NBS CIRCULAR 539

VOLUME IV

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

Standard X-ray Diffraction Powder Patterns

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Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, Ruth K. Fuyat, and George M. Ugrinic

National Bureau of Standards Circular 539

Volume IV, Issued March 1, 1955

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5. Halides and halide hydrates—Continued

ERRATA

Vol. I. Page 51, table 27, Swanson and Tatge pattern. The value for the *d*-spacing at 1.303 should read 1.503.

Vol. II. Page 33, second sentence in text for uranium dioxide should begin by reading: Chemical analysis at the NBS showed 88.0 percent of uranium.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. IV.—Data for 42 Inorganic Substances

Howard E. Swanson, Ruth K. Fuyat,[1] and George M. Ugrinic

Forty-two standard X-ray diffraction powder patterns are presented in revision of the ninety-five corresponding patterns in the ASTM card file, a system for the identification of unknown crystalline materials based on the three strongest reflections of each material or structurally distinct phase. Patterns for seven compounds not represented in the file are also included. A comparison is made between 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-two substances: α-Fe, Ru, Ba, Os, Ir, α-MnS (alabandite). CuS (covellite), CdS (greenockite), HgS (cinnabar), HgS (metacinnabar), Bi_2S_3, α-Ga_2O_3, Nd_2O_3, PdO, SnO, LiBr, NaI, MgF_2, CuCl, CuBr, CuI, $SrCl_2$, RbCl, RbI, AgCl (cerargyrite), AgBr, CsI, HgI, TlCl, orthorhombic TlI, BiOCl (bismoclite), NH_4I, $SrCl_2 \cdot 6H_2O$, $SrBr_2 \cdot 6H_2O$, $Ag_7O_8NO_3$, $NaNO_2$, $NH_4H_2PO_4$, $CaSO_4$, (anhydrite), $ZrSiO_4$ (zircon), AlSb, and InSb.

1. INTRODUCTION

The National Bureau of Standards 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 fourth in a series[3] of standard powder diffraction patterns, data for 5 elements, 35 inorganic compounds, and 2 intermetallic compounds. These patterns are recommended to replace 95 cards now in the file. Seven compounds, gallium oxide, neodymium oxide, strontium chloride, thallium iodide, silver oxynitrate, aluminum antimony, and indium antimony, 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, 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. The data for the various substances are grouped according to their chemical nature as follows: Elements, sulfides, oxides, halides and halide hydrates, nitrates and nitrites, phosphates, sulfates silicates, and intermetallic compounds, and within each group according to increasing atomic number.

ASTM cards. Each section of this Circular, devoted to one substance, 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 second supplement.

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. A phase-purity check was made on the nonopaque materials during the refractive-index determination. Another excellent check on phase purity was provided by the X-ray pattern itself because it was indexed by comparison with theoretical *d*-values.

The quality of most of the patterns was greatly improved by appropriate annealing procedures. The majority of the samples that were too coarse for X-ray analysis could be reduced to the proper

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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, and the British Institute of Physics. 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; and 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.

size and then annealed to remove the strain caused by grinding or filing.

At least two intensity patterns were prepared to check reproducibility of measured values. The grain sizes of samples used were less than 25 microns. A flat piece of glass was held temporarily over the face of an open cell while the 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 used for exposure to the X-ray beam. For a few powder samples that did not flow readily or were prone to orient badly, approximately 50 percent finely ground silica-gel was added as diluent. The intensity values of each pattern were measured as peak height above background and were expressed as percentages of the strongest line.

Separate 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, whose lattice constant at 25° C is 3.1648 A, as determined by Jette and Foote [1] [4]. All of the NBS patterns were made by using copper $K_{\alpha 1}$ radiation having a wavelength of 1.5405 A.

Interplanar spacing and intensity measurements. Interplanar spacing data presented in the tables were converted to angstroms as internationally defined in 1946 [2]. The conversions were from Bragg angle data, from *d*-spacings in kX units, using the factor 1.00202, or from *d*-spacings with specifically stated wavelengths other than kX. In each case the type of conversion made was indicated. The wavelength values in the the tables of *d*-spacings and intensities are given in angstroms, whereas the values listed under the first section of the reports, ASTM cards, are the original values taken from the literature. The tables of patterns contain data from the original literature except in those instances where there is no reference other than an ASTM card.

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 particular 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. Indexing of the noncubic patterns was accomplished by comparing the NBS *d*-spacings with theoretical values of all possible Miller indices of a particular cell calculated with the aid of IBM punched card machines. The unit cells used for these calculations were obtained either through a review of the literature or with an estimated cell based on partial indexing of the NBS pattern. The noncubic indexing as it appears in the tables 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.

The intensities of the strongest lines are of particular importance, because the ASTM card-file system of identification depends upon comparing the three strongest lines of an unknown X-ray pattern with those on the file cards, which are arranged according to their first, second, and third, strongest lines, respectively. Therefore, a table of the three strongest lines of each pattern is listed for comparison with the NBS values.

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 an IBM-Card Program Calculator.

The conversion of published unit-cell data to angstroms followed the same pattern as that used for the *d*-spacings. The unit-cell dimensions were converted to 25° or 26° C for comparison with the NBS values if the temperature of measurement and the thermal expansion were known. The coefficient of linear thermal expansion as used is defined as the change in length per unit length per degree Celsius 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 invalid.

The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter, and the refractive-index measurements were made in white light by grain-immersion methods, using oils standardized in sodium light.

References

[1] E. R. Jette and F. Foote, Precision determination of lattice constants, J. Chem. Phys. **3**, 605–16 (1935).

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

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

2. ELEMENTS

Alpha-**Iron, α-Fe (cubic)**

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
3347	3539 1-1252 1-1252	2.05 1.16 1.43	Tungsten, 0.212 A.	Hull [1] 1917.
3381	3591 1-1269 1-1262	2.03 1.17 0.91	Molybdenum	Davey [2] 1925.
-----	3592 3-1056 3-1050	2.02 1.17	Iron, 1.93 A.	Jung [3] 1927.
3399	3590 1-1268 1-1267	2.01 1.17 1.43	Molybdenum	Hanawalt, Rinn, and Frevel [4] 1938.

The Hull pattern was made by using tungsten radiation rather than molybdenum as the ASTM card states.

Additional published patterns

Source	Radiation	Wave-length
		A
Wever [5] 1921	Iron	-------
Westgren and Lindh [6] 1921	Iron	1.932
Eisenhut and Kaupp [7] 1928	Molybdenum	-------

NBS sample. The iron used for the NBS sample was an exceptionally pure rolled sheet prepared by G. A. Moore of the NBS by a method described in the Journal of Metals [8]. The sample was annealed at 1,100° C for 3 days in a hydrogen atmosphere and slowly cooled in an atmosphere of helium. The impurities reported are less than 0.0013 percent of total foreign metals and about the same order of magnitude of nonmetals, including carbon.

Because the iron pattern contains so few lines, each one was scanned separately at very low speed where 1-degree increments of 2θ were equal to 4 inches of chart paper. The *d*-spacings for iron were corrected by comparison with a similarly prepared pattern of silver made by using an annealed bar of high purity and the unit cell, 4.08611 A, at 25° C, as determined by Jette and Foote [9].

Interplanar spacings and intensity measurements. The Hull, the Davey, and the Hanawalt, Rinn, and Frevel *d*-spacings were converted from kX to angstrom units, the Jung, the Wever, the Westgren, and Lindh, and the Eisenhut and Kaupp *d*-spacings were calculated from Bragg angle data.

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

	1	2	3
Hull	110	211	200
Davey	110	211	310
Jung	110	200	211
Hanawalt, Rinn, and Frevel	110	211	200
Wever	211	220	110
Westgren and Lindh	110	211	220
Eisenhut and Kaupp	110	211	----
Swanson, Fuyat, and Ugrinic	110	211	200

Lattice constant. The structure was determined by Davey [10] in 1924. The space group is O_h^9-Im3m with tungsten-type structure and 2 (Fe) per unit cell.

A group of unit-cell values containing four or more decimal places were converted from kX to angstrom units and from the temperatures indicated in parentheses to 25° C for comparison with the NBS values. The linear coefficient of expansion in the room-temperature range is 11.7×10^{-6} according to Owen and Yates [11]. A large number of less-accurate unit-cell determinations were omitted, as they contributed little in the way of a comparison.

