Additional published patterns

Source	Radiation	Wavelength
Byström [2] 1947-----------	Chromium--	------------

A pattern by Kolderup [3] was found in the literature, but as it was in poor agreement with the other patterns, and contained many impossible lines, it was not included in the table.

NBS sample. The lead fluoride was prepared at the NBS by adding dilute hydrofluoric acid to a solution of lead nitrate. This orthorhombic form is converted to the cubic form above 250° C [3]. Spectrographic analysis of the sample showed the following impurities: 0.001 to 0.01 percent each of aluminum, arsenic, calcium, copper, iron, magnesium, and silicon; and 0.0001 to 0.001 percent of silver.

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

Interplanar spacings and intensity measurements. The *d*-spacings of the Ketelaar and of the Byström patterns were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Ketelaar----------------------------	012	111	121
Byström----------------------------	012	111	101
Swanson, Gilfrich, and Ugrinic---------	012	111	020

Lattice constants. The structure of orthorhombic lead fluoride was determined by Kolderup [3] in 1924. The lattice has the space group D_{2h}^{16}–Pmnb with lead chloride-type structure and 4(PbF_2) per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units, and the lattice constants of Sauka [4] have been temperature corrected from 18° to 25° C for comparison with the NBS values. Sauka gives the thermal coefficient of expansion of orthorhombic lead fluoride as 31.9×10^{-6} parallel to the *a* axis, 37.1×10^{-6} parallel to the *b* axis, and 13.6×10^{-6} parallel to the *c* axis.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1932	Ketelaar [1]	3. 81	6. 42	7.62
1947	Byström [2]	3. 897	6. 441	7.648
1951	Sauka [4]	3. 89971	6. 44154	7.6519 at 25° C.
1955	Swanson, Gilfrich, and Ugrinic.	3. 8990	6. 4421	7.6514 at 25° C.

The density of orthorhombic lead fluoride calculated from the NBS lattice constant is 8.473 at 25° C.

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alpha-**Lead Fluoride, α–PbF_2 (orthorhombic)**

hkl	1932 Ketelaar Cr, 2.2909 A		1947 Byström Cr, 2.2909 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
002	3. 81	w	3. 83	m	3. 824	10
101	3. 42	s	3. 464	s	3. 475	26
012	3. 280	s	3. 280	vs	3. 290	100
020	3. 214	w	3. 223	s	3. 222	40
111	3. 024	s	3. 058	vs	3. 058	57
022	-----	--	2. 459	w	2. 464	5
121	2. 348	m	2. 359	s	2. 364	31
103	2. 127	m	2. 135	s	2. 134	22
113	2. 019	w	2. 024	w	2. 026	9
200	-----	--	1. 949	s	1. 949	7
004	1. 906	m	1. 912	s	1. 912	16
032	1. 868	m	1. 871	s	1. 873	18
014	1. 821	m	1. 834	w	1. 8332	16
---	-----	--	1. 826	s	------	--
123	-----	--	1. 778	s	1. 7791	18
---	1. 704	m	1. 736	vw	------	--
212	1. 670	mw	1. 676	s	1. 6774	15
220	-----	--	1. 667	m	1. 6676	10
024	1. 637	m	1. 644	s	1. 6445	13
040	1. 616	w	1. 610	w	1. 6101	4
---	-----	--	1. 527	w	------	--
133	-----	--	1. 514	w	1. 5134	2
141	-----	--	-----	--	1. 4611	5
034	-----	--	-----	--	1. 4283	2
223	-----	--	-----	--	1. 4112	<1
115	-----	--	-----	--	1. 3908	10
204	-----	--	-----	--	1. 3672	3
143	-----	--	-----	--	1. 2854	5
006	-----	--	-----	--	1. 2752	7
224 311	-----	--	-----	--	1. 2570	3
016	-----	--	-----	--	1. 2510	6
044	-----	--	-----	--	1. 2319	6
052	-----	--	-----	--	1. 2212	4
151	-----	--	-----	--	1. 2079	4
135	-----	--	-----	--	1. 1870	6
026	-----	--	-----	--	1. 1858	7
234	-----	--	-----	--	1. 1520	6
036	-----	--	-----	--	1. 0965	1
060	-----	--	-----	--	1. 0737	4
054	-----	--	-----	--	1. 0687	1

beta-Lead Fluoride, β-PbF_2 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
1504	1451	3.44	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
	1–0627	2.10		
	1–0606	1.78		

Additional published patterns

Source	Radiation	Wavelength
		A
Kolderup [2] 1924	Copper	1.541
Schumann [3] 1933	Copper	1.539

The Schumann pattern included in this report is a combination of two patterns given in the literature. The *d*-spacings of the one pattern made without an internal standard were used only where there were no values in the second pattern made with an internal standard.

NBS sample. The lead fluoride used for the pattern was prepared at the NBS by the action of hydrofluoric acid on lead carbonate. A pattern of the orthorhombic form of PbF_2, which is easily prepared at room temperature by precipitation, is given also in this publication. The orthorhombic form was converted to the cubic form by heating at 400° C for 18 hours. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, arsenic, calcium, copper, iron, magnesium, and silicon; and 0.0001 to 0.001 percent of silver.

The sample is colorless. Consistent index of refraction readings were not obtained from the cubic phase; values were over 1.84. However, the diffraction pattern was unusually sharp, showing no strain or doublet-peaks.

Interplanar spacings and intensity measurements. The Hanawalt, Rinn, and Frevel pattern was converted from kX to angstrom units and the Kolderup and the Schumann patterns were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	220	311
Kolderup	220	311	400
Schumann	220	311	331
Swanson, Gilfrich, and Ugrinic	111	220	311

Lattice constant. The structure of cubic lead fluoride was determined by Kolderup [2] in 1924. The space group is O_h^5–Fm3m with calcium fluoride-type structure and 4(PbF_2) per unit cell. Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		A	
1924	Kolderup [2]	5.94	
1929	Natta and Passerini [3]	5.94	
1933	Schumann [4]	5.954	at 24° C
1947	Byström [5]	5.935	
1955	Swanson, Gilfrich, and Ugrinic.	5.940	at 26° C

The density of the lead fluoride calculated from the NBS lattice constant is 7.770 at 26° C.

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beta-**Lead Fluoride, β-PbF_2(cubic)**

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1924 Kolderup Cu, 1.542 A			1933 Schumann Cu, 1.542 A, 24° C			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	3. 45	100	5. 98	3. 42	s	5. 92	3. 43	vs	5. 94	3. 428	100	5. 938
200	2. 97	13	5. 94	2. 95	ms	5. 90	2. 968	s	5. 936	2. 970	56	5. 940
220	2. 10	53	5. 94	2. 097	vs	5. 931	2. 090	vvs	5. 911	2. 100	73	5. 941
311	1. 78	53	5. 90	1. 788	vs	5. 930	1. 791	vvs	5. 940	1. 791	64	5. 940
222	1. 71	7	5. 93	1. 715	w	5. 941	1. 712	s	5. 930	1. 715	14	5. 941
400	1. 486	7	5. 944	1. 480	vs	5. 920	1. 482	s^-	5. 928	1. 485	10	5. 940
331	1. 365	20	5. 950	1. 360	vs	5. 928	1. 365	vs^+	5. 950	1. 362	27	5. 939
420	1. 327	13	5. 934	1. 326	vs	5. 930	1. 329	vs	5. 943	1. 328	21	5. 940
422	1. 214	13	5. 947	1. 208	vs	5. 918	1. 209	s^+	5. 923	1. 212	26	5. 940
511	1. 144	7	5. 944	1. 141	vs	5. 929	1. 146	vs	5. 954	1. 143	20	5. 941
440	------	----	------	1. 050	s	5. 942	1. 050	s	5. 942	1. 050	8	5. 942
531	1. 005	7	5. 946	1. 003	vs	5. 934	1. 007	vs^+	5. 957	1. 0043	20	5. 942
600	------	----	------	0. 9882	vs	5. 929	0. 9930	vs	5. 958	0. 9903	13	5. 942
620	------	----	------	. 9376	vs	5. 930	. 9381	vs	5. 933	. 9394	10	5. 941
533	------	----	------	. 9052	vs	5. 936	. 9083	vs	5. 956	. 9059	8	5. 940
622	------	----	------	. 8945	vs	5. 933	. 8979	vs	5. 956	. 8957	9	5. 941
444	------	----	------	------	----	-------	. 8625	s^-	5. 976	. 8574	4	5. 940
711	------	----	------	------	----	-------	-------	----	------	. 8318	18	5. 940
640	------	----	------	------	----	-------	-------	----	------	. 8238	7	5. 940
642	------	----	------	------	----	-------	-------	----	------	. 7938	21	5. 940
Average value of last five lines----------			5. 944	------	----	5. 932	-------	----	5. 956	-------	----	5. 940

Lead (II) Iodide, PbI_2 (hexagonal)

ASTM cards.

Card numbers		New index lines	Radiation	Source
Old	New			
1512	1434 1–0618 1–0608	3. 43 2. 62 2. 27	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Terpstra and Westenbrink [2] 1926.	Copper---	1. 537

NBS sample. The lead iodide was prepared at the NBS by the action of hydriodic acid on lead carbonate. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, bismuth, iron, and silicon; and 0.0001 to 0.001 percent each of silver, calcium, chromium, copper, and magnesium.

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

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the *d*-spacings of the Terpstra and Westenbrink pattern were calculated from Bragg angle data.

The Terpstra and Westenbrink pattern did not include intensity values.

The three strongest lines for the two patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	101	102	110
Swanson, Gilfrich, and Ugrinic	101	102	110

Lattice constants. The structure of lead iodide was determined by van Arkel [3] in 1926. The hexagonal lattice has the space group D_{3d}^{3}-$P\bar{3}m1$ with cadmium iodide-type structure and 1(PbI_2) per unit cell.

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

Lattice constants

		a	c
		A	*A*
1926	van Arkel [3]	4. 60	7. 03
1926	Terpstra and Westenbrink [2]	4. 60	6. 79
1929	Ferrari and Giorgi [4]	4. 54	6. 94
1943	Pinsker, Tatarinova, and Novikova [5].	4. 55	6. 90
1955	Swanson, Gilfrich, and Ugrinic.	4. 557	6. 979 at 25° C.

The density of lead iodide calculated from the NBS lattice constants is 6.098 at 25° C.

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Lead (II) Iodide, PbI_2 (hexagonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1926 Terpstra and Westenbrink Cu, 1.542 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
001	7. 0	13	----	--	6. 98	23
---	---	---	4. 30	--	----	--
100	3. 96	2	----	--	3. 945	6
002	---	---	----	--	3. 489	3
101	3. 44	100	3. 41	--	3. 435	100
102	2. 63	40	2. 61	--	2. 614	55
003	---	---	----	--	2. 327	6
110	2. 27	27	2. 25	--	2. 278	43
111	2. 16	7	2. 15	--	2. 1661	13
103	2. 00	11	1. 98	--	2. 0052	15
210	1. 90	13	1. 88	--	1. 8997	18
004	---	---	----	--	1. 7449	5
202	1. 71	8	1. 71	--	1. 7172	13
113	1. 63	5	1. 61	--	1. 6276	8
104	---	---	----	--	1. 5951	1
203	1. 50	3	1. 48	--	1. 5043	4
211	1. 457	8	1. 44	--	1. 4582	11
114	1. 384	8	----	--	1. 3852	7
212	1. 373	8	1. 37	--	1. 3712	9
105 300	1. 317	4	1. 30	--	1. 3158	8
301	1. 290	1	----	--	1. 2928	2
213	1. 261	3	1. 25	--	1. 2556	4
303	---	---	----	--	1. 1449	2
205 220	1. 139	3	1. 13	--	1. 1394	4
106	---	---	----	--	1. 1159	2
311	1. 082	2	----	--	1. 0811	3
304	---	---	----	--	1. 0504	3
312	1. 047	2	1. 02	--	1. 0442	3
223	1. 022	1	----	--	1. 0233	1
215	---	---	----	--	1. 0190	3
313	---	---	----	--	0. 9904	1
401	---	---	----	--	. 9769	<1
224	---	---	----	--	. 9541	2
402	---	---	----	--	. 9494	1
314	---	---	----	--	. 9273	1
216	---	---	----	--	. 9172	1
321	---	---	----	--	. 8977	2
315 410	---	---	----	--	. 8612	2

Lead Nitrate, $Pb(NO_3)_2$ (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
712	0731 1–0335 1–0327	4. 54 2. 36 3. 92	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Vegard [2] 1922	Copper	1.54 A

NBS sample. The lead nitrate was obtained from Johnson, Matthey and Co., Ltd., London. Their spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of calcium and sodium.

The sample is colorless. The index of refraction is 1.780.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units, and the *d*-spacings of the Vegard pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	311	200
Vegard	311	531	111
Swanson, Gilfrich, and Ugrinic	111	311	220

Lattice constant. The structure of lead nitrate was determined by Nishikawa and Hudinuki [3] in 1917. The cubic lattice has the space group T_h^6—Pa3 with $4(Pb(NO_3)_2$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units, and the measurements of Ieviņš and Straumanis and Vegard and Roer have been temperature corrected to 25° C for comparison with the NBS value. Vegard and Roer [4] give the linear coefficient of expansion of lead nitrate as 27.6×10^{-6} from 10° to 70° C.

Lattice constants

		A
1922	Vegard [2]	7.86
1936	Ieviņš and Straumanis [5]	7.8569 at 25° C
1940	Felipe [6]	7.8556
1941	Vegard and Roer [4]	7.8579 at 25° C
1955	Swanson, Gilfrich, and Ugrinic	7.8568 at 25° C

The density of lead nitrate calculated from the NBS lattice constant is 4.535 at 25° C.

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Lead Nitrate, $Pb(NO_3)_2$ (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1922 Vegard Cu, 1.54 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	4. 55	100	7. 88	4. 52	s	7. 83	4. 537	100	7. 858
200	3. 93	33	7. 86	3. 92	s	7. 84	3. 929	36	7. 858
210	--------	----	--------	-------	----	-------	3. 514	7	7. 859
211	--------	----	--------	-------	----	-------	3. 208	6	7. 857
220	2. 78	33	7. 86	2. 77	m	7. 83	2. 778	40	7. 856
311	2. 36	67	7. 83	2. 36	vs	7. 83	2. 370	71	7. 859
222	2. 26	33	7. 83	2. 26	s	7. 83	2. 268	40	7. 858
400	1. 96	13	7. 84	1. 96	m	7. 84	1. 964	11	7. 856
331	1. 80	27	7. 85	1. 80	s	7. 85	1. 802	23	7. 856
420	1. 75	30	7. 83	1. 75	s	7. 83	1. 757	18	7. 857
422	1. 60	17	7. 84	1. 60	m	7. 84	1. 604	14	7. 856
511	1. 50	23	7. 79	1. 51	m	7. 85	1. 512	12	7. 857
440	1. 39	10	7. 87	1. 38	m	7. 83	1. 389	7	7. 856
531	1. 33	20	7. 86	1. 33	vs	7. 84	1. 328	12	7. 856
600	1. 304	7	7. 82	1. 30	m	7. 82	1. 309	7	7. 856
620	1. 243	7	7. 861	1. 24	w	7. 84	1. 242	4	7. 856
533	1. 198	7	7. 856	1. 20	m	7. 85	1. 1980	5	7. 856
622	1. 185	3	7. 860	1. 18	m	7. 85	1. 1844	3	7. 857
444	--------	----	--------	1. 14	w	7. 87	1. 1341	1	7. 857
711	1. 100	7	7. 856	1. 10	s	7. 86	1. 1001	4	7. 856
640	--------	----	--------	-------	----	-------	1. 0895	3	7. 856
642	1. 050	7	7. 857	1. 05	s	7. 86	1. 0499	3	7. 857
731	1. 024	7	7. 865	1. 024	s	7. 865	1. 0228	5	7. 857
800	--------	----	--------	-------	----	-------	0. 9820	<1	7. 856
733	--------	----	--------	-------	----	-------	. 9598	2	7. 856
820	--------	----	--------	0. 9525	s	7. 855	. 9527	3	7. 856
822	--------	----	--------	. 9263	s	7. 860	. 9259	4	7. 856
751	--------	----	--------	. 9065	s	7. 851	. 9071	4	7. 856
662	--------	----	--------	-------	----	-------	. 9012	2	7. 857
840	--------	----	--------	. 8797	w	7. 868	. 8783	2	7. 856
911	--------	----	--------	. 8634	s	7. 859	. 8623	3	7. 856
842	--------	----	--------	. 8580	m	7. 864	. 8571	2	7. 856
664	--------	----	--------	-------	----	-------	. 8375	2	7. 8566
931	--------	----	--------	-------	----	-------	. 8236	2	7. 8567
844	--------	----	--------	-------	----	-------	. 8019	1	7. 8569
933	--------	----	--------	-------	----	-------	. 7897	2	7. 8570
10·0·0	--------	----	--------	-------	----	-------	. 7857	1	7. 8570
Average value of last five lines--			7. 859	-------	----	7. 860	--------	----	7. 8568

Lead Selenide (clausthalite), PbSe (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
II–1275	2007	3.08	Copper	Olshausen [1] 1925.
	2–0600	2.18		
	2–0588	3.56		
II–1302	2009	3.06	Copper	Harcourt [2] 1942.
	2–0602	2.17		
	2–0603	1.37		

The Harcourt pattern was made using copper rather than molybdenum radiation as indicated on the ASTM cards.