Lattice constants

		A
1925	Blake [12]	2.8661
1929	Mayer [13]	2.86693 at 25° C (22° C)
1931	Van Arkel and Burgers [14]	2.8672
1932	Bradley and Jay [15]	2.8663
1933	Esser and Müller [16]	2.8669
1933	Owen and Yates [11]	2.86675 at 25° C (18° C)
1935	Jette and Foote [9]	2.86626 at 25° C
1936	Straumanis and Ieviņš [17]	2.8664 at 25° C (22° C)
1937	Montoro [18]	2.86665 at 25° C (20° C)
1941	Van Bergen [19]	2.86651
1941	Lu and Chang [20]	2.8665 at 25° C (20° C)
1948	Thomas [21]	2.86659 at 25° C (20° C)
1949	Kochanovska [22]	2.8667 at 25° C (22° C)
1953	Swanson, Fuyat, and Ugrinic.	2.8664 at 25° C

The density of iron calculated from the NBS lattice constant, assuming the atomic weight of iron to be 55.85, is 7.874 at 25° C.

Alpha-**Iron,** α-**Fe** (cubic)

hkl	1917 Hull W, 0.212 A			1926 Davey Mo, 0.709 A			1927 Jung Fe, 1.93597 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
110	2. 05	100	2. 90	2. 02	100	2. 86	2. 037	vs	2. 881	2. 01	100	2. 84
200	1. 43	46	2. 86	1. 432	50	2. 864	1. 437	vs	2. 874	1. 431	15	2. 862
211	1. 16	54	2. 84	1. 169	80	2. 865	1. 174	vs	2. 876	1. 168	38	2. 861
220	1. 007	24	2. 849	1. 012	50	2. 863	---	---	---	1. 012	10	2. 862
310	0. 912	18	2. 884	0. 906	60	2. 865	---	---	---	0. 906	8	2. 865
222	. 825	16	2. 857	. 828	20	2. 867	---	---	---	. 827	3	2. 865
------	. 759	22	---	. 766	60	---	---	---	---	. 766	10	-------
------	---	---	---	. 715	10	---	---	---	---	---	---	-------
------	. 666	12	---	. 674	30	---	---	---	---	. 677	3	-------
------	. 634	3	---	. 639	20	---	---	---	---	---	---	-------
------	. 601	2	---	. 609	20	---	---	---	---	---	---	-------
------	. 573	2	---	. 583	20	---	------	---	---	---	---	-------
------	. 556	10	---	---	---	---	---	---	---	---	---	-------
------	. 523	2	---	---	---	---	---	---	---	---	---	-------
Average unit-cell vlaue for last five lines------			2. 860	---	---	2. 865	---	---	2. 877	---	---	2. 863

hkl	1921 Wever Fe, 1.93597 A			1921 Westgren and Lindh Fe, 1.93597 A			1928 Eisenhut and Kaupp Mo, 0.709 A			1953 Swanson, Fuyat, 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	2. 016	m	2. 851	1. 98	s	2. 80	2. 042	m	2. 888	2. 0268	100	2. 8663
200	1. 427	w	2. 854	1. 41	m	2. 82	1. 424	w	2. 848	1. 4332	19	2. 8664
211	1. 166	vs	2. 856	1. 16	s	2. 84	1. 163	mw	2. 849	1. 1702	30	2. 8664
220	1. 011	s	2. 860	1. 01	s	2. 86	1. 007	w	2. 848	1. 0134	9	2. 8663
310	---	---	---	---	--	---	0. 905	w	2. 862	0. 9064	12	2. 8663
222	---	---	---	---	--	---	---	---	---	. 8275	6	2. 8665
------	---	---	---	---	--	---	. 765	mw	---	----	---	-------
------	---	---	---	---	--	---	---	---	---	----	---	-------
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------	---	---	---	---	--	---	---	---	---	----	---	-------
Average unit-cell value for last five lines------			2. 855	---	--	2. 83	---	---	2. 859	----	---	[a] 2. 8664

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[a] An average of six lines.

References

[1] A. W. Hull, A new method of X-ray crystal analysis, Phys. Rev. **10**, 661–96 (1917).

[2] W. P. Davey, Präzisionsmessungen der Gitterkonstanten verbreiteter Metalle, Z. Krist. **63**, 316–7 (1926).

[3] A. O. Jung, Die Raumgitterstruktur und Gitterkonstanten des künstlichen und natürlichen Nickeleisens, Z. Krist. **65**, 309–34 (1927).

[4] 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).

[5] F. Wever, Die Atomanordnung des Eisens in austenitischen Stahlen, Mitt. Kaiser-Wilhelm-Inst. Eisenforsch. Düsseldorf **3**, 45–56 (1921).

[6] A. Westgren and A. E. Lindh, Zum Kristallbau des Eisens und Stahls, Z. physik. Chem. **98**, 181–210 (1921).

[7] O. Eisenhut and E. Kaupp, Röntgenographische Untersuchungen über Eisenkatalysatoren für die Ammoniaksynthese, Z. physik. Chem. **133**, 456–471 (1928).

[8] G. A. Moore, Preparation of metallic iron of high purity, J. Metals **5**, 1443–9 (1953).

[9] E. R. Jette and F. Foote, Precision determination of lattice constants, J. Chem. Phys. **3**, 605–16 (1935).

[10] W. P. Davey, Precision measurements of the lattice constants of pure metals, Phys. Rev. **23**, 292 (1924).

[11] E. A. Owen and E. L. Yates, Precision measurements of crystal parameters, Phil. Mag. **15**, 472–88 (1933).

[12] F. C. Blake, Precision X-ray measurements by the powder method, Phys. Rev. **26**, 60–70 (1925).

[13] G. Mayer, Die Gitterkonstante von reinem α-Eisen, Z. Krist. **70**, 383–384 (1929).

[14] A. E. van Arkel and W. G. Burgers, Eine zur Bestimmung von kleinen Änderungen in der Gitterkonstante des α-Eisens geeignete Röntgenstrahlung, Z. Metallkunde **23**, 149–151 (1931).

[15] A. J. Bradley and A. H. Jay, A method for deducing accurate values of the lattice spacing from X-ray powder photographs taken by the Debye-Scherrer method, Proc. Phys. Soc. (London) **44**, 563–79 (1932).

[16] H. Esser and G. Müller, Die Gitterkonstanten von reinem Eisen und Eisen-Kohlenstoff-Legierungen bei Temperaturen bis 1100° C, Arch. Eisenhüttenw. **7**, 265–268 (1933).

[17] M. Straumanis and A. Ieviņš, Präzisionsaufnahmen nach dem Verfahren von Debye und Scherrer, II, Z. Physik. **98**, 461–75 (1936).

[18] V. Montoro, Misure di precisione della costante reticolare del ferro, Merallurgia ital. **29**, 8–11 (1937).

[19] H. van Bergen, Präzisionsmessung von Gitterkonstanten mit einer Kompensations-methode II, Ann. Physik **39**, 553–72 (1941).

[20] S. S. Lu and Y. L. Chang, The accurate evaluation of lattice spacings from back-reflection powder photographs, Proc. Phys. Soc. (London) **53**, 517–28 (1941).

[21] D. E. Thomas, Precision measurements of crystal lattice parameters, J. Sci. Instr. **25**, 440–4 (1948).

[22] A. Kochanovska, Investigation of thermal dilatation of cubic metals, Physica **15**, 191–6 (1949).

Ruthenium, Ru (hexagonal)

ASTM cards

Old card numbers	New card numbers	New index lines	Radiation	Source
3360	3581	2.04	Molybdenum, 0.712A.	Hull [1] 1921.
	1–1265	1.34		
	1–1256	1.21		
II–2909	3585	2.04	------------	British Museum.
	2–1266	1.22	Copper	Levi and Haardt [2] 1926.
	2–1258	1.15		
3358	3557	2.04	Molybdenum	Hanawalt, Rinn and Frevel [3] 1938.
	1–1256	2.33		
	1–1253	2.13		

The Levi and Haardt pattern was made with copper radiation. The British Museum pattern was not available and therefore was not included in the table.

NBS sample. The ruthenium used for the NBS pattern was obtained from the Baker Chemical Co. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of boron and palladium; 0.001 to 0.01 percent each of aluminum, magnesium, and silicon; 0.0001 to 0.001 percent each of calcium, copper, iron, and lead; and less than 0.0001 percent of barium.

Interplanar spacings and intensity measurements. The *d*-spacings for the Levi and Haardt and the Barth and Lunde patterns were calculated from Bragg angle data; the *d*-spacings for the Hull and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units, and the Hull spacings were converted from Mo radiation of 0.71354 A to Mo K_{α_1} radiation, 0.70926 A.

Additional published patterns

Source	Radiation	Wavelength
Barth and Lunde [4] 1926	Copper	1.539A.

The Levi and Haardt pattern contains *d*-spacings at 1.227 A and 0.922 A, which are not permissible in the ruthenium structure.

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

	1	2	3
Hull	101	110	103
Levi and Haardt	101	211	114
Hanawalt, Rinn, and Frevel	101	100	002
Barth and Lunde	101	112	203
Swanson, Fuyat, and Ugrinic	101	100	002

Lattice constants. The structure was determined by Barth and Lunde [4] in 1926. The space group is D_{6h}^4-C6/mmc with magnesium-type structure and 2(Ru) per unit cell.

A group of unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	A
1921	Hull [1]	2. 691	4.279
1926	Levi and Haardt [2]	2. 685	4.270
1926	Barth and Lunde [4]	2. 700	4.282
1937	Owen and Roberts [5]	2. 70389	4.28168 at 20° C
1953	Swanson, Fuyat, and Ugrinic	2. 7058	4.2819 at 27° C

The density of ruthenium calculated from the NBS lattice constants is 12.438 at 27° C.

Ruthenium, Ru (hexagonal)

hkl	1921 Hull Mo, 0.709 A		1926 Levi and Haardt Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1926 Barth and Lunde Cu, 1.5405 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A , 27° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A	
100	2. 311	30	2. 252	28	2. 33	40	2. 343	30	2. 343	41
002	2. 156	3	2. 074	31	2. 13	30	2. 142	30	2. 142	37
101	2. 036	100	1. 979	100	2. 04	100	2. 051	100	2. 056	100
102	1. 569	20	1. 534	31	1. 57	25	1. 578	40	1. 5808	23
110	1. 341	50	1. 323	54	1. 348	25	1. 348	60	1. 3530	25
----	-----	-----	1. 227	11	-----	-----	-----	-----	------	-----
103	1. 209	50	1. 196	59	1. 215	30	1. 218	70	1. 2189	24
200	-----	-----	1. 151	13	1. 167	4	1. 169	10	1. 1715	5
112	1. 137	50	1. 125	75	1. 142	30	1. 142	80	1. 1434	26
201	1. 121	40	1. 111	59	1. 130	15	1. 128	70	1. 1299	20
004	-----	-----	1. 055	14	1. 071	3	1. 071	10	1. 0705	4
202	1. 022	5	1. 014	20	1. 027	4	1. 027	20	1. 0278	7
104	0. 966	10	0. 963	21	0. 973	4	0. 974	20	0. 9738	6
----	-----	-----	. 922	11	-----	-----	-----	-----	------	-----
203	. 901	20	. 898	59	. 907	10	. 905	80	. 9056	15
210	-----	-----	. 879	25	. 886	2	. 884	20	. 8857	6
211	. 863	30	. 861	98	. 869	20	-----	-----	. 8673	26
114	. 837	20	. 835	78	. 841	10	-----	-----	. 8395	18
212	. 815	3	-----	-----	. 820	4	-----	-----	. 8185	10
105	[a]. 802	5	-----	-----	[b]. 805	6	-----	-----	. 8043	15

[a] Three additional lines were omitted.
[b] Seven additional lines were omitted.

References

[1] A. W. Hull, X-ray crystal analysis of thirteen common metals, Phys. Rev. **17,** 571–88 (1921).

[2] G. R. Levi and R. Haardt, La struttura cristallina del rutenio e dell'osmio, Gazz. chim. ital. **56,** 369 (1926).

[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] T. Barth and G. Lunde, Die Gitterkonstanten der Platinmetalle, Silber, und Gold, Z. Physik. Chem. **121,** 78–102 (1926).

[5] E. A. Owen and E. W. Roberts, The crystal parameters of osmium and ruthenium at different temperatures, Z. Krist. **96A,** 497–498 (1937).

Barium, Ba (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1363	1318 1-0568 1-0543	3. 56 2. 05 1. 34	Molybdenum, K_α	King and Clark [1] 1929.
1382	1319 1-0569 1-0550	3. 54 2. 04 2. 51	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns

Source	Radiation	Wave-length
Ebert and Hartmann [3]	Copper	K_α

NBS sample. The barium used for the NBS pattern was obtained from the American Firstoline Corp. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of calcium, magnesium, sodium, silicon, and strontium; 0.001 to 0.01 percent each of aluminum, iron, and manganese; and 0.0001 to 0.001 percent of copper.

Interplanar spacings and intensity measurements. The d-spacings for the Ebert and Hartmann pattern were calculated from Bragg angle data; d-spacings for the King and Clark and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units.

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

	1	2	3
King and Clark	110	211	321
Hanawalt, Rinn, and Frevel	110	211	200
Ebert and Hartmann	321	411	510
Swanson, Fuyat, and Ugrinic	110	211	200

Lattice constant. The structure was determined by Clark, King, and Hyde [4] in 1928. The space group is O_h^9-Im3m with tungsten-type structure and 2(Ba) per unit cell.

Lattice constants

		A
1929	Ebert and Hartmann [3]	5. 02
1929	King and Clark [1]	5. 025
1941	Klemm and Mika [5]	5. 019
1953	Swanson, Fuyat, and Ugrinic	5. 025 at 26° C

The density of barium calculated from the NBS lattice constant is 3.595 at 26° C.

Barium, Ba (cubic)

hkl	1929 King and Clark Mo, 0.709A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709A			1929 Ebert and Hartmann Cu, 1.5405A			1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
110	3. 563	100	5. 039	3. 55	100	5. 02	3. 56	mw	5. 03	3. 55	100	5. 02
200	2. 515	20	5. 030	2. 52	50	5. 04	---	---	---	2. 513	20	5. 026
211	2. 054	70	5. 031	2. 04	100	5. 00	2. 04	ms	5. 02	2. 051	40	5. 024
220	1. 777	30	5. 026	1. 77	50	5. 01	1. 77	w	5. 04	1. 776	18	5. 023
310	1. 587	20	5. 019	1. 58	50	5. 00	1. 58	m	5. 01	1. 590	12	5. 028
222	1. 450	10	5. 023	1. 446	5	5. 009	1. 449	vw	5. 02	1. 451	5	5. 026
321	1. 342	40	5. 021	1. 343	44	5. 025	1. 341	vs	5. 02	1. 343	14	5. 025
411	1. 183	10	5. 019	1. 183	15	5. 019	1. 181	s	5. 01	1. 1852	5	5. 028
420	1. 123	7. 5	5. 022	1. 122	5	5. 018	1. 128	w	5. 04	1. 1236	4	5. 025
332	1. 071	10	5. 023	1. 068	3	5. 009	1. 072	mw	5. 03	1. 0717	3	5. 027
422	1. 025	10	5. 021	1. 024	3	5. 017	1. 025	w	5. 02	1. 0257	1	5. 025
510	0. 985	10	5. 023	0. 983	8	5. 012	0. 983	s	5. 01	0. 9856	6	5. 026
521	. 917	7. 5	5. 023	. 917	3	5. 023	---	---	---	. 9174	2	5. 025
530	. 862	5	5. 026	---	---	---	---	---	---	. 8615	8	5. 023
Average of last five lines			5. 023	---	---	5. 016	---	---	5. 02	---	---	5. 025

References

[1] A. J. King and G. L. Clark, The crystal structure of barium, J. Am. Chem. Soc. **51**, 1709–1711 (1929).

[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] F. Ebert and H. Hartmann, Die Kristallstruktur des Strontiums und Bariums, Z. anorg. u. allgem. Chem. **179**, 418–420 (1929).