Additional published patterns

Source	Radiation	Wave-length
Wilman [3] 1948	Electron Diffraction	

NBS sample. The lead selenide was obtained from A. D. Mackay, New York. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent of silicon; 0.001 to 0.01 percent each of aluminum and iron; and 0.0001 to 0.001 percent each of silver, calcium, and magnesium.

The sample has a metallic blue-gray color and is opaque.

Interplanar spacings and intensity measurements. The *d*-spacings of the Harcourt and the Wilman patterns were converted from kX to angstrom units, and the *d*-spacings of the Olshausen pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Olshausen	200	220	111
Harcourt	200	220	420
Wilman	220	422	222
Swanson, Gilfrich, and Ugrinic	200	220	111

Lattice constant. The structure of lead selenide was determined by Olshausen [1] in 1925. The cubic lattice has the space group O_h^5-Fm3m, with sodium chloride-type structure and 4(PbSe) per unit cell.

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

Lattice constants

		A
1925	Olshausen [1]	6.174
1925	Ramsdell [4]	6.15
1926	Goldschmidt [5]	6.147
1948	Wilman [3]	6.129
1955	Swanson, Gilfrich, and Ugrinic.	6.1243 at 25° C.

The density of lead selenide calculated from the NBS lattice constant is 8.273 at 25° C.

References

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Lead Selenide (clausthalite), PbSe (cubic)

hkl	1925 Olshausen Cu, 1.5418 A			1942 Harcourt Cu, 1.5418 A			1948 Wilman Electron diffraction			1955 Swanson, Gilfrich, and Ugrinic 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. 61	m	6. 25	3. 52	33	6. 12	3. 539	m	6. 130	3. 536	31	6. 125
200	3. 13	s	6. 26	3. 07	100	6. 13	3. 064	m	6. 128	3. 062	100	6. 124
---	----	--	----	2. 87	3	-----	-----	--	-----	------	--	------
220	2. 22	s	6. 28	2. 169	78	6. 135	2. 163	s	6. 118	2. 165	70	6. 124
311	1. 88	m	6. 24	1. 854	22	6. 149	1. 848	mw	6. 129	1. 846	17	6. 124
222	1. 80	m	6. 24	1. 774	33	6. 145	1. 770	ms	6. 131	1. 768	22	6. 124
400	1. 56	m	6. 24	1. 533	22	6. 132	1. 532	vw	6. 128	1. 531	14	6. 124
331	1. 41	w	6. 15	1. 408	5	6. 137	1. 406	mw	6. 129	1. 405	6	6. 125
420	1. 40	m	6. 26	1. 373	44	6. 140	1. 371	mw	6. 131	1. 369	26	6. 124
422	1. 27	m	6. 22	1. 253	33	6. 138	1. 251	s	6. 129	1. 250	15	6. 124
511	1. 19	vw	6. 18	1. 182	5	6. 142	1. 179	w	6. 126	1. 179	4	6. 125
440	1. 09	w	6. 17	1. 085	5	6. 138	----	--	----	1. 082	5	6. 124
531	1. 05	w	6. 21	1. 037	2	6. 135	----	--	----	1. 035	3	6. 125
600	1. 03	m	6. 18	1. 022	11	6. 132	----	--	----	1. 021	8	6. 125
620	0. 978	m	6. 19	0. 970	11	6. 135	----	--	----	0. 9685	7	6. 125
622	. 936	m	6. 21	. 925	5	6. 136	----	--	----	. 9233	6	6. 1245
444	. 896	w	6. 21	-----	--	-----	----	--	----	. 8840	1	6. 1245
711	. 861	m	6. 15	-----	--	-----	----	--	----	. 8576	2	6. 1245
640	----	--	----	. 851	3	6. 137	----	--	----	. 8492	3	6. 1237
642	----	--	----	. 820	3	6. 136	----	--	----	. 8184	5	6. 1243
Average value of last five lines----------			6. 19	-----	--	6. 135	----	--	6. 129	----	--	6. 1243

Lead Titanate, $PbTiO_3$ (tetragonal)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
----	2578 2–0828 2–0804	2. 83 1. 60 2. 30	Copper---- 1.539 A.	Cole and Espenschied [1] 1937.
----	2576 3–0747 3–0721	2. 84 1. 61 2. 73	Copper----	Megaw, Philips Lamps Ltd.

Cole and Espenschied believed lead titanate to be orthorhombic at room temperature as indicated on ASTM card number 2–0804, but later investigations by Náray-Szabó [2], Megaw [3], and Shirane, Hoshino, and Suzuki [4] show it to be tetragonal.

Additional published patterns. None.

NBS sample. The sample of lead titanate was prepared at the NBS by George R. Shelton. It was heated in a lead oxide-rich atmosphere to 1,250° C for one-half hour. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent of silicon; 0.001 to 0.01 percent each of aluminum, boron, calcium, copper, iron, magnesium, and tin; and 0.0001 to 0.001 percent of silver.

The sample is yellow-brown. The indices of refraction were too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-spacings of the Cole and Espenschied and the Megaw patterns were converted from kX to angstrom units.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Cole and Espenschied	101	211	111
Megaw	101	211	110
Swanson, Gilfrich, and Ugrinic	101	110	100

Lattice constants. The structure of lead titanate was determined by Náray-Szabó [2] in 1943. The tetragonal lattice has the space group D_{4h}^1–P4/mmm with perovskite-type structure and 1 ($PbTiO_3$) per unit cell.

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

Lattice constants

		a	c
		A	A
1943	Náray-Szabó [2]	3. 90	4.14
1946	Megaw [3]	3. 904	4.152
1950	Shirane, Hoshina, and Suzuki [4].	3. 899	4. 149
1955	Swanson, Gilfrich, and Ugrinic.	3. 8993	4.1532 at 26° C.

The density of lead titanate calculated from the NBS lattice constants is 7.969 at 26° C.

References

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Lead Titanate, $PbTiO_3$ (tetragonal)

hkl	1937 Cole and Espenschied Cu, 1.539 A		---- Megaw Cu, 1.5405 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C	
	d	I	d	I	d	I
	A		A		A	
001	4. 040	10	4. 15	70	4. 150	26
100	3. 858	20	3. 91	70	3. 899	49
---	3. 261	5	-----	----	-------	---
---	3. 055	5	-----	----	-------	---
---	2. 912	20	-----	----	-------	---
101	2. 831	100+	2. 85	100	2. 842	100
110	2. 763	40	2. 74	85	2. 758	52
111	2. 298	50	2. 29	85	2. 297	40
002	-----	---	2. 07	70	2. 076	15
200	1. 951	40	1. 91	85	1. 950	32
102	1. 856	5	1. 83	70	1. 833	13
201	1. 761	10	1. 77	70	1. 765	10
210	1. 730	10	1. 75	70	1. 744	11
112	1. 653	50	1. 65	85	1. 6581	19
211	1. 607	80	1. 61	100	1. 6075	42
202	1. 417	50	1. 42	85	1. 4213	13
003	-----	---	-----	----	1. 3841	3
220	1. 372	40	1. 38	70	1. 3787	9
212	1. 331	30	1. 34	70	1. 3351	7
221	-----	---	1. 31	70D	1. 3081	3
103	-----	---	-----	----	1. 3045	5
300	1. 299	30	-----	----	1. 3000	11
301	-----	---	1. 24	70	1. 2403	10
113	-----	---	-----	----	[a] 1. 237	3
310	1. 234	30	1. 23	70	1. 2333	7
---	1. 218	10	-----	----	-------	---
311	1. 179	20	1. 18	70	1. 1819	10
222	1. 145	20	1. 15	70	1. 1484	5
203	1. 127	10	1. 13	60	1. 1287	3
302	-----	---	1. 10	50	1. 1016	2
213	1. 080	10	1. 08	85D	1. 0841	7
320	------	---	-----	----	1. 0816	3
312	1. 057	30	1. 06	85	1. 0601	9
321	-----	---	1. 05	85	1. 0465	8
004	-----	---	1. 01	50	1. 0383	1
104	-----	---	-----	----	1. 0031	2
223	------	---	-----	----	0. 9766	3
400	-----	---	0. 978	60D	. 9747	4
114	-----	---	-----	----	. 9715	1
322	-----	---	. 962	60	. 9593	3
401	-----	---	. 949	70	. 9491	2
303	-----	---	-----	----	. 9476	2
410	-----	---	-----	----	. 9457	4
411	-----	---	. 926	85	. 9222	6
330	-----	---	-----	----	. 9192	1
204	-----	---	. 923	85	. 9168	3
331	-----	---	. 901	50	. 8975	3
214	------	---	. 895	60	. 8922	2

[a] The $K\alpha_1$ peak for 113 is superimposed on the $K\alpha_2$ peak for 301.

Magnesium Tin, Mg_2Sn (cubic)

ASTM card

Card numbers		New index lines	Radiation	Source
Old	New			
1099	1056 1–0468 1–0470	3. 90 2. 38 2. 03	Molybde-num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wave-length
Sacklowski [2] 1925	Copper	----------
Zintl and Kaiser [3] 1933	Copper	1.539 A

NBS sample. The magnesium tin was prepared at the NBS by William R. Hosler. Spectrographic analysis of the sample showed the following impurities: 0.001 to 0.01 percent each of aluminum, barium, calcium, iron, manganese, silicon, and titanium; and 0.0001 to 0.001 percent each of silver and lead.

The NBS sample is opaque and has a blue metallic luster.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units, and the *d*-spacings of the Sacklowski and the Zintl and Kaiser patterns were calculated from Bragg angle data. The Sacklowski pattern did not include intensity values.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Zintl and Kaiser	220	111	311
Hanawalt, Rinn, and Frevel	111	220	311
Swanson, Gilfrich, and Ugrinic	111	220	311

Lattice constant. The structure of magnesium tin was determined by Pauling [4] in 1923. The cubic lattice has the space group O_h^5–Fm3m with calcium fluoride-type structure and 4(Mg_2Sn) per unit cell.

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

Latice constants

		A
1923	Pauling [4]	6.79
1925	Sacklowski [2]	6.76
1933	Zintl and Kaiser [3]	6.779
1955	Swanson, Gilfrich, and Ugrinic	6.7630 at 26° C

The density of magnesium tin calculated from the NBS lattice constant is 3.592 at 26° C.

References

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Magnesium Tin, Mg_2Sn (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1925 Sacklowski Cu, 1.5405 A			1933 Zintl and Kaiser Cu, 1.5405 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	3.91	100	6.77	3.85	----	6.67	3.90	s	6.76	3.906	100	6.765
200	3.39	24	6.78	3.36	----	6.72	3.40	w	6.79	3.382	23	6.765
220	2.38	100	6.73	2.40	----	6.78	2.49	vs	6.76	2.391	76	6.764
311	2.03	80	6.73	2.04	----	6.77	2.043	s	6.776	2.039	51	6.764
222	1.95	8	6.75	1.98	----	6.86	1.955	s	6.772	1.952	5	6.764
400	1.69	24	6.76	1.69	----	6.76	1.693	mw	6.772	1.691	12	6.763
331	1.55	40	6.76	1.544	----	6.73	1.553	m	6.769	1.552	15	6.764
420	1.51	12	6.75	1.507	----	6.74	1.515	w	6.775	1.5122	4	6.763
422	1.383	60	6.753	1.38	----	6.76	1.383	s	6.775	1.3805	14	6.763
511	1.303	24	6.771	1.30	----	6.75	1.304	m	6.776	1.3016	10	6.763
440	1.196	10	6.766	1.19	----	6.73	1.198	m	6.778	1.1955	6	6.763
531	1.144	20	6.768	1.140	----	6.74	1.145	m	6.774	1.1432	8	6.763
600	1.127	2	6.762	-------	----	-------	1.129	w	6.774	1.1273	2	6.764
620	1.070	16	6.767	1.07	----	6.77	1.072	m	6.780	1.0694	7	6.763
533	1.033	6	6.774	1.03	----	6.75	1.034	w	6.780	1.0315	3	6.764
622	------	----	------	-------	----	------	------	----	------	1.0197	2	6.764
444	0.977	4	6.769	0.976	----	6.76	0.979	vw	6.782	0.9762	2	6.763
711	.948	8	6.770	.947	----	6.76	.949	mw	6.774	.9471	4	6.764
640	------	----	------	-------	----	------	------	----	------	.9379	1	6.763
642	.905	12	6.772	.904	----	6.76	.906	m	6.779	.9039	7	6.764
731	.882	10	6.775	.881	----	6.77	.882	mw	6.776	.8805	4	6.7632
800	------	----	------	-------	----	------	------	----	------	.8454	3	6.7632
733	------	----	------	-------	----	------	------	----	------	.8263	2	6.7636
820	------	----	------	-------	----	------	------	----	------	.8201	2	6.7627
822	------	----	------	-------	----	------	------	----	------	.7970	3	6.7628
751	------	----	------	-------	----	------	------	----	------	.7809	3	6.7628
Average value of last five lines----------			6.772	-------	----	6.76	------	----	6.778	-------	----	6.7630

Magnesium Titanate (geikielite), $MgTiO_3$ (hexagonal)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
II–1828	2743	2.74	Molybdenum.	Posnjak and Barth [1] 1934.
	2–0896	1.72		
	2–0874	2.23		
	2716	2.71	Molybdenum.	General Electric Co.
	2–0882	2.21		
	2–0901	1.70		

The pattern of the New Jersey Zinc Co. on ASTM card 1–0571 is for $MgTi_2O_5$ and not $MgTiO_3$ as indicated on the card. This error has been corrected in the fifth supplement to the card file.

Additional published patterns

Source	Radiation	Wavelength
Büssem, Schusterius, and Ungewiss [2] 1937	Copper	

NBS sample. The magnesium titanate was prepared at the NBS by Leslie Coughanour [3]. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum and calcium; 0.001 to 0.01 percent each of copper, iron, and silicon; and 0.0001 to 0.001 percent each of barium, and manganese.

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

Interplanar spacings and intensity measurements. The *d*-spacings of the Posnjak and Barth and the General Electric Co. patterns were converted from kX to angstrom units, and the *d*-spacings of the Büssem, Schusterius, and Ungewiss pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Posnjak and Barth	104	116	113
General Electric Co	104	113	116
Büssem, Schusterius, and Ungewiss	104	113	116
Swanson, Gilfrich, and Ugrinic	104	113	110

Lattice constants. The structure of magnesium titanate was determined by Zachariasen [4] in 1928. The rhombohedral lattice has the space group C_{3i}^2–$R\bar{3}$ with ilmenite-type structure and $2(MgTiO_3)$ per unit cell.

A group of rhombohedral measurements have been referred to hexagonal axes and converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1928	Zachariasen [4]	5.00	13.73
1936	Glocker [5]	5.00	13.73
1939	Tanaka [6]	5.05	13.93
1947	Yamaguchi [7]	5.08	14.09
1955	Swanson, Gilfrich, and Ugrinic.	5.054	13.898 at 26° C

The density of the magnesium titanate calculated from the NBS lattice constants is 3.895 at 26° C.

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Magnesium Titanate (geikielite), $MgTiO_3$ (hexagonal)

hkl	1934		----		1937		1955	
	Posnjak and Barth		General Electric Co.		Büssem, Schusterius, and Ungewiss		Swanson, Gilfrich, and Ugrinic	
	Mo, 0.7107 A		Mo, 0.7107 A		Cu, 1.5418 A		Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
003	4.71	40	4.62	50	4.52	ms	4.64	32
101	4.23	40	4.16	50	4.07	m	4.18	31
012	3.74	50	3.69	50	3.63	m	3.703	43
--------	--------	------	--------	------	[a] 3.41	w	--------	------
104	2.75	100	2.72	100	2.67	vs	2.722	100
110	2.56	70	2.52	80	2.48	ms	2.527	57
113	2.23	80	2.21	90	2.18	s	2.218	70
202	2.07	10	2.09	40	--------	------	2.090	10
024	1.864	60	1.84	80	1.82	ms	1.852	40
107	1.819	5	--------	------	--------	------	1.809	4
116	1.718	90	1.70	90	1.68	s	1.708	55
211	1.650	20	1.64	10	--------	------	1.6434	5
018	1.623	25	1.61	20	1.59	ms	1.6148	12
--------	1.548	5	--------	------	--------	------	--------	------
214	1.504	50	1.48	30	1.48	m	1.4938	29
027	1.468	60	--------	------	--------	------	1.4708	6
030	1.436	5	1.45	80	1.44	m	1.4592	38
303	1.403	10	1.38	10	1.38	vw	1.3919	2
208	--------	------	1.36	10	1.35	vw	1.3606	2
1·0·10	1.331	30	1.32	20	1.31	s	1.3247	13
119							1.3174	8
217	1.272	20	--------	------	--------	------	1.2708	4
220	--------	------	1.26	20	1.25	w	1.2634	9
223	1.122	------	1.21	30	--------	------	1.2191	4
131	--------	------	--------	------	1.20	vw	1.2085	2
128	1.202	20	1.19	30	--------	------	1.1978	6
0·2·10	1.177	20	1.17	20	--------	------	1.1735	5
134	--------	------	1.14	30	1.16	w	1.1462	11
315	1.113	30	1.10	30	--------	------	1.1125	10
226	--------	------	--------	------	1.10	w	1.1093	10
042	--------	------	--------	------	--------	------	1.0809	2
2·1·10	1.068	30	--------	------	1.06	mw	1.0642	13
1·1·12	--------	------	--------	------	--------	------	1.0528	1
404	--------	------	--------	------	--------	------	1.0441	2
1·0·13	--------	------	--------	------	--------	------	1.0385	1
318	0.999	5	--------	------	0.990	w	0.9950	5
0·2·13	--------	------	--------	------	--------	------	.9683	3
324	.972	10	--------	------	.961	mw	.9646	5
140	--------	------	--------	------	.950	w	.9552	5
143	--------	------	--------	------	.931	vw	.9356	3
048	--------	------	--------	------	.920	vw	.9260	2
1·3·10	--------	------	--------	------	.911	w	.9143	5
1·2·13	--------	------	--------	------	.900	w	.9043	3
327	--------	------	--------	------	[b] .879	mw	.8962	3

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[a] Strongest line for $MgTi_2O_5$.
[b] Six additional lines were omitted.

Manganese (II) Oxide (manganosite), MnO (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
-------	3826 3–1146 3–1145	1.55 0.99 .90	Copper, 1.54 A.	Levi [1] 1924.
II–2635	3312 2–1151 2–1158	2.20 1.56 2.55	Chromium	Fontana [2] 1926.
3166	3290 1–1197 1–1206	2.22 2.56 1.57	Molybdenum.	Hanawalt, Rinn, and Frevel [3] 1938.

Additional published patterns

Source	Radiation	Wave length
		A
Broch [4] 1927	Iron	1.934
Holgersson [5] 1927	Iron	1.935
Natta and Passerini [6] 1929	Iron	----------
Le Blanc and Wehner [7] 1933	Iron	----------
Ellefson and Taylor [8] 1934	Iron	----------

NBS sample. The manganous oxide developed on a sample of powdered manganese that was annealed for 24 hours at 750° C. in a hydrogen atmosphere. The formation of the oxide was apparently due to a small amount of water vapor in the hydrogen. The manganese powder was prepared by Johnson, Matthey and Co., Ltd., London. Spectrographic analysis of the oxide at the NBS showed the following impurities: 0.01 to 0.1 percent each of aluminum, magnesium, and silicon; 0.001 to 0.01 percent each of barium, calcium, and iron; and 0.0001 to 0.001 percent each of silver and copper.

The color of the sample is green. The index of refraction is too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel and the Natta and Passerini patterns were converted from kX to angstrom units and the *d*-spacings of the Levi, the Fontana, the Broch, and the Le Blanc and Wehner patterns were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Levi	220	420	422
Fontana	200	220	111
Hanawalt, Rinn, and Frevel	200	111	220
Broch	200	220	222
Holgersson	200	220	420
Natta and Passerini	200	220	311
Le Blanc and Wehner	200	220	311
Ellefson and Taylor	111	220	200
Swanson, Gilfrich, and Ugrinic	200	111	220

Lattice constant. The structure of manganous oxide was determined by Levi [1] in 1924. The cubic lattice has the space group O_h^5–Fm3m with sodium chloride-type structure and 4(MnO) per unit cell.

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

Lattice constants

1924	Levi [1]	4.41
1926	Fontana [2]	4.418
1926	Ott [8]	4.48
1927	Holgersson [5]	4.477
1929	Natta and Passerini [6]	4.424
1930	Passerini [10]	4.444
1933	Le Blanc and Wehner [7]	4.440
1934	Ellelfson and Taylor [8]	4.445 at 26° C
1935	Ruheman [11]	4.4434 at 17° C
1940	Montoro [12]	4.447
1946	Rigamonti [13]	4.444
1946	Pettersson [14]	4.44 to 4.45
1955	Swanson, Gilfrich, and Ugrinic	4.4448 at 26° C

The density of manganous oxide calculated from the NBS lattice constant is 5.365 at 26° C.

Manganese(II) Oxide (manganosite), MnO (cubic)

hkl	1925 Levi Cu, 1.5418 A			1926 Fontana Cr, 2.2909 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1927 Broch Fe, 1.9373 A			1927 Holgersson Fe, 1.935 A			1929 Natta and Passerini Fe, 1.9373 A			1933 LeBlanc and Wehner Fe, 1.9373 A			1934 Elletson and Taylor Fe, 1.9373 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*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*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	2.48	d	4.30	2.558	s	4.431	2.57	66	4.45	2.564	m	4.441	2.58	s	4.48	2.490	ms	4.313	2.535	80	4.391	2.553	vs	4.422	2.568	62	4.448
200	2.18	m	4.36	2.204	vs	4.408	2.22	100	4.44	2.220	vvs	4.440	2.24	vs	4.47	2.175	vs	4.350	2.178	100	4.356	2.212	s	4.424	2.223	100	4.446
220	1.55	s	4.38	1.559	vs	4.410	1.57	66	4.44	1.571	vvs	4.443	1.580	vs	4.469	1.543	vs	4.364	1.549	100	4.381	1.564	vs	4.424	1.571	58	4.443
311	1.32	m	4.38	1.334	s	4.424	1.342	23	4.45	1.340	m	4.444	1.347	w	4.471	1.320	vs	4.378	1.337	90	4.434	1.334	s	4.424	1.340	21	4.444
222	1.27	m	4.40	1.276	s	4.420	1.284	17	4.45	1.282	vs	4.441	1.292	w	4.479	1.265	ms	4.382	1.278	90	4.427	1.278	s	4.427	1.283	13	4.444
400	1.10	d	4.40				1.112	7	4.45				1.118	w	4.476	1.099	m	4.396	1.108	70	4.432	1.106	s	4.424	1.1112	11	4.4448
331	1.01	m	4.40				1.021	7	4.45				1.025	w	4.472	1.012	m	4.411							1.0198	10	4.4452
420	0.987	s	4.41				0.996	17	4.45				0.9983	vs	4.468				0.9978	100	4.462				0.9938	18	4.4444
422	.903	s	4.42				.908	7	4.45																.9074	15	4.4448
511	.852	m	4.43				.8550	3	4.44																.8554	13	4.4448
440	.782	md	4.42																						.7857	4	4.4448
Average value of last five lines			4.42			4.419			4.45			4.442			4.473			4.386			4.427			4.425			4.4448

References

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Molybdenum Disulfide (molybdenite), MoS_2 (hexagonal)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
II–220	0376	6. 16	Copper	British Museum.
	2–0137	2. 26		
	2–0132	1. 03		
II–2564	3267	2. 27	Copper	Harcourt [1] 1942.
	2–1128	1. 82		
	2–1133	1. 53		

The Harcourt pattern was made using copper radiation rather than molybdenum radiation as stated on the ASTM card.

Additional published patterns. A pattern by Montoro [2] was found in the literature, but as it was in poor agreement with the other patterns, it was not included in the table.

NBS sample. The molybdenum disulfide was obtained from the Alpha Corporation, Greenwich, Connecticut. It was heated in a closed tube with sulfur to 850° C. and cooled slowly. Spectrographic analysis of the sample shows the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, copper, iron, and silicon; 0.001 to 0.01 percent each of magnesium, lead, and titanium; and 0.0001 to 0.001 percent manganese.

The sample is lead-gray and opaque.

Interplanar spacings and intensity measurements. The *d*-spacings of the British Museum and the Harcourt patterns were converted from kX to angstrom units.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
British Museum	002	103	210
Harcourt	103	105	008
Swanson, Gilfrich, and Ugrinic	002	103	105

The first two lines of the Harcourt pattern are not possible in molybdenum disulfide structure.

Lattice constants. The structure of molybdenum disulfide was determined by Dickinson and Pauling [3] in 1923. The hexagonal lattice has the space group D^4_{6h}—$P6_3/mmc$ with 2(MoS_2) per unit cell. Molybdenite has been used as a structure type.

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

Molybdenum Disulfide (molybdenite), MoS_2 (hexagonal)

hkl	----		1942		1955	
	British Museum		Harcourt		Swanson, Gilfrich, and Ugrinic	
	Cu, 1.5418 A		Cu, 1.5418 A		Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
---	-----	---	6. 62	38	------	---
002	6. 17	100	-----	---	6. 15	100
---	-----	---	5. 63	62	------	---
004	3. 01	50	-----	---	3. 075	4
100	2. 72	70	2. 74	25	2. 737	16
101	2. 64	50	2. 67	6	2. 674	9
102	2. 53	70	2. 50	12	2. 501	8
103	2. 26	100	2. 28	100	2. 277	45
006	2. 04	50	2. 044	25	2. 049	14
105	1. 831	70	1. 824	88	1. 830	25
----	1. 753	20	-----	---	------	--
----	1. 702	20	-----	---	------	--
106	1. 638	20	1. 638	6	1. 641	4
110	1. 578	50	1. 581	25	1. 581	11
008	1. 532	70	1. 533	75	1. 538	12
107	1. 480	20	1. 478	4	1. 4784	2
----	1. 434	20	-----	---	------	--
200	1. 365	20	1. 368	4	1. 3688	2
108	1. 336	50	1. 338	25	1. 3401	4
203	1. 292	70	1. 298	25	1. 2983	5
116	1. 250	50	1. 254	25	1. 2513	4
0·0·10	-----	---	-----	---	1. 2295	2
109	1. 223	50	1. 224	4	1. 2224	1
205	1. 193	50	1. 197	12	1. 1960	4
----	1. 148	20	-----	---	------	--
----	1. 123	20	-----	---	------	--
118	1. 099	70	1. 102	25	1. 1015	6
210	1. 035	100	1. 036	38	1. 0347	6
208	1. 023	20	1. 023	12	1. 0215	1
213	1. 002	50	1. 004	25	1. 0029	5
1·1·10	-----	---	0. 970	6	0. 9704	2
215	-----	---	. 955	25	. 9534	3
300	-----	---	. 914	6	. 9124	2
302	-----	---	. 903	4	. 9024	1
1·0·13	-----	---	. 896	25	. 8939	3
0·0·14	-----	---	. 867	12	. 8783	2
2·0·11	-----	---	. 860	6	. 8658	1
1·0·14	-----	---	. 836	2	. 8362	<1

Lattice constants

		a	*c*
		A	*A*
1923	Dickinson and Pauling [3]	3. 16	12.32
1925	Hassel [4]	3. 15	12.32
1926	Natta [5]	3 09	12.24
1955	Swanson, Gilfrich, and Ugrinic.	3. 1604	12.295 at 26° C

The density of molybdenum disulfide calculated from the NBS lattice constants is 4.998 at 26° C.

References

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Potassium Chloroplatinate, K_2PtCl_6 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
366	0419 1–0177 1–0192	5. 6 4. 87 3. 44	Molybdenum.	Hanawalt, Rinn, and Frevel [1] (1938).

Additional published patterns. None.

NBS sample. The potassium chloroplatinate was prepared at the NBS from potassium chloride and chloroplatinic acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium and barium; 0.001 to 0.01 percent each of aluminum, calcium, chromium, and silicon; and 0.0001 to 0.001 percent each of silver, iron, magnesium, and manganese.

The sample is bright yellow. The index of refraction is 1.823.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	200	220
Swanson, Gilfrich, and Ugrinic	111	400	220

Lattice constant. The structure of potassium chloroplatinate was determined by Ewing and Pauling [2] in 1928. The cubic lattice has the space group O_h^5–Fm3m with 4(K_2PtCl_6) per unit cell. Potassium chloroplatinate is used as a structure type.

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

Lattice constants

		A
1922	Scherrer and Stoll [3]	9.7
1928	Frederikse and Verweel [4]	9.75
1928	Ewing and Pauling [2]	9.75
1933	Bødtker-Naess and Hassel [5]	9.752
1935	Engel [6]	9.745
1955	Swanson, Gilfrich, and Ugrinic	9.755 at 25° C

The density of potassium chloroplatinate calculated from the NBS lattice constant is 3.478 at 25° C.