[4] G. L. Clark, A. J. King, and J. F. Hyde, The crystal structures of the alkaline earth metals, Proc. Nat. Acad. Sci. U. S. **14**, 617–8 (1928).

[5] W. Klemm and G. Mika, Über das Verhalten der Erdalkalimetalle zueinander, Z. anorg. u. allgem. Chem. **248**, 155–166 (1941).

Osmium, Os (hexagonal)

ASTM cards

Old card number	New card number	New index lines	Radiation	Source
II–2879	3540 2–1252 2–1249	2. 06 1. 15 1. 22	Copper	Levi and Haardt [1] 1926.
3324	3473 1–1239 1–1245	2. 07 2. 36 2. 16	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns

Source	Radiation	Wavelength
Barth and Lunde [3] 1926	Copper	1.539A

NBS sample. The osmium used for the NBS sample was obtained from the Baker Chemical Co. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of iridium; 0.001 to 0.01 percent each of iron, magnesium, and silicon; and 0.0001 to 0.001 percent each of silver, aluminum, calcium, and copper.

Interplanar spacings and intensity measurements. The *d*-spacings for the Levi and Haardt and the Barth and Lunde patterns were calculated from Bragg angle data; the *d*-spacings for the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units. The Levi and Haardt pattern contains *d*-spacings at 1.251 A and 0.932 A, which are not possible in the osmium structure.

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

	1	2	3
Levi and Haardt	101	112	211
Barth and Lunde	211	101	203
Hanawalt, Rinn, and Frevel	101	100	002
Swanson, Fuyat, and Ugrinic	101	100	002

Lattice constants. The structure was determined by Barth and Lunde [3] in 1926. The space group is D^4_{6h}-C6/mmc with magnesium-type structure and 2(Os) per unit cell.

Several unit-cell values were converted from kX to angstrom units for comparison with the NBS values. The Owen and Roberts values were converted from 20° C to 26° C. The coefficient of thermal expansion near 50° C is 5.8×10^{-6} parallel to the *c*-axis and 4.0×10^{-6} perpendicular to it, according to Owen and Roberts [4].

Lattice constants

		a	*c*
		A	*A*
1921	Hull [5]	2. 719	4.33
1926	Levi and Haardt [1]	2. 719	4.325
1926	Barth and Lunde [3]	2. 730	4.323
1937	Owen and Roberts [4]	2. 7353	4.3191 at 26° C
1953	Swanson, Fuyat, and Ugrinic.	2. 7341	4.3197 at 26° C

The density of osmium calculated from the NBS lattice constants is 22.583 at 26° C.

Osmium, Os (hexagonal)

hkl	1926 Levi and Haardt Cu, 1.5405 A		1926 Barth and Lunde Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
100	2.31	31	2.367	20	2.36	20	2.367	34
002	2.11	38	2.163	20	2.16	15	2.160	33
101	2.03	100	2.072	90	2.07	100	2.076	100
102	1.569	37	1.601	30	1.59	10	1.595	18
110	1.348	64	1.364	40	1.366	13	1.3668	20
-------	1.251	7	-----	-----	-----	-----	------	-----
103	1.216	71	1.228	40	1.233	13	1.2300	20
200	1.171	14	1.182	10	1.180	3	1.1840	4
112	1.143	84	1.155	60	1.160	10	1.1551	21
201	1.129	66	1.139	50	1.146	8	1.1416	17
004	1.071	17	1.080	10	1.084	3	1.0799	3
202	1.029	22	1.037	20	1.041	3	1.0383	4
104	0.975	23	0.983	20	0.983	3	0.9827	4
-------	.932	13	-----	-----	-----	-----	------	-----
203	.908	52	.913	70	.917	4	.9145	10
210	.891	19	-----	30	-----	-----	.8949	3
211	.871	74	.874	100	.878	5	.8764	16
114	.843	56	-----	-----	-----	-----	.8474	11
212	-----	-----	-----	-----	-----	-----	.8268	6
105	-----	-----	-----	-----	-----	-----	.8116	9

References

[1] G. R. Levi and R. Haardt, La Struttura cristallina del rutenio e dell'osmio, Gazz. chim. ital. **56,** 369 (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] T. Barth and G. Lunde, Die Gitterkonstanten der Platinmetalle, Silber und Gold, Z. physik. Chem. **121,** 78–102 (1926).

[4] E. A. Owen and E. W. Roberts, The crystal parameters of osmium and ruthenium at different temperatures, Z. Krist. **69A,** 497–498 (1937).

[5] A. W. Hull, The crystal structures of Ti, Zr, Ce, Th, and Os, Phys. Rev. **18,** 88–89 (1921).

Iridium, Ir (cubic)

ASTM cards

Old card number	New card number	New index lines	Radiation	Source
3203	3366 1–1222 1–1216	2.19 1.35 1.15	Molybdenum 0.712A.	Hull [1] 1921.
II–2630	3332 2–1164 2–1155	2.21 1.15 1.91	Molybdenum	Wyckoff [2] 1924.
3186	3302 1–1204 1–1212	2.20 1.91 1.15	Molybdenum	Hanawalt, Rinn, and Frevel [3] 1938.

Additional published patterns

Source	Radiation	Wavelength
Barth and Lunde [4] 1925	Copper	1.539A

NBS sample. The iridium used for the NBS pattern was obtained from the Baker Chemical Co. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent of silicon; 0.0001 to 0.001 percent each of aluminum, calcium, and magnesium; and less than 0.0001 percent each of copper and iron.

Interplanar spacing and intensity measurements. The *d*-spacings for the Barth and Lunde pattern were calculated from Bragg angle data; the Hull, the Wyckoff, and the Hanawalt, Rinn, and Frevel *d*-spacings were converted from kX to angstrom units, and the Hull d-spacings were converted from Mo radiation at 0.713 A to Mo Kα_1 radiation at 0.709 A.

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

	1	2	3
Hull	111	220	311
Wyckoff	111	311	200
Hanawalt, Rinn, and Frevel	111	200	311
Barth and Lunde	111	311	200
Swanson, Fuyat, and Ugrinic	111	200	311

Lattice constant. The structure was determined by Hull [5] in 1920. The space group is O_h^5-Fm3m with copper-type structure and 4(Ir) per unit cell.

A group of unit-cell values were converted from kX to angstrom units for comparison with the NBS values, and the Owen and Yates value was converted from 18° C to 26° C. The coefficient of expansion in the room-temperature range is 6.5×10^{-6} according to Owen and Yates [6].

Lattice constants

		a
		A
1921	Hull [1]	3. 813
1923	Wyckoff [2]	3. 831
1926	Barth and Lunde [4]	3. 831
1933	Owen and Yates [6]	3. 8390 at 26° C
1953	Swanson, Fuyat, and Ugrinic	3. 8394 at 26° C

The density of iridium calculated from the NBS lattice constant is 22.661 at 26° C.

Iridium, Ir (cubic)

hkl	1921			1924			1938			1926			1953		
	Hull			Wyckoff			Hanawalt, Rinn, and Frevel			Barth and Lunde			Swanson, Fuyat, and Ugrinic		
	Mo, 0.709 A			Mo, 0.709 A			Mo, 0.709 A			Cu, 1.5405 A			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*
111	2. 18	100	3. 78	2. 22	100	3. 84	2. 20	100	3. 81	2. 208	100	3. 824	2. 2170	100	3. 8399
200	1. 90	50	3. 79	1. 92	60	3. 84	1. 91	50	3. 82	1. 914	90	3. 827	1. 9197	50	3. 8394
220	1. 34	100	3. 80	1. 360	60	3. 85	1. 355	28	3. 833	1. 353	90	3. 827	1. 3575	41	3. 8396
311	1. 15	100	3. 81	1. 151	80	3. 82	1. 155	36	3. 831	1. 153	100	3. 824	1. 1574	47	3. 8387
222	1. 09	25	3. 78	1. 108	20	3. 84	1. 106	8	3. 831	1. 104	50	3. 824	1. 1082	15	3. 8389
400	------	----	------	0. 9545	5	3. 82	------	----	------	0. 957	30	3. 827	0. 9598	10	3. 8392
331	0. 871	50	3. 80	. 8780	30	3. 827	0. 880	8	3. 836	. 878	50	3. 826	. 8808	39	3. 8393
420	. 846	12	3. 78	. 8561	30	3. 829	. 859	8	3. 842	. 856	50	3. 827	. 8586	39	3. 8398
422	. 775	----	3. 80	. 7804	20+	3. 823	. 784	4	3. 841	------	----	------	. 7838	45	3. 8397
511	. 730	----	3. 79	. 7367	20+	3. 828	. 738	4	3. 835	------	----	------	------	----	------
440	------	----	------	. 6791	3	3. 842	------	----	------	------	----	------	------	----	------
600	. 641	----	3. 85	------	----	------	. 648	4	3. 888	------	----	------	------	----	------
------	------	----	------	. 6374	2	------	------	----	------	------	----	------	------	----	------
Average unit cell value for last five lines			3. 803	------	----	3. 830	------	----	3. 848	------	----	3. 826	------	----	3. 8394

References

[1] A. W. Hull, X-ray crystal analysis of thirteen common metals, Phys. Rev. **17,** 571–88 (1921).

[2] R. W. G. Wyckoff, Die Kristallstruktur des metallischen Iridiums, Z. Krist. **59,** 55–61 (1923).

[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] T. Barth and G. Lunde, Der Einfluss der Lanthanidenkontraktion auf die Gitterdimensionen der kubischen Platinmetalle, Z. physik. Chem. **117,** 478–490 (1925).

[5] A. W. Hull, Arrangement of the atoms in some common metals, Science **52,** 227 (1920).

[6] E. A. Owen and E. L. Yates, Precision measurements of crystal parameters, Phil. Mag. **15,** 472–88 (1933).

3. SULFIDES

Alpha-Manganese Sulfide (alabandite), α-MnS (Cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2724	2906 1-1093 1-1089	2.61 1.85 1.17	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
II-2103	2909 2-0981	2.60 1.84	Iron	Lyubimtsev and Lyamina [3] 1938.
	2-0990	1.17	Copper	Harcourt [2] 1942.
--------	2905 3-0835 3-0833	2.61 1.85 1.50	Copper	Harcourt [2] 1942.

The following ASTM card *d*-spacings labeled alpha-manganese sulfide, and alabandite, are predominantly the beta-cubic form with a small amount of the beta-hexagonal form. The unit cell and the space group given for the alpha-form are therefore incorrect for that pattern. The date of the reference should be 1933 rather than 1932.

--------	3605 3-1063 3-1065	1.98 3.24 1.69	Iron	Schnaase [4] 1933.

The Harcourt and the Lyubimtsev and Lyamina patterns are presented on one ASTM card, and the same Harcourt pattern appears alone on another. These patterns were made by using copper and iron rather than molybdenum radiation, as the card states.

Additional published patterns

Source	Radiation	Wavelength
Weiser and Milligan [5] 1931	----------	----------

NBS sample. The alabandite used for the NBS pattern was prepared by heating manganese and sulfur in a closed tube at 675° C for about 2 hours. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of aluminum; 0.001 to 0.01 percent each of chromium, iron, magnesium, silicon, and tin; 0.0001 to 0.001 percent each of boron, calcium, copper, and nickel; and less than 0.0001 percent of silver. The refractive indices of alabandite are too high to be measured by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The Hanawalt, Rinn, and Frevel, the Lyubimtsev and Lyamina, the Harcourt, and the Weiser and Milligan *d*-spacings were converted from kX to angstrom units. The *d*-spacings at 2.84 and 1.999 A, found only in the Harcourt pattern, are possible copper K_β lines. The very wide line extending from 1.795 to 1.765 angstrom units in the Lyubimtsev and Lyamina pattern is not possible in the face-centered alabandite structure.

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

	1	2	3
Hanawalt, Rinn, and Frevel	200	220	420
Lyubimtsev and Lyamina	200	220	420
Harcourt	200	220	222
Weiser and Milligan	200	220	420
Swanson, Fuyat, and Ugrinic	200	220	222

Lattice constant. The structure was determined by Ott [6] in 1926. The space group is O_h^5-Fm3m with sodium-chloride-type structure and 4(MnS) per unit cell. A beta-cubic zinc-sulfide-type structure and a beta-hexagonal zinc-oxide-type structure are also known, according to Wyckoff [7].

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

Lattice constants

		a A
1926	Ott [6]	5.25
1931	Weiser and Milligan (5)	5.21
1933	Schnaase [4]	5.223
1938	Mehmed and Haraldsen [8]	5.222
1939	Kröger [9]	5.219
1953	Swanson, Fuyat, and Ugrinic	5.2236 at 26° C

The density of alabandite calculated from the NBS lattice constants is 4.053 at 26° C.

Alpha-**Manganese Sulfide, MnS, (alabandite) (cubic)**

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1938 Lyubimtsev and Lyamina Fe, 1.93597 A			1942 Harcourt Cu, 1.5405 A			1931 Weiser and Milligan --------			1953 Swanson, Fuyat, 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*
111	3.03	11	5.25	3.025	5	5.239	3.0	4	5.2	------	----	------	3.015	13	5.222
------	------	----	------	------	----	------	[b]2.84	4	------	------	----	------	------	----	------
200	2.62	100	5.24	2.608	100	5.216	2.62	100	5.24	2.605	100	5.21	2.612	100	5.224
------	------	----	------	------	----	------	[b]1.999	3	------	------	----	------	------	----	------
220	1.85	67	5.23	1.847	100	5.224	1.849	57	5.230	1.839	90	5.20	1.847	48	5.224
------	------	----	------	[a]1.795	----	------	------	----	------	------	----	------	------	----	------
------	------	----	------	[a]1.765	10	------	------	----	------	------	----	------	------	----	------
311	1.58	4	5.24	1.637	10	5.429	------	----	------	------	----	------	1.575	6	5.224
222	1.51	20	5.23	1.507	50	5.220	1.505	14	5.213	1.504	30	5.21	1.509	19	5.227
400	1.312	8	5.248	1.305	40	5.220	1.305	3	5.220	1.303	10	5.21	1.306	8	5.224
331	1.202	1	5.239	------	----	------	------	----	------	------	----	------	------	----	------
420	1.172	23	5.241	1.167	70	5.219	1.167	7	5.219	1.164	60	5.21	1.1682	19	5.224
422	1.072	11	5.252	1.065	70	5.217	1.067	4	5.227	1.064	50	5.21	1.0662	15	5.2233
440	0.929	3	5.255	------	----	------	------	----	------	.919	1	5.20	.9235	1	5.2241
600	.875	5	5.250	------	----	------	------	----	------	.864	20	5.18	.8705	7	5.2230
620	.830	3	5.249	------	----	------	------	----	------	.820	10	5.17	.8260	8	5.2241
622	.792	3	5.254	------	----	------	------	----	------	------	----	------	.7875	3	5.2237
------	.729	1	------	------	----	------	------	----	------	------	----	------	------	----	------
------	.701	3	------	------	----	------	------	----	------	------	----	------	------	----	------
Average unit cell value for last five lines-------			5.252	-------	----	5.220	-------	----	5.220	------	----	5.20	-------	----	5.2236

[a] Band edges of wide line. [b] Possible CuK$_\beta$ lines.

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. Mineralogist **27,** 63–113 (1942).

[3] A. I. Lyubimtsev and A. N. Lyamina, Data for the X-ray determination of minerals, Works of the all-union institute of mineral resources, Trudy Vsesoyuzn. Inst. Min. Syrya (1938).

[4] H. Schnaase, Kristallstruktur der Manganosulfide und ihrer Mischkristalle mit Zinksulfid und Cadmiumsulfid, Z. physik. Chem. **B20,** 89–117 (1933).

[5] H. B. Weiser and W. O. Milligan, The transformation from rose to green manganous sulfide, J. Phys. Chem. **35,** 2330–2344 (1931).

[6] H. Ott, Die Strukturen von MnO, MnS, AgF, NiS, SnJ_4, $SrCl_2$, BaF_2; Präzisionsmessungen einiger Alkalihalogenide, Z. Krist. **63,** 222–230 (1926).

[7] R. W. G. Wyckoff, Crystal Structures, vol. I (Interscience Publishers, Inc., New York, N. Y., 1948).

[8] F. Mehmed and H. Haraldsen, Das magnetische Verhalten der allotropen Modifikationen des Mangan (II)-Sulfids, Z. anorg. Chem. **235,** 193–200 (1938).