Potassium Chloroplatinate, K_2PtCl_6 (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	5. 6	100	9. 7	5. 632	100	9. 756
200	4. 88	33	9. 76	4. 878	60	9. 756
220	3. 45	33	9. 76	3. 449	70	9. 755
311	2. 94	33	9. 75	2. 942	66	9. 755
222	-----	---	---	2. 816	10	9. 755
400	2. 43	33	9. 72	2. 439	73	9. 756
331	2. 23	13	9. 72	2. 238	26	9. 756
420	2. 18	13	9. 75	2. 182	30	9. 756
422	1. 99	17	9. 75	1. 991	27	9. 756
511	1. 87	17	9. 72	1. 877	33	9. 754
440	1. 72	17	9. 73	1. 724	39	9. 755
531	1. 65	13	9. 76	1. 649	24	9. 756
600	-----	---	---	1. 626	13	9. 755
620	1. 54	3	9. 74	1. 542	11	9. 755
533	1. 488	3	9. 76	1. 488	9	9. 756
444	1. 407	5	9. 75	1. 408	10	9. 756
711	1. 368	7	9. 77	1. 366	14	9. 754
640	-----	---	---	1. 353	6	9. 757
642	1. 305	5	9. 77	1. 303	10	9. 754
731	1. 271	5	9. 76	1. 270	12	9. 754
800	-----	---	---	1. 219	4	9. 755
733	-----	---	---	1. 192	2	9. 755
820	-----	---	---	1. 1829	8	9. 754
822	-----	---	---	1. 1496	6	9. 755
751	-----	---	---	1. 1264	8	9. 755
840	-----	---	---	1. 0906	11	9. 755
911	-----	---	---	1. 0708	9	9. 755
842	-----	---	---	1. 0644	6	9. 755
664	-----	---	---	1. 0400	4	9. 756
931	-----	---	---	1. 0226	7	9. 755
844	-----	---	---	0. 9956	9	9. 755
933	-----	---	---	. 9804	6	9. 755
10·0·0	-----	---	---	. 9756	3	9. 756
10·2·0	-----	---	---	. 9567	6	9. 756
951	-----	---	---	. 9431	7	9. 756
953	-----	---	---	. 9097	4	9. 755
10·4·0	-----	---	---	. 9058	4	9. 756
10·4·2	-----	---	---	. 8905	3	9. 755
11·1·1	-----	---	---	. 8796	2	9. 755
880	-----	---	---	. 8623	3	9. 756
11·3·1	-----	---	---	. 8524	7	9. 756
10·4·4	-----	---	---	. 8491	5	9. 755
10·6·0	-----	---	---	. 8365	4	9. 755
11·3·3	-----	---	---	. 8275	5	9. 756
12·0·0	-----	---	---	. 8130	6	9. 756
11·5·1	-----	---	---	. 8046	2	9. 755
12·2·2	-----	---	---	. 7912	3	9. 755
11·5·3	-----	---	---	. 7835	6	9. 754
Average value of last five lines			9. 76	--------	-----	9. 755

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] F. J. Ewing and L. Pauling, The crystal structure of potassium chloroplatinate, Z. Krist. **68**, 223–230 (1928).

[3] P. Scherrer and P. Stoll, Confirmation de la théorie de la coordination de Werner a l'aide d'analyse de rayons, Arch. sci. phys. et nat. **4**, 232 (1922).

[4] W. A. Frederikse and H. J. Verweel, The crystal structure of potassium-chloroplatinate, Rec. trav. chim. **47**, 904–908 (1928).

[5] G. Bødtker-Naess and O. Hassel, Ionerabstände in Kristallen von Komplexsalzen mit Fluoritstruktur, Avhandl. Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1933,** No. 7 (1933).

[6] G. Engel, Die Kristallstrukturen einiger Hexachlorokomplexsalze, Z. Krist. **90**, 341–773 (1935).

Potassium Fluosilicate (hieratite), K_2SiF_6 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
3035	3177 1–1169 1–1171	2. 35 2. 03 4. 71	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The potassium fluosilicate was prepared at the NBS from silica gel, hydrofluoric acid and potassium oxalate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of cesium and sodium; 0.001 to 0.01 percent each of aluminum, calcium, and iron; and 0.0001 to 0.001 percent each of barium, lead, and magnesium.

The sample is colorless. The index of refraction is too low to be determined by the liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	222	400	111
Swanson, Gilfrich, and Ugrinic	111	222	220

Lattice constant. The structure of potassium fluosilicate was determined by Ketelaar [2] in 1935. The cubic lattice has the space group O_h^5–Fm3m with potassium chloroplatinate-type structure and $4(K_2SiF_6)$ per unit cell.

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

Lattice constants

		A
1935	Ketelaar [2]	8.184
1955	Swanson, Gilfrich, and Ugrinic	8.133 at 26° C

The density of potassium fluosilicate calculated from the NBS lattice constant is 2.719 at 26° C.

Potassium Fluosilicate (hieratite), K_2SiF_6 (cubic)

hkl	1938			1955		
	Hanawalt, Rinn, and Frevel			Swanson, Gilfrich, and Ugrinic		
	Mo, 0.7107 A			Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	4. 72	63	8. 17	4. 699	100	8. 138
220	2. 89	50	8. 17	2. 877	65	8. 137
311	2. 45	1	8. 12	2. 453	5	8. 134
222	2. 35	100	8. 14	2. 349	71	8. 136
400	2. 03	75	8. 12	2. 034	52	8. 135
331	1. 86	1	8. 11	1. 866	<1	8. 135
420	1. 82	1	8. 14	1. 819	4	8. 135
422	1. 66	20	8. 13	1. 661	12	8. 135
511	1. 56	25	8. 10	1. 565	13	8. 133
440	1. 441	30	8. 15	1. 438	15	8. 134
531	1. 368	8	8. 09	1. 375	5	8. 134
600	----	---	----	1. 356	3	8. 134
620	1. 288	20	8. 15	1. 286	9	8. 135
622	1. 227	7	8. 14	1. 2262	3	8. 134
444	1. 177	6	8. 15	1. 1741	2	8. 134
711	1. 136	6	8. 11	1. 1390	3	8. 134
642	1. 087	10	8. 13	1. 0869	5	8. 134
731	1. 058	1	8. 13	1. 0588	2	8. 133
800	1. 016	1	8. 13	1. 0167	1	8. 134
733	0. 998	1	8. 17	0. 9936	<1	8. 133
820	. 986	1	8. 13	. 9864	1	8. 134
822	. 959	2	8. 14	. 9585	2	8. 133
751	. 938	1	8. 12	. 9391	1	8. 133
662	----	---	----	. 9331	<1	8. 135
840	. 910	2	8. 14	. 9094	2	8. 134
911	----	---	----	. 8927	<1	8. 133
842	----	---	----	. 8873	1	8. 132
664	----	---	----	. 8670	2	8. 133
931	----	---	----	. 8525	<1	8. 132
844	----	---	----	. 8302	2	8. 134
933	----	---	----	. 8175	<1	8. 134
10·0·0	----	---	----	. 8134	<1	8. 134
10·2·0	----	---	----	. 7975	4	8. 133
Average value of last five lines			8. 14	------	---	8. 133

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] J. A. A. Ketelaar, Die Kristallstruktur von K-, Rb- Cs-und Tl-Silicofluorid und von $LiMnO_4 \cdot 3H_2O$, Z. Krist. **92**, 155–156 (1935).

Potassium Zinc Fluoride, $KZnF_3$ (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
----	2452 3-0706 3-0700	2. 87 2. 03 4. 05	Molybdenum.	The Dow Chemical Co.

Additional published patterns. None.

NBS sample. The potassium zinc fluoride was prepared at the NBS from potassium cyanide, zinc carbonate, and hydrofluoric acid. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent each of aluminum and silicon; 0.001 to 0.01 percent each of silver, calcium, iron, and magnesium; and 0.0001 to 0.001 percent each of barium, chromium, copper, manganese, and lead.

The sample is colorless. The index of refraction is too low to be measured by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-spacings of the Dow Chemical Co. pattern were converted from kX to angstrom units.

The three strongest lines of the two patterns are as follows:

Pattern	1	2	3
The Dow Chemical Co	110	200	100
Swanson, Gilfrich, and Ugrinic	110	200	100

Lattice constant. The structure of potassium zinc fluoride according to Náray-Szabó [1] is monoclinic having the space group C_{2h}^2–$P2_1/m$ with perovskite-type structure, $8(KZnF_3)$ per unit cell, and the angle beta equal to 90° and, *a*, *b*, and *c* as approximately equal. The NBS pattern has been indexed as cubic having the space group O_h^1–Pm3m with $1(KZnF_3)$ per unit cell as it was first reported by Goldschmidt [2] in 1926. Neither microscopic examination nor the X-ray powder pattern showed any indication of other than an isometric arrangement.

A group of unit-cell measurements have been converted from kX to angstrom units, and the Náray-Szabó [1] measurement has been halved for comparison with the other values.

Lattice constants

		A
1926	Goldschmidt [2]	4.06
1928	Natta and Passerini [3]	4.06
1947	Náray-Szabó [1]	4.06
1955	Swanson, Gilfrich, and Ugrinic	4.056 at 25° C

The density of potassium zinc fluoride calculated from the NBS lattice constant is 4.018 at 25° C.

Potassium Zinc Fluoride, $KZnF_3$ (cubic)

hkl	-----			1955		
	Dow Chemical Co.			Swanson, Gilfrich, and Ugrinic		
	Mo, 0.7107 A			Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
100	4. 06	40	4. 06	4. 055	35	4. 055
110	2. 88	100	4. 07	2. 869	100	4. 057
111	-----	--	-----	2. 343	15	4. 058
200	2. 03	80	4. 06	2. 029	60	4. 057
210	1. 81	20	4. 04	1. 814	14	4. 056
211	1. 65	40	4. 04	1. 656	31	4. 056
220	1. 44	40	4. 08	1. 434	26	4. 056
300	1. 35	10	4. 05	1. 352	5	4. 056
310	1. 28	20	4. 05	1. 283	10	4. 056
222	1. 18	10	4. 09	1. 171	6	4. 057
320	-----	--	-----	1. 125	1	4. 056
321	-----	--	-----	1. 084	11	4. 056
400	-----	--	-----	1. 014	3	4. 055
410	-----	--	-----	0. 9839	2	4. 057
411	-----	--	-----	. 9561	6	4. 056
420	-----	--	-----	. 9070	8	4. 056
421	-----	--	-----	. 8850	2	4. 056
332	-----	--	-----	. 8648	3	4. 056
422	-----	--	-----	. 8279	6	4. 056
510	-----	--	-----	. 7955	7	4. 056
Average value of last five lines			4. 06	-----	---	4. 056

References

[1] S. Náray-Szabó, The perovskite structure family, Müegyetemi Közlemények **1,** 30–41 (1947).

[2] V. M. Goldschmidt, Geochemische Verteilungsgesetze der Element IV, Untersuchungen über Bau und Eigenschaften von Krystallen, Skrifter Norske Videnskaps-Akad. Oslo. I. Mat.-Naturv. Kl. **1926,** No. 8 (1926).

[3] G. Natta and L. Passerini, Isomorfismo, polimorfismo e morfotropia.—I. Composti del tipo ABX_3, Gazz. chim. ital. **58,** 472–484 (1928).

Praseodymium Fluoride, PrF_3 (hexagonal)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
----	3629	1.99	Copper 1.5405	Oftedal [1] 1929.
	3-1074	1.78		
	3-1063	1.17		

Since a large part of the low angle portion of the Oftedal pattern, including two of the strongest lines for praseodymium fluoride, is missing, the card is useless for identification purposes.

A structure study by Oftedal [1] showed that the unit cell values, a=4.085 A and c=7.232 A, as indicated on the ASTM card and in the earlier part of the literature reference were incorrect and they were changed to the larger unit cell, a=7.061 A and c=7.218 A. A later article by Oftedal [2] postulated a new structure D_{6h}^3 instead of the D_6^6 found on the ASTM card.

Additional published patterns. None.

NBS sample. The praseodymium fluoride sample used for the NBS pattern was prepared by J. H. Kluckhohn and T. P. Perros of the George Washington University in Washington, D. C. In preparation, the sample was dried at 100° C in an atmosphere of fluorine. Spectrographic analysis at the NBS showed the following impurities: 0.1 to 0.5 percent each of aluminum and silicon; 0.01 to 0.1 percent each of magnesium and nickel; and 0.0001 to 0.001 percent each of boron, calcium, iron, and lead. The other rare earth elements were reported as less than 0.1 percent which was the limit of detection for them in the spectrographic analysis.

The sample is pale green. The refractive indices are approximately 1.583 and 1.602. The crystals are too fine to allow determination of the sign.

Interplanar spacings and intensity measurements. The d-spacings of the Oftedal pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Oftedal	113	302	413
Swanson, Gilfrich, and Ugrinic	111	113	110

Lattice constants. The structure of praseodymium fluoride was redetermined by Oftedal [2] in 1931. The postulated structure is D_{6h}^3–$P6_3/mcm$ with lanthanum fluoride-type structure and 6(PrF_3) per unit cell. According to Wyckoff [3], the structure very nearly approximates an arrangement which reduces to a bimolecular cell, space group D_{6h}^4–$P6_3/mmc$, with smaller unit-cell values.

The unit-cell measurements of Oftedal were converted from kX to angstrom units for comparison with the NBS cell.

Lattice constants

		a	c
		A	A
1929	Oftedal [1]	7.075	7.233
1955	Swanson, Gilfrich, and Ugrinic.	7.075	7.238 at 26° C

The density of praseodymium fluoride calculated from the NBS lattice constants is 6.283 at 26° C.

Praseodymium Fluoride, PrF_3 (hexagonal)

hkl	1929 Oftedal Cu, 1.5405 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*
	A		A	
002	-------	----	3.622	36
110	-------	----	3.542	37
111	-------	----	3.180	100
112	-------	----	2.531	10
300	-------	----	2.042	51
113	1.996	m+	1.993	42
302	1.777	m	1.779	30
221	1.716	w	1.718	21
114	-------	----	1.612	5
222	-------	----	1.591	4
223	1.426	w	1.427	12
304	-------	----	1.354	9
115	-------	----	1.339	7
411	1.314	m−	1.314	12
330	-------	----	1.1795	6
413	1.170	m	1.1696	10
332	1.121	m	1.1210	8
306	1.038	w	1.0386	7
600	-------	----	1.0212	<1
415	0.983	m	0.9824	9

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).

[3] R. W. G. Wyckoff, Crystal Structures **1,** V text p. 21 (1951).

Rubidium Chloroplatinate, Rb_2PtCl_6 (cubic)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wave-length
Natta and Pirani [1] 1932	Iron	Kα

NBS sample. The rubidium chloroplatinate was prepared at the NBS from rubidium nitrate and chloroplatinic acid. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of potassium[5]; 0.01 to 0.1 percent each of aluminum, iron, and silicon; and 0.001 to 0.01 percent each of calcium, copper, and magnesium.

The sample is yellow. The index of refraction is 1.817.

Interplanar spacings and intensity measurements. The *d*-spacings of the Natta and Pirani pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Natta and Pirani	440	642	840
Swanson, Gilfrich, and Ugrinic	111	200	311

Lattice constant. The structure of rubidium chloroplatinate was determined by Natta and Pirani [1] in 1932. The cubic lattice has the space group O_h^5–Fm3m with potassium chloroplatinate-type structure and 4(Rb_2PtCl_6) per unit cell.

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

Lattice constants

		A
1932	Natta and Pirani [1]	9.85
1933	Bødtker-Naess and Hassel [2]	9.901
1935	Engel [3]	9.904
1955	Swanson, Gilfrich, and Ugrinic	9.901 at 25° C

The density of rubidium chloroplatinate calculated from the NBS lattice constant is 3.958 at 25° C.