[9] F. A. Kröger, Formation of solid solutions in the system zincsulfide-manganesesulfide, Z. Krist. **A100,** 543–545 (1939).

Copper (II) Sulfide (covellite), CuS (hexagonal)

ASTM cards

Old card number	New card number	New index lines	Radiation	Source
II–1715	2555	2.81	Molybdenum	Roberts and Ksanda [1] 1929.
	2-0818	1.89	No data	Waldo [2] 1935.
	2-0820	1.56	--------------	
--------	3656	1.90	Copper	Harcourt [3] 1942.
	3–1081	2.82		
	1–1090	3.02		
3513	3694	1.89	Molybdenum	New Jersey Zinc Co.
	1–1284	2.81		
	1–1281	1.56		
--------	2554	2.83	Copper	British Museum.
	3–0740	1.90		
	3–0724	3.03		

Additional published patterns

Date	Source	Radiation	Wave-length
1931	Alsén [4]	Iron	----------

NBS samples. The cupric sulfide used for the NBS pattern was obtained from the Fisher Scientific Co. The CuS was annealed by heating in a closed tube and in an atmosphere of sulfur at 400° C for several hours. It was annealed again at 500° C in a closed tube without additional sulfur.

Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of silicon and zinc; 0.001 to 0.01 percent each of silver, aluminum, calcium, iron, magnesium, and nickel; and 0.0001 to 0.001 percent each of boron, manganese, and lead.

Interplanar spacings and intensity measurements. The *d*-spacings for the Roberts and Ksanda and the Alsén patterns were calculated from Bragg angle data, and the *d*-spacings for the Waldo, the Harcourt, the New Jersey Zinc Co., and the British Museum patterns were converted from kX to angstrom units.

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

	1	2	3
Roberts and Ksanda	103	110	203, 116
Waldo	103	110	102
Harcourt	110	103	102
New Jersey Zinc Co	110	103	203, 116
British Museum	103	110	102
Alsén	006	110	1·0·14
Swanson, Fuyat, and Ugrinic	103	110	102

The New Jersey Zinc Co. and the Alsén patterns contain a number of lines not belonging to the cupric-sulfide pattern and not otherwise identifiable.

Lattice constants. The structure was determined by Gossner and Mussgnug [5] in 1927. The space group is D_{6h}^4-Pb_3/mmc with 6(CuS) per unit cell. Cupric sulfide (covellite) is a prototype for other similar structures.

A group of unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1927	Gossner and Mussgnug [5]	3.82	16.49
1929	Roberts and Ksanda [1]	3.810	16.46
1932	Oftedal [6]	3.76	16.2
1953	Swanson, Fuyat, and Ugrinic.	3.792	16.344 at 26° C

The density of cupric sulfide calculated from the NBS lattice constants is 4.680 at 26° C.

Copper (II) Sulfide (covellite), CuS (hexagonal)

hkl	1929 Roberts and Ksanda Mo, 0.709 A		1935 Waldo ---------		1942 Harcourt Cu, 1.5405 A		-------- New Jersey Zinc Co. Mo, 0.709 A		-------- British Museum Cu, 1.5405 A		1931 Alsén Fe, 1.93597 A		1953 Swanson, Fuyat, 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*	
002	---	--	---	--	---	-	--	-	--	--	---	--	8.18	7
-----	---	--	---	--	---	-	4.77	2	--	--	---	--	----	--
-----	---	--	---	--	---	-	4.48	2	--	--	---	--	----	--
-----	---	--	---	--	---	-	3.98	4	--	--	---	--	----	--
-----	---	--	---	--	---	-	3.73	4	--	--	---	--	----	--
-----	---	--	3.34	vw	---	-	--	-	3.40	40	---	--	----	--
100	3.247	m	3.25	w	3.23	22	3.27	12	3.22	40	3.281	w−	3.285	14
101	---	--	---	--	---	-	--	-	--	--	3.208	w−	3.220	28
102	3.053	s	3.05	m	3.03	78	3.04	20	3.04	80	3.046	m−	3.048	67
103	2.881	vvs	2.82	s	2.83	89	2.82	60	2.84	100	2.806	m+	2.813	100
006	2.728	m	2.73	m	2.73	67	2.72	14	2.73	80	2.716	s+	2.724	56
-----	---	--	---	--	---	-	--	-	--	--	2.551	w−	----	--
105	2.326	w	2.30	w	2.31	6	--	-	2.32	20	2.314	w	2.317	10
-----	---	--	---	--	---	-	--	-	--	--	2.275	w−	----	--
106	2.111	vw	2.09	vvw	---	-	--	-	2.10	40	2.092	w	2.097	6
008	2.038	vw	2.03	vw	---	-	--	-	2.04	20	2.036	w	2.043	7
107	---	--	---	--	---	-	--	-	--	--	---	--	1.902	25
110	1.896	vs	1.894	s	1.90	100	1.89	100	1.90	100	1.888	s+	1.896	75
108	1.730	s	1.733	m	1.739	44	1.73	10	1.74	70	1.722	s	1.735	34
-----	---	--	---	--	---	-	--	-	--	--	1.703	w	----	--
201	---	--	---	--	---	-	--	-	--	--	1.622	w−	1.634	3
202	---	--	---	--	---	-	--	-	--	--	1.600	w+	1.609	8
203	1.559	vs	1.558	m	1.563	67	1.56	30	1.56	60	1.564	w	1.572	15
116											1.548	s	1.556	37
1·0·10	1.463	vw	1.468	vw	---	-	--	-	1.46	20	1.485	w+	1.463	5
-----	---	--	---	--	---	-	--	-			1.456	m	----	--
-----	1.402	w	---	--	---	-	--	-	--	--	1.402	w−	----	--
118	---	--	1.385	vw	---	-	--	-	1.39	20	1.383	w−	1.390	6
1·0·11	1.351	w	1.350	w	1.355	6	--	-	1.35	40	1.348	s−	1.354	7
207	---	--	---	--	---	-	--	-	--	--	1.339	w−	1.343	5
208	1.277	w	1.275	w	1.283	6	1.28	4	1.28	20	1.274	m+	1.280	9
212	1.232	vw	---	--	---	-	--	-	--	--	1.209	m+	1.227	5
213	1.206	w	1.212	w	---	-	1.21	4	1.21	40B	1.171	w+	1.210	9
-----	---	--	---	--	---	-	--	-	1.16	20	1.165	m	----	--
1·0·14	1.157	vw	---	--	1.100	6	1.09	8	1.10	60	1.099	s+	1.0998	8
300	1.098	m	1.095	m	---	-	--	-	--	--	---	--	1.0946	10
218	---	--	1.058	w	1.063	6	1.06	4	1.06	40	1.059	w	1.0607	9
-----	---	--	---	--	---	-	--	-	--	--	1.033	w	----	--
306	---	--	1.016	w	---	-	1.01	4	1.02	40	1.019	w	1.0155	7
-----	---	--	0.992	vw	---	-	--	-	--	--	0.993	w	----	--
-----	---	--	.952	w	---	-	--	-	--	--	---	--	----	--
-----	---	--	.895	vvw	---	-	--	-	--	--	---	--	----	--
-----	---	--	.849	vvw	---	-	--	-	--	--	---	--	----	--

References

[1] H. S. Roberts and C. J. Ksanda, The crystal structure of covellite, Am. J. Sci. **17**, 489–503 (1929).

[2] A. W. Waldo, Identification of the copper ore minerals by means of X-ray powder diffraction pattern, Am. Mineralogist **20**, 575–597 (1935).

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

[4] N. Alsén, Über die Kristallstrukturen von Covellin (CuS) und Kupferglanz (Cu_2S), Geol. Fören. i Stockholm Förh. **53**, 111–120 (1930).

[5] B. Gossner and F. Mussgnug, Über die Kristallstruktur von Zinnober und Covellin, Centralblatt für mineralogie, geologie und paleontologie, Stuttgart, **1927A**, 410–413 (1927).

[6] I. Oftedal, Die Kristallstruktur des Covellins (CuS), Z. Krist. **83**, 9–25 (1932).