Rubidium Chloroplatinate, Rb_2PtCl_6 (cubic)

hkl	1932 Natta and Pirani Fe, 1.937 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	-----	---	---	5. 72	100	9. 90
200	-----	---	---	4. 95	67	9. 90
220	3. 41	w	9. 64	3. 501	32	9. 902
311	2. 90	w	9. 62	2. 986	60	9. 902
222	2. 79	vw	9. 66	2. 859	4	9. 904
400	2. 41	ms	9. 64	2. 476	43	9. 904
331	-----	---	---	2. 272	21	9. 904
420	2. 18	vw	9. 75	2. 2144	38	9. 903
----	2. 06	vw	---	------	---	-----
422	1. 99	s	9. 75	2. 0213	12	9. 902
511	1. 88	ms	9. 77	1. 9061	25	9. 904
440	1. 72	vs	9. 73	1. 7505	26	9. 902
531	1. 65	ms	9. 76	1. 6737	19	9. 902
600	-----	---	---	1. 6504	16	9. 902
620	1. 54	ms	9. 74	1. 5659	5	9. 904
533	1. 49	w	9. 77	1. 5103	8	9. 904
622	-----	---	---	1. 4929	1	9. 903
444	1. 41	ms	9. 77	1. 4295	5	9. 904
711	1. 37	m	9. 78	1. 3866	9	9. 902
640	-----	-----	---	1. 3730	7	9. 901
642	1. 31	vs	9. 80	1. 3232	6	9. 902
731	1. 27	ms	9. 76	1. 2890	8	9. 901
800	1. 23	mw	9. 84	1. 2378	4	9. 902
733	-----	---	---	1. 2098	2	9. 903
820	1. 19	w	9. 81	1. 2007	5	9. 901
822	1. 16	ms	9. 84	1. 1669	2	9. 902
751	1. 13	m	9. 79	1. 1433	7	9. 901
840	1. 100	vs	9. 84	1. 1070	8	9. 901
911	1. 079	mw	9. 83	1. 0868	5	9. 901
842	-----	---	---	1. 0803	1	9. 901
664	1. 050	mw	9. 85	1. 0555	3	9. 902
931	1. 032	ms	9. 84	1. 0380	3	9. 902
844	-----	---	---	1. 0107	4	9. 903
933	-----	---	---	0. 9952	2	9. 904
10·0·0	-----	---	---	. 9903	1	9. 903
10·2·0	-----	---	---	. 9710	4	9. 902
951	-----	---	---	. 9573	3	9. 902
953	-----	---	---	. 9234	2	9. 902
10·4·2	-----	---	---	. 9040	2	9. 903
11·1·1	-----	---	---	. 8927	1	9. 900
880	-----	---	---	. 8753	2	9. 903
11·3·1	-----	---	---	. 8651	3	9. 902
10·4·4	-----	---	---	. 8618	2	9. 901
10·6·0	-----	---	---	. 8490	3	9. 901
11·3·3	-----	---	---	. 8393	2	9. 901
12·0·0	-----	---	---	. 8251	4	9. 901
11·5·1	-----	---	---	. 8167	1	9. 902
12·2·2	-----	---	---	. 8031	4	9. 901
11·5·3	-----	---	---	. 7953	3	9. 901
12·4·0	-----	---	---	. 7828	4	9. 902
Average value of last five lines			9. 83	------	---	9. 901

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[5] This amount of potassium can be expected to enter into solid solution with the rubidium compound decreasing the size of the cell by not more than one thousandth of an angstrom.

References

[1] G. Natta and R. Pirani, Soluzioni solide per precipitazione ed isomorfismo tra complessi del platino e del tellurio tetravalente.—I. Struttura dei cloroplatinati di cesio e di rubidio, Rend. Accad. Lincei, **15,** 92–98 (1932).

[2] G. Bødtker-Naess and O. Hassel, Ionerabstände in Kristallen von Komplexsalzen mit Fluoritstruktur, Avhandl. Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1933,** No. 7 (1933).

[3] G. Engel, Die Kristallstrukturen einiger Hexachlorokomplexsalze, Z. Krist. **90,** 341–373 (1935).

Selenium, Se (hexagonal)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
3811	3886	1. 43	Copper____ 1.539	Bradley [1] 1924.
	1–1303	1. 08		
	1–1298	1. 50		
_______	0898	4. 29	Copper____ 1.53923	Olshausen [2] 1925.
	3–0237	3. 79		
	3–0233	3. 01		
2082	2057	3. 01	Molybdenum.	Slattery [3] 1925.
	1–0841	3. 77		
	1–0853	2. 07		
II–1421	2233	2. 98	Copper____	Parravano and Caglioti [4] 1930.
	2–0696	2. 06		
	2–0677	1. 76		
2070	2118	3. 02	Molybdenum.	Hanawalt, Rinn, and Frevel [5] 1938.
	1–0861	2. 07		
	1–0848	3. 78		

The data of the pattern for Bradley agrees with that for the hexagonal system, and not the monoclinic as reported on the ASTM card.

The Bradley and the Parravano and Caglioti patterns were made using copper radiation rather than molybdenum as indicated on the ASTM cards.

Additional published patterns

Source	Radiation	Wavelength
Tanaka [6] 1934________________	Copper___	__________

A pattern by Gupta, Das, and Ray [7] was found in the literature, but as this pattern included many *d*-spacings that were not possible for hexagonal selenium it was not included in the table.

NBS sample. The selenium used for the NBS pattern was an especially purified sample contributed by the Mallinckrodt Chemical Works. The sample was annealed at 155° C for 16 hours. Their spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum and silicon; and 0.0001 to 0.001 percent each of boron, barium, calcium, copper, and iron.

The sample is a dark gray opaque powder.

Interplanar spacings and intensity measurements. The *d*-spacing at 4.29 A which is noted as the strongest line on the ASTM card for Olshausen could not be found in the literature.

The *d*-spacings of the Tanaka, the Bradley, the Slattery, and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units, and the *d*-spacings of the Parravano and Caglioti and the Olshausen patterns were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Bradley______________________________	210	213	----
Olshausen____________________________	100	101	----
Slattery_____________________________	101	100	102
Parravano and Caglioti_______________	101	102	201
Hanawalt, Rinn, and Frevel___________	101	102	100
Tanaka_______________________________	200	-----	105
Swanson, Gilfrich, and Ugrinic_________	101	100	102

Lattice constants. Work was done on the structure of selenium by Bradley [1] in 1924. The hexagonal lattice has the space group D_3^4–$P3_121$ or D_3^6–$P3_221$ with 3(Se) per unit cell. Selenium is used as a structure type.

Several unit-cell determinations have been converted from kX to angstrom units and the rhombohedral unit cell was converted to hexagonal cells for comparison with the NBS values. The linear coefficient of expansion at 20° is 74.09×10^{-6} parallel to the *a*-axis and -17.89×10^{-6} parallel to the *c*-axis, according to Straumanis [8]. The lattice constants determined by Straumanis and by Krebs [9] were temperature corrected from 20° to 26° C for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1925__	Slattery [3]__________	4. 35	4. 96
1930__	Parravano and Caglioti [4].	4. 346	4. 952
1934__	Tanaka [6]__________	4. 369	4. 972
1937__	Prins and Dekeyser [10].	4. 35	4. 96
1949__	Krebs [9]____________	4. 35536	4. 94885 at 26° C
1949__	Straumanis [8]_______	4. 3642	4. 9588 at 26° C
1955__	Swanson, Gilfrich, and Ugrinic.	4. 3662	4. 9536 at 26° C

The density of the selenium calculated from the NBS lattice constants is 4.809 at 26° C.

Selenium, Se (hexagonal)

hkl	1924 Bradley Cu, 1.5405 A		1925 Olshausen Cu, 1.5405 A		1925 Slattery Mo, 0.7107 A		1930 Parravano and Caglioti Cu. 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1934 Tanaka Cu, 1.5405 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*		*A*	
100	3.72	38	3.78	s	3.78	80	------	---	3.79	33	3.78	10	3.78	53
----	--------	--	3.35	m	------	---	------	---	------	---	------	--	------	--
101	2.99	13	3.00	s	3.02	100	2.98	vs	3.03	100	3.01	5	3.005	100
110	2.18	--	2.19	m	2.17	20	2.17	m	2.18	27	2.186	35	2.184	16
102	2.07	25	2.07	m	2.07	25	2.06	vs	2.07	40	2.074	25	2.072	35
111	2.00		------	---	2.001	20	1.988	s	2.00	33	2.002	30	1.998	21
200	1.90	--	1.88	w	1.883	2	1.888	w	------	---	1.889	100	1.890	3
-----	------	--	1.81	vw	------	---	------	---	------	---	------	--	------	--
201	1.76	50	1.76	m	1.774	17	1.757	vs	1.77	27	1.767	15	1.766	21
003	1.64	63	------	---	1.641	15	1.644	s	1.64	20	1.645	45	1.650	9
112							1.635	s					1.637	12
103	1.51	78	1.50	m	1.508	15	1.511	ms	1.51	27	1.512	40	1.5127	7
202							1.500	ms					1.5029	10
210	1.43	100	------	---	1.428	15	1.426	s	1.433	20	1.435	20	1.4291	9
211	1.373	--	1.376	w	------	---	1.371	m	------	---	1.382	65	1.3727	4
113	1.318	--	1.317	w	1.313	3	1.319	s	1.323	13	1.325	80	1.3170	5
-----	1.274	--	------	---	------	---	------	---	------	---	-------	---	------	--
203	1.244	--	------	---	------	---	1.243	mw	1.242	7	1.254	75	1.2439	2
212	------	--	------	---	------	---	------	---	------	---	1.239	70	1.2387	3
301	1.222	--	1.224	w	------	---	1.207	m	------	---	1.191	85	1.2215	3
104	1.179	--	1.182	vw	1.177	3	1.179	s	1.182	7	1.184	85	1.1769	5
302	1.124	--	------	---	------	---	1.126	m	1.127	7	1.126	55	1.1232	3
213	1.081	88	------	---	1.077	2	1.081	s	1.086	13	1.086	50	1.0803	6
-----	1.063	88	------	---	------	---	------	---	------	---	------	--	------	--
204	1.045	--	1.038	vw	------	---	1.039	m	1.040	7	1.034	60	1.0365	2
311	1.027	--	1.029	w	------	---	1.025	m	------	---	------	--	1.0261	2
-----	0.999	--	1.000	w	------	---	------	---	------	---	1.007	95	------	--
105	.965	--	0.966	m	------	---	0.961	m	------	---	0.970	90	0.9593	2
-----	------	--	.944	vw	------	---	.947	m	------	---	------	--	------	--
-----	------	--	.914	w	------	---	.905	m	------	---	------	--	------	--
-----	------	--	.887	m	------	---	.879	m	------	---	------	--	------	--
-----	------	--	.859	w	------	---	------	---	------	---	------	--	------	--

References

[1] A. J. Bradley, The crystal structures of the rhombohedral forms of selenium and tellurium, Phil. Mag. **48,** 477–496 (1924).

[2] S. v. Olshausen, Strukturuntersuchungen nach der Debye-Scherrer-Method, Z. Krist. **61,** 463–514 (1925).

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[4] N. Parravano and V. Caglioti, Ricerche sul sistema bismutoselenio, Gazz. chim. ital. **60,** 923–932 (1930).

[5] 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).

[6] K. Tanaka, The X-ray examination of selenium crystals, Mem. Coll. Sci. Univ. Kyoto **17,** 59–78 (1934).

[7] K. D. Gupta, S. R. Das, and B. B. Ray, A study of allotropes of selenium by the X-ray diffraction method, Indian J. Phys. **15,** 389–399 (1944).

[8] M. E. Straumanis, The precision determination of lattice constants by the powder and rotation crystal methods and applications, J. Appl. Phys. **20,** 726–734 (1949).

[9] H. Krebs, Über das schwarze Selen. Die Gitterstörungen des hexagonalen Selens, Z. Physik. **126,** 769–780 (1949).

[10] J. A. Prins and W. Dekeyser, Étude aux rayons X du sélénium vitreux et de sa crystalisation, Physica **4,** 900–908 (1937).

Silver Arsenate, Ag_3AsO_4 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
II–1818	2704 2–0876 2–0868	2. 74 2. 51 1. 64	Molybdenum.	Wyckoff [1] 1925.
-------	2703 3–0787 3–0779	2. 74 2. 51 1. 64	Molybdenum.	Wyckoff [2] 1925.
2538	2705 1–1042 1–1031	2. 74 2. 50 1. 63	Molybdenum.	Hanawalt, Rinn, and Frevel [3] 1938.

The pattern on ASTM card 2–0868 for Wyckoff has been corrected, indexed and reissued on card 3–0779 in the fifth set of cards, and the older card has been marked for deletion. The two Wyckoff references are to the same paper—the first being a German republication of the second.

Additional published patterns. None.

NBS sample. The sample of silver arsenate was prepared at the NBS. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of iron and silicon; 0.001 to 0.01 percent each of aluminum, calcium, copper, magnesium, nickel, and lead; and 0.0001 to 0.001 percent of boron.

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

Interplanar spacings and intensity measurements. The d-spacings of the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units and the d-spacings of the Wyckoff pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Wyckoff	210	211	321
Hanawalt, Rinn, and Frevel	210	211	321
Swanson, Gilfrich, and Ugrinic	210	211	321

Lattice constant. In 1925, Wyckoff [2] determined the space group of silver phosphate to be either O_h^3–Pm3n or T_d^4–$P\bar{4}3n$. He favored the latter, although he could not establish the positions of the oxygen atoms. Helmholz and Levine [4], in 1942, established the space group of silver arsenate as T_d^4–$P\bar{4}3n$ with silver phosphate-type structure and 2(Ag_3AsO_4) per unit cell.

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

Lattice constants

		A
1925	Wyckoff [2]	6.13
1947	Vegard [5]	6.129
1955	Swanson, Gilfrich, and Ugrinic.	6.1328 at 26° C

The density of silver arsenate calculated from the NBS lattice constant is 6.658 at 26° C.

References

[1] R. W. G. Wyckoff, Kristallstruktur des Silberphosphats und Silberarsenats, Z. Krist. **62,** 529–539 (1925).

[2] R. W. G. Wyckoff, Crystal structure of silver phosphate and silver arsenate, Am. J. Sci. **10,** 107–118 (1925).

[3] 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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[5] L. Vegard, The crystal structure of Ag_3PO_4 and Ag_3AsO_4, Skrifter Norske Videnskaps-Akad. Oslo. I. Mat.-Naturv. Kl. **1947,** No. 2, 67–72 (1947).