Cadium Sulfide (greenockite), CdS (hexagonal)

ASTM cards

Old card number	New card number	New index lines	Radiation	Source
1896	1918 1-0797 1-0783	3.14 2.06 3.55	Copper, 1.539 A.	Ulrich and Zachariasen [1] 1925.
II-1193	1802	3.15	No data	Milligan [2] 1934.
	2-0533 2-0549	3.57 2.06		General Electric Wembley, England.
II-1231	1919 2-0572 2-0563	3.12 2.06 1.89	Copper	Harcourt [3] 1942.
1890	1871 1-0783 1-0780	3.14 3.56 2.07	Molybdenum	New Jersey Zinc Co.

The Ulrich and Zachariasen ASTM card pattern is not the same pattern as that found in the literature reference given on that card, but closely resembles Milligan's published data in both *d*-spacings and intensities. The Milligan and the General Electric Co. patterns have been combined on one ASTM card with one line from the Ulrich and Zachariasen pattern. The General Electric Co. pattern, which is not available from the literature, was not included in the comparison table. The Harcourt pattern was made by using copper radiation rather than molybdenum as the ASTM card states.

Additional published patterns. None.

NBS sample. The cadmium sulfide used for the NBS pattern was obtained from the Radio Corporation of America. This material is a mixture of cubic and hexagonal forms of cadmium sulfide. The cubic phase position was eliminated by heating the sample at 400° C for 30 hours in a sulfur atmosphere. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of aluminum, boron, iron, magnesium, and silicon; and 0.0001 to 0.001 percent each of calcium and copper. The refractive indices of cadmium sulfide are too high to be measured by the ordinary grain-oil immersion methods.

Interplanar spacings and intensity measurements. The *d*-spacings for the Ulrich and Zachariasen pattern were calculated from Bragg angle data, and *d*-spacings for the Milligan, the Harcourt, and the New Jersey Zinc Co. patterns were converted from kX to angstrom units.

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

	1	2	3
Ulrich and Zachariasen	215, 312	213	116
Milligan	101	110	100
Harcourt	101	110	103
New Jersey Zinc Co	101	100	110
Swanson, Fuyat, and Ugrinic	101	100	002

The *d*-spacing of 3.04 A in the New Jersey Zinc Co. pattern is not a permissible hexagonal cadmium sulfide line.

Lattice constants. The structure was determined by Bragg [4] in 1920. The space group is C_{6v}^{4}-$P6_3mc$ with zinc-oxide-type structure and 2(CdS) per unit cell.

Several unit cell values were converted from kX to angstrom units for comparison with the NBS pattern.

Lattice constants

		a	*c*
		A	*A*
1925	Ulrich and Zachariasen [1]	4.150	6.738
1940	Kröger [5]	4.139	6.705
1953	Swanson, Fuyat, and Ugrinic.	4.136	6.713 at 25° C

The density of cadmium sulfide calculated from the NBS lattice constants is 4.824 at 25° C.

(Cadmium Sulfide, CdS hexagonal)

hkl	1925 Ulrich and Zachariasen Cu, 1.5405 A		1934 Milligan --------------		1942 Harcourt Cu, 1.5405 A		-------- New Jersey Zinc Co. --------------		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
100	3. 625	80	3. 56	90	3. 56	50	3. 57	80	3. 583	75
002	3. 371	40	3. 35	80	3. 33	25	3. 36	48	3. 357	59
101	3. 174	80	3. 15	100	3. 13	100	3. 15	100	3. 160	100
----	------	----	-----	-----	-----	-----	3. 04	1	------	-----
102	2. 467	40	2. 43	40	2. 42	25	2. 45	24	2. 450	25
110	2. 075	80	2. 06	100	2. 06	75	2. 07	60	2. 068	57
103	1. 903	80	1. 892	80	1. 89	75	1. 899	48	1. 898	42
200	1. 798	20	-----	-----	-----	-----	-----	-----	1. 791	17
112	1. 767	80	1. 754	90	1. 75	50	1. 762	44	1. 761	45
210	1. 736	30	-----	-----	-----	-----	1. 727	12	1. 731	18
004	1. 684	<10	1. 671	10	-----	-----	-----	-----	1. 679	4
202	1. 588	20	1. 570	10	1. 57	8	1. 579	2	1. 581	7
104	1. 525	<10	-----	-----	-----	-----	-----	-----	1. 520	2
203	1. 401	±65	1. 393	20	1. 398	25	1. 400	15	1. 398	15
201	1. 357	30	-----	-----	-----	-----	1. 357	3	1. 3536	6
211	1. 332	60	1. 323	10	1. 325	25	1. 329	7	1. 3271	11
114	1. 308	±25	-----	-----	1. 303	8	1. 304	3	1. 3032	7
105	1. 260	70	1. 251	20	1. 258	25	1. 256	15	1. 2572	11
204	1. 229	<20	-----	-----	-----	-----	-----	-----	1. 2247	1
300	1. 197	50	1. 189	10	1. 192	13	1. 194	5	1. 1940	8
213	1. 162	90	1. 152	10	1. 157	25	1. 158	14	1. 1585	12
302	1. 128	50	1. 127	10	1. 124	13	1. 124	5	1. 1249	8
205	1. 077	50	1. 068	10	1. 074	13	1. 074	3	1. 0743	6
214	------	----	-----	-----	-----	-----	-----	-----	1. 0540	1
220	1. 037	±45	-----	-----	1. 034	8	1. 034	2	1. 0340	4
310	0. 9967	20	-----	-----	-----	-----	-----	-----	0. 9934	4
222	------	----	-----	-----	-----	-----	-----	-----	. 9881	5
116	. 9872	90	0. 984	10	0. 984	8	-----	-----	. 9842	6
311	------	----	-----	-----	-----	-----	-----	-----	. 9827	5
304	. 9759	30	-----	-----	-----	-----	-----	-----	. 9729	2
215	} . 9547	100	-----	-----	. 954	8	-----	-----	. 9533	9
312										
107	. 9303	30	-----	-----	-----	-----	-----	-----	. 9265	2
313	. 9109	90	-----	-----	. 908	8	-----	-----	. 9081	7
400	. 8989	20	-----	-----	-----	-----	-----	-----	. 8956	1
401	. 8881	50	-----	-----	-----	-----	-----	-----	. 8878	1
224	. 8833	40	-----	-----	-----	-----	-----	-----	. 8804	3
402	} . 8646	70	-----	-----	-----	-----	-----	-----	{ . 8653	<1
216									{ . 8624	<1
403	. 8575	50	-----	-----	-----	-----	-----	-----	. 8315	3
306	------	----	-----	-----	. 817	5	-----	-----	. 8166	4
321	------	----	-----	-----	-----	-----	-----	-----	. 8158	4
315	------	----	-----			-----	-----	-----	. 7986	7

References

[1] F. Ulrich and W. Zachariasen, Über die Kristallstruktur des α- und β-CdS, sowie des Wurtzits, Z. Krist. **62**, 260–273 (1925).

[2] W. O. Milligan, The color and crystal structure of precipitated cadmium sulfide, J. Phys. Chem. **38**, 797–800 (1934).

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

[4] W. L. Bragg, The crystalline structure of zinc oxide, Phil. Mag. **39**, 647-651 (1920).

[5] F. A. Kröger, Solid solutions in the ternary system Zns–CdS-MnS, Z. Krist. **102A**, 132–135 (1940).

Mercury (II) Sulfide (cinnabar), HgS (red) (hexagonal)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
2332	2398	2. 87	Copper, 1.5374 A.	Buckley and Vernon [1] 1925.
	1–0948	3. 63		
	1–0951	2. 38		
--------	1503	3. 35	Copper, 1.53923 A.	Olshausen [2] 1925.
	3–0416	2. 84		
	3–0424	3. 13		
2361	2403	2. 85	Molybdenum	Hanawalt, Rinn, and Frevel [3] 1938.
	1–0949	3. 36		
	1–0970	1. 97		
II–1013	1570	3. 34	Copper	Harcourt [4] 1942. British Museum.
	2–0465	2. 85		
	2–0461	1. 68		

The intensities of the Buckley and Vernon pattern, shown on the old ASTM card, are listed in order of decreasing value, from 1 to 28, and the three strongest lines given are those published in the orginal article. On the new ASTM card the strongest line was given a value of 100 and the two 28's, the weakest lines of the pattern, were taken as second and third strongest lines, thus placing the pattern in the wrong section of the file.