Silver Arsenate, Ag_3AsO_4 (cubic)

hkl	1925 Wyckoff Mo, 0.7107 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
200	3.065	35	6.130	3.08	17	6.16	3.066	25	6.132
210	2.738	>100	6.122	2.75	100	6.15	2.743	100	6.134
211	2.509	80	6.146	2.50	67	6.12	2.504	55	6.133
310	--------	--	--------	1.94	5	6.13	1.940	4	6.135
222	1.771	30	6.135	1.77	13	6.13	1.7704	11	6.1328
320	1.699	50	6.126	1.70	33	6.13	1.7010	21	6.1330
321	1.625	60	6.080	1.63	53	6.10	1.6391	28	6.1329
400	1.533	30	6.132	1.53	20	6.12	1.5333	9	6.1332
420	1.371	25	6.131	1.372	13	6.14	1.3714	8	6.1331
421	1.341	40	6.145	1.338	23	6.131	1.3384	12	6.1333
332	1.308	10	6.135	1.308	11	6.135	1.3076	4	6.1332
520	1.137	50	6.123	1.139	20	6.134	1.1389	9	6.1332
521	1.116	20	6.113	1.120	12	6.134	1.1197	6	6.1328
440	1.081	30	6.115	1.082	11	6.121	1.0842	6	6.1332
600	--------	--	--------	1.023	7	6.138	1.0222	2	6.1332
611	--------	--	--------	0.996	9	6.140	0.9949	5	6.1330
622	--------	--	--------	--------	--	--------	.9246	1	6.1331
630	--------	--	--------	.917	5	6.151	.9143	1	6.1333
631	--------	--	--------	--------	--	--------	.9043	1	6.1333
444	--------	--	--------	--------	--	--------	.8852	2	6.1328
640	--------	--	--------	--------	--	--------	.8505	3	6.1330
720	--------	--	--------	--------	--	--------	.8424	5	6.1327
721	--------	--	--------	--------	--	--------	.8346	6	6.1330
650	--------	--	--------	--------	--	--------	.7852	3	6.1326
Average value of last five lines			6.13	--------	--	6.14	--------	--	6.1328

Silver Bromate, $AgBrO_3$ (tetragonal)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
II–1482	[a] 2253 2–0708 2–0716	2.95 1.74 3.06	Chromium 2.285 A.	Harang [1] 1928.
2212	2179 1–0879 1–0904	2.95 3.04 1.74	Molybdenum.	Hanawalt, Rinn, and Frevel [2] 1938.

[a] The ASTM card for Harang has been deleted in the 1954 index.

Additional published patterns. None.

NBS sample. The silver bromate was obtained from A. D. Mackay Inc., New York. Spectrographic analysis of the sample showed the following impurities: 0.001 to 0.01 percent each of iron, nickel, and silicon; and 0.0001 to 0.001 percent each of barium, calcium, copper, magnesium, and lead.

The sample is colorless, and it is optically positive with the refractive indices N_o=1.845 and N_e=1.918.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the *d*-spacings of the Harang pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Harang	202	422	220
Hanawalt, Rinn, and Frevel	202	220	422
Swanson, Gilfrich, and Ugrinic	202	220	211

Lattice constants. In 1942 Náray-Szabó and Pócza [3] determined the structure of silver chlorate, which is isostructural with silver bromate. The tetragonal lattice has the space group C_{4h}^5–I4/m with 8($AgBrO_3$) per unit cell.

The unit-cell measurements of Harang have been converted from kX to angstrom units and compared with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1927	Harang [1]	8. 61	8.10
1955	Swanson, Gilfrich, and Ugrinic	8. 609	8.092 at 25° C

The density of silver bromate calculated from the NBS lattice constants is 5.222 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] 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).

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

Silver Bromate, $AgBrO_3$ (tetragonal)

hkl	1927 Harang Cr, 2.2909 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
101	-----	---	-----	---	5. 90	2
200	-----	---	-----	---	4. 306	5
211	3. 48	m	3. 49	13	3. 479	41
220	3. 06	s	3. 05	27	3. 044	56
202	2. 96	vs	2. 96	100	2. 950	100
310	2. 74	w	2. 71	3	2. 722	5
301	-----	---	-----	---	2. 706	9
103	-----	---	2. 59	1	2. 576	4
222	-----	---	-----	---	2. 433	4
321	2. 29	vw	2. 28	2	2. 292	9
213	2. 21	vw	2. 22	8	2. 210	13
400	2. 15	s	2. 15	20	2. 152	28
411 004	2. 03	m	2. 05	5	2. 024	10
420	1. 91	m	1. 92	5	1. 925	9
402	-----	---	-----	---	1. 900	2
323	1. 79	m	1. 79	7	1. 788	10
422	1. 74	vs	1. 74	27	1. 738	29
224 501 431	1. 68	s	1. 69	11	1. 685	15
413	-----	---	1. 65	1	1. 651	6
314	-----	---	-----	---	1. 624	2
521	1. 57	vw	1. 56	3	1. 568	4
512	-----	---	-----	---	1. 558	2
440	1. 52	w	1. 52	3	1. 522	3
215	1. 49	w	1. 493	1	1. 4927	3
404	1. 47	w	1. 473	3	1. 4742	4
503 433	1. 45	vw	1. 453	3	1. 4515	3
442	-----	---	-----	---	1. 4242	<1
305	-----	---	1. 414	1	1. 4099	2
611	1. 39	vw	1. 393	1	1. 3937	2
532	-----	---	-----	---	1. 3868	1
620	1. 36	s	1. 361	5	1. 3609	4
602	1. 35	s	-----	---	1. 3525	4
622	-----	---	-----	---	1. 2906	4
613	-----	---	-----	---	1. 2535	2
444	-----	---	-----	---	1. 2162	3
316	-----	---	-----	---	1. 2085	1
543	-----	---	-----	---	1. 2033	3
640 534	-----	---	-----	---	1. 1938	1
505 435	-----	---	-----	---	1. 1796	2
712 552	-----	---	-----	---	1. 1661	1
633	-----	---	-----	---	1. 1588	3
406 642	-----	---	-----	---	1. 1440	3

Silver Nitrate, $AgNO_3$ (orthorhombic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
2095	2045	3. 00	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
	1–0836	4. 51		
	1–0856	4. 08		

Additional published patterns. None.

NBS sample. The silver nitrate was obtained from Johnson Matthey and Co., Ltd. The sample was recrystallized by atomizing a water solution. Their spectographic analysis showed the following impurities: 0.001 to 0.01 percent each of magnesium and copper; and 0.0001 to 0.001 percent each of iron and calcium.

The sample is colorless, optically positive, and $2V \simeq 60°$. The indices of refraction are $\alpha = 1.731$ and $\beta = 1.741$, and $\gamma \simeq 1.788$. γ could not be accurately determined as the index oils in the range of γ reacted with the sample.

Interplanar spacings and intensity measurements. The *d*-spacings of Hanawalt, Rinn, and Frevel were converted from kX to angstrom units.

The three strongest lines for the two patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	211	111	102
Swanson, Gilfrich, and Ugrinic	211	020	102

Lattice constants. Work was done on the structure of silver nitrate by Zachariasen [2] in 1928. The orthorhombic lattice has one of the four space groups D_2^1 to D_2^4. There are 8($AgNO_3$) per unit cell.

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

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1928	Zachariasen [2]	6. 98	7. 35	10.16
1955	Swanson, Gilfrich, and Ugrinic.	6. 995	7. 328	10.118 at 26° C

The density of silver nitrate calculated from the NBS lattice constants is 4.351 at 26° 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 Kristallstruktur von Sesquioxyden und Verbindungen ABO_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1928**, No. 4 (1928).

Silver Nitrate, $AgNO_3$ (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*
	A		*A*	
111	4. 52	50	4. 525	56
102	4. 09	50	4. 099	54
020	3. 67	38	3. 666	62
112	-------	----	3. 580	6
021	-------	----	3. 446	10
210	------	---	3. 157	11
121	-------	---	3. 092	7
211	3. 01	100	3. 013	100
113	2. 81	38	2. 806	38
122	2. 74	44	2. 733	56
212	------	----	2. 678	4
220	}2. 54	38	2. 531	43
004				
023	-------	----	2. 482	3
213	2. 29	31	2. 305	33
131	2. 24	25	2. 249	28
311	2. 15	15	2. 170	12
302	2. 11	10	2. 118	12
024	2. 08	50	2. 082	31
231	1. 96	18	1. 965	16
133	1. 90	10	1. 904	10
115	-------	----	1. 879	9
313	-------	----	1. 855	20
322	1. 83	25	1. 833	22
224	-------	----	1. 789	4
144	-------	----	1. 747	9
233	-------	----	1. 721	11
215	1. 70	15	1. 703	20
142	1. 66	15	1. 676	15
331	-------	----	1. 663	7

Silver Nitrate, $AgNO_3$ (orthorhombic)—Con.

hkl	1938 Hanawalt, Rinn and Frevel Mo, 0.7107 A		1955 Swanson, Gilfrich and Ugrinic Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*
106	-------	----	1. 639	5
420	1. 57	5	1. 578	7
333	-------	----	1. 508	7
126	}1. 493	10	1. 496	11
315				
044	-------	----	1. 4835	10
404	-------	----	1. 4381	9
430	}1. 423	8	1. 4230	5
235				
052	-------	----	1. 4065	<1
117	}------	----	1. 3893	3
036				
501	}1. 385	5	1. 3855	4
342				
502	-------	----	1. 3483	4
251	}1. 343	13	1. 3392	9
424				
217	1. 313	3	1. 3139	1
326	-------	----	1. 2803	1
522	}------	----	1. 2650	9
008				
440	}------	----	1. 2552	<1
441				
227				
351	-------	----	1. 2316	2
146	}------	----	1. 2215	4
060				
317	-------	----	1. 2117	2
028	}------	----	1. 1953	4
161				
162	}------	----	1. 1707	4
155				

Silver Nitrite, $AgNO_2$ (orthorhombic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
1996	1964 1–0813 1–0823	3. 06 3. 95 1. 97	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
	2014 3–0582 3–0572	3. 08 2. 11 1. 97	Copper	Ketelaar [2] 1936.

Additional published patterns. None.

NBS sample. The silver nitrite was obtained from the City Chemical Company, New York. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, and silicon; and 0.0001 to 0.001 percent of copper.

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

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the *d*-spacings of the Ketelaar pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	020, 110	011	022, 112
Ketelaar	020, 110	121	022, 112
Swanson, Gilfrich, and Ugrinic	110	011	020

Lattice constants. The structure of silver nitrite was determined by Ketelaar [2] in 1936. The orthorhombic lattice has the space group C_{2v}^{20}–Imm2 with 2($AgNO_2$) per unit cell.

The Ketelaar unit-cell measurements have been converted from kX to angstrom units and compared with the NBS values.

Lattice constants

		a	b	c
		A	A	A
1936	Ketelaar [2]	3. 51	6. 15	5.17
1955	Swanson, Gilfrich, and Ugrinic.	3. 526	6. 170	5.182 at 25° C.

The density of silver nitrite calculated from the NBS lattice constants is 4.532 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 (9128).

[2] J. A. A. Ketelaar, Die Kristallstruktur des Silbernitrits, Z. Krist. **95,** 383–393 (1936).

Silver Nitrite $AgNO_2$ (orthorhombic)

hkl	1936 Ketelaar Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
011	3. 955	w	3. 96	67	3. 967	48
020	3. 065	vs	3. 07	100	3. 084	35
110					3. 062	100
101	2. 927	vw	2. 91	13	2. 915	16
002	2. 550	w	2. 59	40	2. 592	20
121	2. 112	ms	2. 11	40	2. 118	26
022	1. 972	ms	1. 97	67	1. 984	18
112					1. 979	27
031	1. 902	m	1. 90	13	1. 912	12
130	-----	---	-----	---	1. 777	6
200	1. 764	m⁻	1. 76	7	1. 761	6
013	1. 657	w⁻	1. 66	7	1. 663	3
211	1. 603	w	1. 60	3	1. 610	5
103	1. 541	vw	1. 54	3	1. 5511	4
040	-----	---	-----	---	1. 5424	2
220	1. 527	w	-----	---	1. 5308	3
132	-----	---	1. 464	7	1. 4650	5
202	1. 458	m	-----	---	1. 4576	3
123	1. 381	w	1. 388	5	1. 3855	4
141	1. 356	mw	1. 364	3	1. 3634	4
033	1. 317	m	1. 323	7	1. 3229	4
222	-----	---	-----	---	1. 3186	2
231	1. 295	mw	1. 295	4	1. 2958	6
004						
114	1. 203	vw	1. 194	4	1. 1931	3
150	1. 188	mw	-----	---	1. 1650	2
310	1. 156	w	-----	---	1. 1549	<1
143	1. 089	w	-----	---	1. 0939	1
152	1. 073	vw	-----	---	1. 0622	<1
242	1. 057 ([a])	m	-----	---	1. 0596	1

[a] Eleven additional lines were omitted.

Silver Phosphate, Ag_3PO_4 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
II–1958	2853	2.68	Molybdenum.	Wyckoff [1] 1925.
	2–0952	1.30		
	2–0931	2.44		
-------	2852	2.68	Molybdenum.	Wyckoff [2] 1925.
	3–0829	1.30		
	3–0821	2.45		
2621	2798	2.86	Molybdenum.	Hanawalt, Rinn, and Frevel [3] 1938.
	1–1058	2.45		
	1–1058	1.66		

The pattern on ASTM card 2–0931 for Wyckoff has been corrected, indexed and reissued on card 3–0821 in the 5th set of cards and the older card has been marked for deletion. The two Wyckoff references are to the same paper—the first being a German republication of the second.

Additional published patterns. None.

NBS sample. The sample of silver phosphate was prepared at the NBS in a darkened room. It was rinsed in alcohol and protected from light until it was dry. Spectrographic analysis of the sample showed the following impurities: 0.001 to 0.01 percent each of lead, silicon, aluminum, barium, calcium, iron, and magnesium; and 0.0001 to 0.001 percent each of boron, copper, and manganese.

The NBS sample is yellow. The index of refraction is 1.975.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the *d*-spacings of the Wyckoff pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Wyckoff	210	421	211
Hanawalt, Rinn, and Frevel	210	211	320
Swanson, Gilfrich, and Ugrinic	210	211	320

Lattice constant. In 1925, Wyckoff [2] determined the space group of silver phosphate to be either O_h^3-Pm3n or T_d^4-P$\bar{4}$3n. He favored the latter, although he could not establish the positions of the oxygen atoms. Helmholz [4], in 1936, definitely established the space group as T_d-P$\bar{4}$3n. The cubic lattice has 2(Ag_3PO_4) per unit cell. Silver phosphate is used as a structure type.

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

Lattice constants

		A
1925	Wyckoff [2]	6.01
1936	Glocker [5]	6.00
1936	Helmholz [4]	6.007
1947	Vegard [6]	6.011
1955	Swanson, Gilfrich, and Urginic	6.013 at 26° C

The density of silver phosphate calculated from the NBS lattice constant is 6.394 at 26° C.

References

[1] R. W. G. Wyckoff, Kristallstruktur des Silberphosphats und Silberarsenats, Z. Krist. **62,** 529–539 (1925).

[2] R. W. G. Wyckoff, Crystal structure of silver phosphate and silver arsenate, Am. J. Sci. **10,** 107–118 (1925).

[3] 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).

[4] L. Helmholz, The crystal structure of silver phosphate, J. Chem. Physics **4,** 316–322 (1936).

[5] R. Glocker, Materialprufung mit Röntgenstrahlen unter besonderer Berucksichtigung der Röntgenmetallkunde, 2d Ed. Berlin, Verlag von Julius Springer (1936).

[6] L. Vegard, The crystal structure of Ag_3PO_4 and Ag_3AsO_4, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl **1947,** No. 2, 67–72 (1947).

Silver Phosphate, Ag_3PO_4 (cubic)

hkl	1925 Wyckoff Mo, 0.7107 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*d*	*d*	*I*	*a*
	A		A	A		A	A		A
110	4. 27	25	6. 039	4. 26	11	6. 02	4. 25	14	6. 010
200	3. 012	20	6. 024	3. 01	17	6. 02	3. 006	18	6. 012
210	2. 678	>100	5. 988	2. 69	100	6. 02	2. 689	100	6. 013
211	2. 453	55	6. 009	2. 45	43	6. 00	2. 454	33	6. 011
220	--------	--	--------	2. 11	3	5. 97	2. 126	3	6. 013
310	1. 897	25	5. 999	1. 89	17	5. 98	1. 9016	9	6. 013
222	1. 732	30	6. 000	1. 73	29	5. 99	1. 7356	13	6. 012
320	1. 661	50	5. 989	1. 66	36	5. 99	1. 6676	20	6. 013
321	1. 601	40	5. 990	1. 60	29	5. 99	1. 6070	14	6. 013
400	--------	--	--------	1. 50	11	6. 00	1. 5034	7	6. 014
411	--------	--	--------	1. 416	2	6. 008	1. 4173	2	6. 013
--------	--------	--	--------	1. 379	1	--------	--------	--	--------
420	--------	--	--------	1. 344	6	6. 011	1. 3444	4	6. 012
421	1. 306	60	5. 985	1. 311	29	6. 008	1. 3121	12	6. 013
332	--------	--	--------	1. 281	5	6. 008	1. 2819	3	6. 013
422	--------	--	--------	1. 228	2	6. 016	1. 2275	1	6. 014
510	--------	--	--------	1. 179	2	6. 012	1. 1793	1	6. 013
520	1. 113	55	5. 994	1. 115	23	6. 004	1. 1167	9	6. 014
521	--------	--	--------	1. 097	5	6. 009	1. 0980	3	6. 014
440	--------	--	--------	1. 062	9	6. 008	1. 0630	4	6. 013
530	--------	--	--------	1. 031	1	6. 012	1. 0314	1	6. 014
600	--------	--	--------	1. 002	2	6. 012	1. 0022	1	6. 013
610	--------	--	--------	0. 990	2	6. 022	0. 9888	2	6. 014
611	--------	--	--------	. 975	4	6. 010	. 9756	3	6. 014
622	--------	--	--------	-------	--	-------	. 9064	2	6. 012
630	--------	--	--------	-------	--	-------	. 8964	4	6. 013
720	--------	--	--------	-------	--	-------	. 8259	3	6. 013
721	--------	--	--------	-------	--	-------	. 8182	2	6. 012
Average value of last five lines			5. 992	-------	--	6. 013	--------	--	6. 013

Sodium Acid Fluoride, $NaHF_2$ (hexagonal)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
II-1807	2639 2-0854 2-0860	2. 75 2. 03 1. 73	Copper	Michigan Alkali Co., Michigan.
II-1863	2725 2-0889 2-0893	2. 72 2. 02 4. 53	Molybdenum.	Canadian Industries, Ltd., Canada.
-------	2640 3-0766 3-0766	2. 76 2. 02 1. 73	Molybdenum.	Dow Chemical Co.

Additional published patterns

Source	Radiation	Wavelength
Anderson and Hassel [1] 1926	Copper	----------

NBS sample. The sodium acid fluoride was obtained from A. D. Mackay, Inc., New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon; 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, and lead; and 0.0001 to 0.001 percent of manganese.

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

Interplanar spacings and intensity measurements. The *d*-spacings of the Michigan Alkali Company, the Canadian Industries and the Dow Chemical Company patterns were converted from kX to angstrom units and the *d*-spacings of the Anderson and Hassel pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Michigan Alkali Co.	012	015	110
Canadian Industries	012	015	003
Dow Chemical Co.	012	015	110
Anderson and Hassel	012	015	110
Swanson, Gilfrich, and Ugrinic	012	015	003

Lattice constants. The structure of sodium acid fluoride was determined by Rinne, Hentschel, and Leonhardt [2] in 1923. The hexagonal lattice has the space group D_{3d}^5–$R\bar{3}m$ with cesium dichloroiodide-type structure and 3($NaHF_2$) per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1923	Rinne, Hentschel, and Leonhardt [2].	3.44	13.96
1926	Anderson and Hassel [1]	3.47	13.95
1955	Swanson, Gilfrich, and Ugrinic	3.468	13.76 at 25° C.

The density of sodium acid fluoride calculated from the NBS lattice constants is 2.154 at 25° C.

References

[1] C. C. Anderson and O. Hassel, Die Struktur des Kristallisierten Natriumhydrofluorids und die Gestalt des Ions HF-, Z. physik. Chem. **123**, 151–159 (1926).

Sodium Acid Fluoride, $NaHF_2$ (hexagonal)

hkl	---- Michigan Alkali Co. Cu, 1.5418 A		---- Canadian Industries, Ltd. Mo, 0.7107 A		---- Dow Chemical Co. Mo, 0.7107 A		1926 Anderson and Hassel Cu, 1.5418 A		1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
003	4.7	50	4.54	60	4.62	25	4.38	ms	4.593	48
-----	------	----	3.30	5	------	----	------	----	------	----
-----	------	----	3.04	5	------	----	------	----	------	----
101	2.94	20	2.91	10	2.94	7	------	----	2.935	11
012	2.76	100	2.73	100	2.77	100	2.66	s	2.753	100
006	------	----	2.30	7	2.32	7	2.22	vw–w	2.294	3
015	2.03	80	2.02	80	2.02	63	1.99	s	2.029	49
-----	1.92	20	------	----	------	----	------	----	------	----
-----	1.82	10	------	----	------	----	------	----	------	----
-----	1.79	5	1.78	2	------	----	------	----	------	----
110	1.73	70	1.73	60	1.73	40	1.71	ms–s	1.7345	31
107	1.64	50	1.64	60	1.64	20	1.61	ms	1.6453	22
113	1.62	30	1.62	7	------	----	------	----	1.6218	8
009	1.52	3	------	----	1.53	1	------	----	1.5290	2
202	1.46	10	1.46	10	1.47	8	1.45	ms	1.4673	8
-----	1.38	3	------	----	------	----	1.37	vw	------	----
205	1.31	10	1.31	10	1.32	6	1.30	ms	1.3187	7
-----	1.26	3	------	----	------	----	------	----	------	----
1·0·10	1.25	5	1.24	2	1.25	6	1.24	vw–w	1.2515	3
-----	1.24	3	------	----	------	----	------	----	------	----
027	1.19	10	1.19	5	1.19	5	1.18	w–ms	1.1936	3
012	1.14	5	1.14	5	1.15	3	1.14	w	1.1467	2
122	1.12	5	1.12	10	1.12	3	1.11	w	1.1198	3
125	1.05	5	1.05	10	1.05	4	1.04	ms	1.0495	3
0·2·10	1.02	3	------	----	1.01	1	1.01	vw	1.0146	1
030	1.00	3	------	----	1.00	2	0.994	ms	1.0011	2
217	0.979	5	0.981	2	0.982	3	.977	w	0.9833	2
1·1·12	.953	10	.953	5	.957	3	.950	ms	.9567	<1

Sodium Bromate, $NaBrO_3$ (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
2135	2250 1–0902 1–0874	2. 99 1. 78 2. 73	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Kolkmeijer, Bijvoet, and Karssen [2] 1920.	Copper	1.537 A
Vegard [3] 1922	Copper	

NBS sample. The sodium bromate was obtained from the Mallinckrodt Chemical Company. Spectrographic analysis of the sample showed the following impurities: 0.0001 to 0.001 percent each of aluminum, calcium, iron, and silicon.

The sample is colorless. The index of refraction is 1.611.

Interplanar spacings and intensity measurements. The d-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the d-spacings of the Kolkmeijer, Bijvoet, and Karssen pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	210	321	211
Kolkmeijer, Bijvoet, and Karssen	210	321	510
Vegard	321	210	422
Swanson, Gilfrich, and Ugrinic	210	321	110

Lattice constant. The structure of sodium bromate was determined by Dickinson and Goodhue [4] in 1921. The cubic lattice has the space group T^4–$P2_13$ with sodium chlorate-type structure and $4(NaBrO_3)$ per unit cell.

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

Lattice constants

		A
1920	Kolkmeijer, Bijvoet, and Karssen [2].	6.75
1921	Dickinson and Goodhue [4]	6.72
1922	Vegard [3]	6.73
1938	Hamilton [5]	6.72
1955	Swanson, Gilfrich, and Ugrinic	6.705 at 25° C.

The density of sodium bromate calculated from the NBS lattice constant is 3.325 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] N. H. Kolkmeijer, J. M. Bijvoet, and A. Karssen, Investigation by means of X-rays of the crystal-structure of sodium-chlorate and sodium-bromate, Proc. Acad. Sci. Amsterdam **23,** 644–653 (1920).

[3] L. Vegard, Die Lage der Atome in den optisch aktiven Kristallen $NaClO_3$ und $NaBrO_3$, Z. Physik. **12,** 289–303 (1922).

[4] R. G. Dickinson and E. A. Goodhue, The crystal structure of sodium chlorate and sodium bromate, J. Am. Chem. Soc. **43,** 2045–2055 (1921).

[5] J. E. Hamilton, The crystal structure of sodium bromate, Z. Krist. **100,** 104–110 (1938).

Sodium Bromate, $NaBrO_3$ (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1920 Kolkmeijer, Bijvoet, and Karssen Cu, 1.537 A			1922 Vegard Cu, 1.5405 A			1955 Swanson, Gilfrich, and Ugrinic 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*
110	4.76	40	6.73	4.87	mw	6.9	4.71	10	6.66	4.744	46	6.708
111	3.87	27	6.70	3.90	vw	6.8	3.85	50	6.67	3.873	39	6.709
200	3.35	13	6.70	3.38	mw	6.76	3.30	40	6.60	3.354	30	6.709
210	3.00	100	6.71	3.05	vs	6.82	3.05	70	6.82	3.000	100	6.707
211	2.74	53	6.71	2.74	w	6.71	2.79	50	6.83	2.739	40	6.708
221	2.23	20	6.69	2.23	vw	6.69	2.242	30	6.73	2.236	18	6.706
310	2.11	7	6.67	----	--	----	-----	--	----	2.121	6	6.708
311	2.01	20	6.67	----	--	----	2.015	30	6.68	2.022	14	6.707
222	1.93	7	6.69	----	--	----	1.934	30	6.70	1.936	7	6.706
320	1.85	7	6.67	----	--	----	1.874	30	6.76	1.860	8	6.707
321	1.78	83	6.66	1.80	vs	6.73	1.802	100	6.74	1.793	51	6.708
400	-----	--	----	1.68	vw	6.72	-----	--	----	1.677	3	6.708
410	1.62	7	6.68	----	--	----	1.633	25	6.73	1.627	7	6.710
411	1.57	7	6.66	----	--	----	-----	--	----	1.581	5	6.709
331	1.53	20	6.67	1.54	vw	6.71	1.542	25	6.72	1.539	7	6.709
420	1.498	7	6.69	----	--	----	-----	--	----	1.500	4	6.709
421	1.463	27	6.70	1.47	w	6.74	1.464	50	6.71	1.464	3	6.709
422	-----	--	----	1.38	vw	6.76	1.376	15	6.74	1.369	2	6.708
510	1.316	27	6.71	1.32	s	6.73	1.321	70	6.74	1.316	13	6.708
511	1.290	7	6.70	----	--	----	1.292	40	6.71	1.291	7	6.707
520	1.248	13	6.72	----	--	----	1.248	50	6.72	1.246	8	6.707
521	1.222	7	6.69	----	--	----	1.227	20	6.72	1.225	3	6.708
440	-----	--	----	----	--	----	-----	--	----	1.186	1	6.708
522	-----	--	----	----	--	----	1.169	15	6.72	1.168	3	6.707
530	-----	--	----	----	--	----	-----	--	----	1.150	3	6.707
531	-----	--	----	----	--	----	-----	--	----	1.134	2	6.708
600	1.112	7	6.67	----	--	----	1.121	20	6.73	1.118	2	6.707
611	1.084	7	6.68	----	--	----	1.091	30	6.73	1.088	4	6.707
620	-----	--	----	----	--	----	-----	--	----	1.061	1	6.708
621	1.044	13	6.68	----	--	----	1.051	70	6.73	1.048	5	6.708
541	-----	--	----	----	--	----	-----	--	----	1.035	2	6.709
533	-----	--	----	----	--	----	-----	--	----	1.023	1	6.708
630	-----	--	----	----	--	----	-----	--	----	1.0000	3	6.708
631	-----	--	----	----	--	----	-----	--	----	0.9889	2	6.707
632	-----	--	----	----	--	----	-----	--	----	.9582	4	6.707
710	-----	--	----	----	--	----	-----	--	----	.9485	4	6.707
711	-----	--	----	----	--	----	-----	--	----	.9392	5	6.707
640	-----	--	----	----	--	----	-----	--	----	.9300	3	6.706
720	-----	--	----	----	--	----	-----	--	----	.9210	2	6.705
721	-----	--	----	----	--	----	-----	--	----	.9125	4	6.706
642	-----	--	----	----	--	----	-----	--	----	.8961	2	6.706
722	-----	--	----	----	--	----	-----	--	----	.8882	2	6.706
730	-----	--	----	----	--	----	-----	--	----	.8803	1	6.704
731	-----	--	----	----	--	----	-----	--	----	.8726	6	6.703
650	-----	--	----	----	--	----	-----	--	----	.8584	2	6.704
732	-----	--	----	----	--	----	-----	--	----	.8515	2	6.705
810	-----	--	----	----	--	----	-----	--	----	.8317	6	6.705
811	-----	--	----	----	--	----	-----	--	----	.8254	4	6.706
733	-----	--	----	----	--	----	-----	--	----	.8192	2	6.706
820	-----	--	----	----	--	----	-----	--	----	.8131	1	6.705
821	-----	--	----	----	--	----	-----	--	----	.8072	3	6.705
653	-----	--	----	----	--	----	-----	--	----	.8014	3	6.705
822	-----	--	----	----	--	----	-----	--	----	.7902	4	6.705
830	-----	--	----	----	--	----	-----	--	----	.7847	2	6.705
831	-----	--	----	----	--	----	-----	--	----	.7795	7	6.705
Average value of last five lines-----------			6.69	----	--	6.73	-----	--	6.73	-----	--	6.705

Strontium Fluoride, SrF_2 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
1597	1528 1–0650 1–0644	3.37 2.06 1.75	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
van Arkel [2] 1924	Copper	

NBS sample. The strontium fluoride was prepared at the NBS from strontium carbonate and hydrofluoric acid. It was heated at 1,000° C. for 10 minutes. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent each of barium, calcium, and silicon; 0.001 to 0.01 percent each of aluminum, boron, magnesium, and lead; and 0.0001 to 0.001 percent each of copper, iron, and manganese.

The sample is colorless. The refractive index is 1.435.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units, and the *d*-spacings of the van Arkel pattern were calculated from Bragg angle data. The van Arkel pattern did not include intensity values.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	220	311
Swanson, Gilfrich, and Ugrinic	111	220	311

Lattice constant. The structure of strontium fluoride was determined by van Arkel [2] in 1924. The cubic lattice has the space group O_h^5—Fm3m with calcium fluoride-type structure and 4(SrF_2) per unit cell.

Strontium Fluoride, SrF_2 (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1929 van Arkel Cu, 1.5418 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	3.38	100	5.85	3.35	--	5.80	3.352	100	5.806
200	2.92	5	5.84	-------	--	-------	2.900	25	5.801
220	2.06	100	5.83	2.07	--	5.85	2.0508	80	5.800
311	1.75	50	5.80	1.76	--	5.84	1.7486	52	5.7995
222	1.68	5	5.82	1.70	--	5.89	1.6743	5	5.8000
400	1.458	10	5.83	1.47	--	5.88	1.4499	15	5.7996
331	1.339	15	5.84	1.34	--	5.84	1.3303	21	5.7986
420	1.305	5	5.84	1.31	--	5.86	1.2966	10	5.7986
422	1.191	20	5.83	1.19	--	5.83	1.1840	24	5.8004
511	1.123	15	5.84	1.13	--	5.87	1.1164	16	5.8010
440	1.031	5	5.83	1.03	--	5.83	1.0253	7	5, 8000
531	0.981	10	5.80	0.991	--	5.86	0.9803	14	5, 7995
600	--------	--	--------	.978	--	5.87	.9666	7	5.7996
620	--------	--	--------	.927	--	5.86	.9170	10	5.7996
533	--------	--	--------	.896	--	5.88	.8844	7	5.7994
622	--------	--	--------	.883	--	5.86	.8743	4	5.7994
444	--------	--	--------	.846	--	5.86	.8371	3	5.7996
711	--------	--	--------	.820	--	5.86	.8121	15	5.7996
640	--------	--	--------	.811	--	5.85	.8043	4	5.7999
Average value of last five lines			5.83	-------	--	5.86	--------	----	5.7996

A group of unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS valve.

Lattice constants

1924	van Arkel [2]	5.87
1926	Goldschmidt, Barth, Lunde, and Zachariasen [3].	5.81
1927	Thilo [4]	5.82
1930	Rumpf [5]	5.793
1933	Schumann [6]	5.796 at 18° C.
1939	Zintl and Udgård [7]	5.861
1955	Swanson, Gilfrich, and Ugrinic.	5.7996 at 26° C.

The density of strontium fluoride calculated from the NBS lattice constant is 4.277 at 26° 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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[4] F. Thilo, Röntgenographische Untersuchung und eutropische Beziehungen der Fluoride der Erdalkalireihe, Z. Krist. **65**, 720–722 (1927).

[5] E. Rumpf, Über die Mischkristallreihe CaF_2–SrF_2, Z. physik. Chem. (B) **7**, 148–154 (1930).

[6] H. Schumann, Zur Dimorphie des Bleifluorides, Zentr. Mineral. Geol. **1933A**, 122–132 (1933).

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Strontium Oxide, SrO (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
2173	2210 1–0892 1–0886	2.97 2.58 1.82	Molybdenum.	Hanawalt, Rinn, and Frevel, Dow Chemical Company.

Additional published patterns

Source	Radiation	Wave-length
Gerlach [1] 1922	Copper	1.5393

NBS sample. The strontium oxide was obtained from the City Chemical Company, New York. It was heated to 1,150° C for 1 hour. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent of barium; 0.001 to 0.01 percent each of calcium and lithium; and 0.0001 to 0.001 percent each of aluminum, potassium, manganese, and sodium.

The sample is colorless. The index of refraction could not be determined as the surface of the sample grains reacted with the index liquids.

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units, and the *d*-spacings of the Gerlach pattern were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	200	220
Gerlach	200	220	311
Swanson, Gilfrich, and Ugrinic	200	111	220

Lattice constant. The structure of strontium oxide was determined by Gerlach [1] in 1922. The cubic lattice has the space group O_h^5-Fm3m with sodium chloride-type structure, and 4(SrO) per unit cell.

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

Lattice constants

		A
1922	Gerlach [1]	5.114
1927	Goldschmidt [2]	5.156
1928	Wilson [3]	5.083
1933	Burgers [4]	5.154
1942	Huber and Wagener [5]	5.15
1955	Swanson, Gilfrich, and Ugrinic	5.1602 at 25° C

The density of strontium oxide calculated from the NBS lattice constant is 5.008 at 25° C.

Strontium Oxide, SrO (cubic)

hkl	Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1922 Gerlach Cu, 1.542 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	2. 98	100	5. 16	--------	--	--------	2. 980	90	5. 161
200	2. 59	86	5. 18	2. 62	s	5. 24	2. 581	100	5. 162
220	1. 82	71	5. 15	1. 81	s	5. 10	1. 825	80	5. 162
311	1. 55	43	5. 14	1. 54	s	5. 12	1. 556	51	5. 161
222	1. 49	14	5. 16	1. 48	mw	5. 11	1. 490	26	5. 161
400	1. 29	14	5. 16	1. 278	mw	5. 112	1. 2901	13	5. 1604
331	1. 18	29	5. 14	1. 174	mw	5. 117	1. 1841	20	5. 1614
420	1. 15	14	5. 14	1. 148	ms	5. 134	1. 1540	28	5. 1608
422	1. 05	29	5. 14	1. 048	ms	5. 134	1. 0535	20	5. 1611
511	--------	--	--------	0. 989	ms	5. 140	0. 9932	15	5. 1608
440	--------	--	--------	. 908	mw	5. 138	. 9122	10	5. 1602
531	--------	--	--------	. 870	s	5. 144	. 8723	20	5. 1606
600	--------	--	--------	. 858	s	5. 146	. 8600	18	5. 1600
620	--------	--	--------	. 815	s	5. 154	. 8159	18	5. 1602
533	--------	--	--------	--------	--	--------	. 7869	9	5. 1600
Average value of last five lines			5. 15	--------	--	5. 144	--------	--	5. 1602

References

[1] W. Gerlach, Die Gitterstruktur der Erdalkalioxyde, Z. Physik. **9,** 184–192 (1922).

[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).

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Thallium Chloroplatinate, Tl_2PtCl_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The thallium chloroplatinate was prepared at the NBS from thallium nitrate and chloroplatinic acid. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent each of sodium and nickel; 0.001 to 0.01 percent each of aluminum, iron, lead, and silicon; and 0.0001 to 0.001 percent each of calcium and magnesium.

The sample has an orange color. The index of refraction is too high to be determined by the usual liquid grain immersion method.

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

Pattern	1	2	3
Swanson, Gilfrich, and Ugrinic	220	400	111

Lattice constant. The structure of thallium chloroplatinate was determined by Engel [1] in 1934. The cubic lattice has the space group O_h^5-Fm3m with potassium chloroplatinate-type structure and $4(Tl_2PtCl_6)$ per unit cell.

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

Lattice constants

		A
1934	Engel [1]	9.775
1955	Swanson, Gilfrich, and Ugrinic	9.779 at 25° C.

The density of thallium chloroplatinate calculated from the NBS lattice constant is 5.800 at 25° C.

Thallium Chloroplatinate, Tl_2PtCl_6 (cubic)

hkl	1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 25 °C.		
	d	*I*	*a*
	A		*A*
111	5. 65	42	9. 79
200	4. 90	8	9. 79
220	3. 46	100	9. 78
331	2. 95	19	9. 78
222	2. 82	29	9. 78
400	2. 44	45	9. 78
331	2. 25	8	9. 80
420	2. 192	2	9. 80
422	1. 996	36	9. 78
511	1. 883	8	9. 78
440	1. 729	25	9. 78
531	1. 653	7	9. 78
600	1. 631	1	9. 79
620	1. 5466	11	9. 782
533	1. 4914	3	9. 780
622	1. 4746	5	9. 781
444	1. 4114	6	9. 778
711	1. 3694	3	9. 780
642	1. 3065	10	9. 777
731	1. 2732	3	9. 780
800	1. 2221	3	9. 777
733	1. 1952	1	9. 783
822	1. 1522	4	9. 777
751	1. 1292	2	9. 779
662	1. 1217	1	9. 779
840	1. 0933	5	9. 779
911	1. 0733	<1	9. 778
664	1. 0426	1	9. 780
931	1. 0249	<1	9. 777
844	0. 9981	2	9. 779
933	. 9829	1	9. 780
10·2·0	. 9589	3	9. 779
951	. 9453	2	9. 778
953	. 9117	1	9. 777
10·4·2	. 8926	1	9. 778
11·1·1	. 8816	<1	9. 777
880	. 8643	<1	9. 778
11·3·1	. 8542	1	9. 777
10·6·0	. 8385	2	9. 778
11·3·3	. 8296	<1	9. 781
12·0·0	. 8148	3	9. 778
11·5·1	. 8066	<1	9. 780
12·2·2	. 7931	4	9. 778
11·5·3	. 7854	2	9. 778
Average value of last five lines			9. 779

References

[1] G. Engel, Die Kristallstrukturen einiger Hexachlorosalze, Centr. Mineral. Geol. **1934A,** 285–286 (1934).

Tin (IV) Iodide, SnI_4 (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
-----	3369	2.16	Copper	Ott [1] 1926.
	3–0966	1.25		
	3–0966	3.05		
1395	1313	3.53	Molybdenum.	Hanawalt, Rinn, and Frevel [2] 1938.
	1–0565	2.16		
	1–0557	1.84		

Additional published patterns. None.

NBS sample. The tin iodide was obtained from the City Chemical Company, New York. Spectrographic analysis of the sample showed the following impurities: 0.001 to 0.01 percent each of silver, aluminum, iron, lead, and silicon; and 0.0001 to 0.001 percent each of calcium, copper, and magnesium.

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

Interplanar spacings and intensity measurements. The *d*-spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the *d*-spacings of Ott were calculated from Bragg angle data.

The three strongest lines for each of the patterns are as follows:

Pattern	1	2	3
Ott	400	622	662
Hanawalt, Rinn, and Frevel	222	440	622
Swanson, Gilfrich, and Ugrinic	222	440	400

Lattice constant. The structure of tin iodide was determined by Dickinson [3] in 1923. The cubic lattice has the space group T_h^6–Pa3 with 8(SnI_4) per unit cell. Tin iodide has been used as a structure type.

Several unit-cell measurements have been converted from kX to angstrom units and the values of Ott and of Mark and Weissenberg [4] have been doubled for comparison with the NBS value.

Lattice constants

		A
1923	Mark and Weissenberg [4]	12.10
1923	Dickinson [3]	12.25
1926	Ott [1]	12.26
1955	Swanson, Gilfrich, and Ugrinic	12.273 at 26° C.

The density of tin iodide calculated from the NBS lattice constant is 4.500 at 26° C.

References

[1] H. Ott, Die Strukturen von MnO, MnS, AgF, NiS, SnI_4, $SrCl_2$, BaF_2; Präzisionsmessungen einiger Alkalihalogenide, Z. Krist. **63,** 222–235 (1926).

[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).

[3] R. G. Dickinson, The crystal structure of tin tetraiodide, J. Am. Chem. Soc. **45,** 958–962 (1923).

[4] H. Mark and K. Weissenberg, Röntgenographische Bestimmung der Struktur des Harnstoffs und des Zinntetrajodids, Z. Physik. **16,** 1–22 (1923).

Tin (IV) Iodide, SnI_4 (cubic)

hkl	1926 Ott Cu, 1.5418 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1955 Swanson, Gilfrich, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	-------	--	-------	6. 9	10	12	7. 09	3	12. 27
102	-------	--	-------	5. 5	27	12	5. 49	10	12. 27
211	-------	--	-------	5. 0	10	12	5. 012	15	12. 277
222	3. 52	m	12. 1	3. 54	100	12. 3	3. 543	100	12. 275
302	-------	--	-------	--------	--	--------	3. 404	5	12. 272
321	-------	--	-------	3. 29	3	12. 3	3. 280	5	12. 274
400	3. 04	s	12. 2	3. 06	23	12. 2	3. 070	32	12. 280
331	-------	--	-------	2. 81	3	12. 2	2. 816	3	12. 274
421	-------	--	-------	2. 66	3	12. 2	2. 678	6	12. 273
332	-------	--	-------	--------	--	--------	2. 617	5	12. 273
502	-------	--	-------	2. 27	3	12. 2	2. 279	5	12. 272
521	-------	--	-------	--------	--	--------	2. 241	4	12. 276
440	2. 16	vs	12. 2	2. 16	50	12. 2	2. 1701	41	12. 276
622	1. 85	s	12. 3	1. 84	33	12. 2	1. 8503	26	12. 274
631	-------	--	-------	--------	--	--------	1. 8097	6	12. 274
444	1. 77	vw	12. 3	1. 76	3	12. 2	1. 7717	2	12. 275
702	-------	--	-------	--------	--	--------	1. 6862	2	12. 276
721	-------	--	-------	1. 66	3	12. 2	1. 6701	<1	12. 273
732	-------	--	-------	1. 56	3	12. 3	1. 5587	5	12. 273
800	1. 53	vw	12. 2	1. 53	5	12. 2	1. 5345	11	12. 276
662	1. 41	s	12. 3	1. 405	10	12. 25	1. 4074	3	12. 269
832	-------	--	-------	--------	--	--------	1. 3983	2	12. 272
840	1. 37	mw	12. 3	1. 371	3	12. 26	1. 3720	4	12. 272
844	1. 25	vs	12. 2	1. 251	7	12. 26	1. 2528	6	12. 275
10·2·2	1. 18	s	12. 3	1. 180	5	12. 26	1. 1807	3	12. 270
10·3·1	-------	--	-------	--------	--	--------	1. 1702	<1	12. 273
-------	1. 09	w	-------	--------	--	--------	--------	--	--------
10·6·2	1. 04 ([a])	s	12. 3	--------	--	--------	1. 0374	3	12. 275
Average value of last five lines			12. 3	--------	--	12. 26	--------	--	12. 273

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[a] Four additional lines omitted.

Zinc Cyanide $Zn(CN)_2$ (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
926	0971 1-0431 1-0412	4.19 2.40 2.08	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
1906	1866 1-0782 1-0788	3.12 4.68 2.30	Molybdenum.	New Jersey Zinc Co.

The pattern of the New Jersey Zinc Company on ASTM card 1-0788 is for zinc cyanamide, and not zinc cyanide as indicated on the card.

The ASTM card for Hanawalt, Rinn, and Frevel states erroneously that zinc cyanide is orthorhombic.

Additional published patterns. None.

NBS sample. The zinc cyanide was obtained from the City Chemical Company of New York. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, cadmium, copper, iron, lead, and silicon; and 0.001 to 0.01 percent each of magnesium and manganese.

The sample is colorless. The refractive index is approximately 1.47, the particle size of the sample being too fine to make an exact determination.

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

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	110	211	220
Swanson, Gilfrich, and Ugrinic	110	211	111

Lattice constant. The structure of zinc cyanide was determined by Zhdanov [2] in 1941. The cubic lattice has the space group T_d^1–$P\bar{4}3m$ with $2(Zn(CN)_2)$ per unit cell.

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

Lattice constants

		A
1941	Zhdanov [2]	5.90
1955	Swanson, Gilfrich, and Ugrinic	5.905 at 25° C

The density of zinc cyanide calculated from the NBS lattice constant is 1.894 at 25° C.

Zinc Cyanide, $Zn(CN)_2$ (cubic)

hkl	1938			1955		
	Hanawalt, Rinn, and Frevel			Swanson, Gilfrich, and Ugrinic		
	Mo, 0.7107 A			Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
110	4.20	100	5.94	4.178	100	5.908
111	3.41	13	5.91	3.410	25	5.906
200	2.96	4	5.92	2.953	5	5.906
211	2.40	40	5.88	2.411	35	5.906
220	2.08	27	5.88	2.087	22	5.904
300	-----	--	-----	1.968	2	5.903
310	1.86	11	5.88	1.867	9	5.904
311	-----	--	-----	1.780	1	5.903
222	1.70	1	5.89	1.704	3	5.905
321	1.57	20	5.87	1.579	17	5.907
400	1.473	1	5.892	1.476	2	5.904
411	1.393	7	5.910	1.392	6	5.907
420	1.318	3	5.894	1.320	3	5.904
332	1.258	1	5.900	1.259	1	5.907
422	1.204	1	5.898	1.205	2	5.905
510	1.159	3	5.910	1.158	3	5.904
521	-----	--	-----	1.078	<1	5.903
611	-----	--	-----	0.958	1	5.906
541	-----	--	-----	.911	2	5.906
Average value of last five lines			5.902	------	--	5.905

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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).

[2] H. S. Zhdanov, The crystalline structure of Zn $(CN)_2$ Compt. rend. acad. sci. U. R. S. S. **31,** 352–354 (1941).

CUMULATIVE INDEX TO VOLUMES I, II, III, IV, AND V [6]

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[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.

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