The Harcourt pattern was made by using copper radiation, and the same is probably true of the British Museum pattern. Both are combined on one ASTM card, which incorrectly indicates that molybdenum radiation was used.

Additional published patterns

Source	Radiation	Wave-length
Kolkmeijer, Bijvoet, and Karssen [5] 1924.	Copper	Kα
Ramsdell [6] 1925	Molybdenum	Kα
De Jong and Willems [7] 1926	Iron	Kα
Aurivillius [8] 1950	Chromium	Kα

NBS sample. The hexagonal mercury sulfide used for the NBS pattern was obtained from the Fisher Scientific Co. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, magnesium, and sodium; 0.001 to 0.01 percent each of iron, manganese, and silicon; and 0.0001 to 0.001 percent each of silver, copper, and lead. The sample was annealed in a closed tube with a sulfur atmosphere at 325° C for 2 hours and cooled slowly. The refractive indices of cinnabar are too high to be determined by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The Olshausen, the Kolkmeijer, Bijvoet and Karssen, the De Jong and Willems, and the Aurivillius *d*-spacings were calculated from Bragg angle data; the Buckley and Vernon, the Hanawalt, Rinn, and Frevel, the Harcourt, and the Ramsdell *d*-spacings were converted from kX to angstrom units. The Kolkmeijer, Bijvoet, and Karssen sample and, probably, the Hanawalt, Rinn, and Frevel sample were laboratory preparations, but the others were natural mineral cinnabar. Because the intensities given by Buckley and Vernon were presented only as 28 steps, they were converted to percentages of the strongest line by assuming each step to be equal. The British Museum pattern, combined with Harcourt's pattern on one ASTM card, was not included in the table because it had no original reference and contained the same lines as the Harcourt pattern except for five *d*-spacings of 3.67, 2.30, 2.18, 1.85, and 1.492 A, none of which is a possible mercury sulfide line. The Ramsdell pattern contained no intensity values.

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

	1	2	3
Buckley and Vernon	102	101	110
Olshausen	101	102	100
Hanawalt, Rinn, and Frevel	102	101	104
Harcourt	101	102	105
Kolkmeijer, Bijvoet, and Karssen	101	102	201
De Jong and Willems	102	101	104
Aurivillius	101	102	003
Swanson, Fuyat, and Ugrinic	101	102	104

Lattice constants. Buckley and Vernon [1] determined the structure in 1925. The space group is D_3^4-$P3_121$ or D_3^6-$P3_221$, according to the rotary sense of the lattice, with 3(HgS) per unit cell. Hexagonal mercury sulfide is a prototype for other similar structures.

Mercury (II) Sulfide (cinnabar), HgS (red) (hexagonal)

hkl	1925 Buckley and Vernon Cu, 1.5405 A		1925 Olshausen Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.70926 A		1942 Harcourt Cu, 1.5405 A		1924 Kolkmeijer, Bijvoet, and Karssen Cu, 1.5405 A	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
100	3.64	4	3.68	m	-------	-------	-------	-------	-------	-------
101	3.375	97	3.35	s	3.37	83	3.35	100	3.31	vs
003	3.185	36	3.13	m	3.17	27	3.17	11	3.17	vw
102	2.875	100	2.84	s	2.86	100	2.86	100	2.87	vs
103	2.388	4	-------	-------	2.35	8	2.36	6	-------	-------
110	2.084	93	2.07	m	2.06	27	2.07	33	2.05	s
111	-------	-------	-------	-------	-------	-------	2.02	11	-------	-------
104	1.994	90	1.97	m	1.97	33	1.984	33	1.96	ms
112	1.917	15	-------	-------	1.89	1	1.904	3	-------	-------
201	1.776	68	1.74	mD	1.76	11	1.769	22	1.74	vs
113	1.748	75	-------	-------	1.72	20	1.739	33	-------	-------
105	1.688	86	1.67	m	1.67	27	1.683	44	1.67	s
006	1.596	36	1.58	wD	1.57	8B	1.584	11	1.57	w
203	-------	-------	-------	-------	-------	-------	1.563	11	-------	-------
204	1.438	61	1.434	w	1.432	9	1.438	22	1.433	mw
115	-------	-------	-------	-------	1.398	3	1.404	6	-------	-------
210	-------	-------	-------	-------	-------	-------	1.363	6	-------	-------
211	1.356	72	1.340	w	1.343	11	1.348	6	1.347	s
212 205	1.315	83	1.303	m	1.303	13	1.308	-------	1.302	ms
107	1.270	83	-------	-------	-------	-------	1.271	11	-------	-------
116	-------	-------	1.256	mD	1.255	11	1.261	11	1.255	ms$^-$
213	-------	-------	-------	-------	-------	-------	1.251	6	-------	-------
300	1.215	29	-------	-------	-------	-------	-------	-------	-------	-------
301 206	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
214	1.191	54	1.184	w	1.181	4B	1.181	6	1.188	w
302	-------	-------	-------	-------	-------	-------	1.163	3	-------	-------
117	1.136	29	-------	-------	-------	-------	-------	-------	-------	-------
108	1.129	43	-------	-------	-------	-------	1.127	3	1.128	m$^+$
303	-------	-------	1.125	w-m	1.123	5	1.122	2	1.113	m
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
215	1.109	43	1.103	w	1.102	5	1.107	11	-------	-------
207	1.062	15	-------	-------	1.082	1	1.085	6	1.085	vw
304	1.042	22	1.074	vw	-------	-------	1.071	6	-------	-------
221	1.033	22	1.034	w	1.029	3	1.033	11	1.034	mw
222 305	1.019	15	-------	-------	-------	-------	1.016	3	-------	-------
311 208	0.995	68	0.992	w-m	-------	-------	0.994	6	-------	-------
223	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
312	-------	-------	.977	w	-------	-------	.977	6	-------	-------
217	.962	61	-------	-------	-------	-------	.962B	6	-------	-------
224 313	-------	-------	.958	w	-------	-------	.952B	6	-------	-------
119	-------	-------	.941	w	-------	-------	.943	6	-------	-------
314 1·0·10	.922	47	.920	m	-------	-------	.920	11	-------	-------
225 209	-------	-------	-------	-------	-------	-------	.912	6	-------	-------
400 307	.902	54	-------	-------	-------	-------	.900B	3	-------	-------
402 315	-------	-------	-------	-------	-------	-------	.884	6	-------	-------
403	-------	-------	-------	-------	-------	-------	.867	6	-------	-------
-------	-------	-------	-------	-------	-------	-------	.842	6	-------	-------
-------	-------	-------	-------	-------	-------	-------	.835	2	-------	-------
-------	-------	-------	-------	-------	-------	-------	.822	2	-------	-------

Mercury (II) Sulfide (cinnabar), HgS (red) (hexagonal)—Continued

hkl	1925 Ramsdell Mo, 0.70926 A		1926 De Jong Fe, 1.93597 A		1950 Aurivillius Cr, 2.28962 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C	
	d	I	d	I	d	I	d	I
	A		A		A		A	
100	---	---	---	---	3.61	w	3.59	5
101	3.36	---	3.42	90	3.379	vs	3.359	100
003	3.17	---	3.19	30	3.177	s	3.165	28
102	2.87	---	2.89	100	2.877	vs	2.863	94
103	---	---	2.38	20	2.379	vw	2.375	9
110	2.08	---	2.08	70	2.073	s	2.074	26
111	---	---	2.03	20	2.024	m	2.026	12
104	1.98	---	1.98	80	1.978	s	1.980	29
112	---	---	1.90	10	1.904	m	1.900	3
201	1.76	---	1.76	60	1.763	s	1.765	21
113	1.73	---	1.72	70	1.733	s	1.735	27
105	1.680	---	1.67	80	1.661	s	1.679	25
006	1.580	---	1.58	30	1.581	w	1.583	5
203	---	---	1.56	20	1.561	m	1.562	6
204	1.440	---	1.42	50	1.432	s	1.433	8
115	---	---	1.39	20	1.401	vvw	1.401	2
210	---	---	1.35	20	1.358	w	1.358	5
211	1.340	---	1.33	50	1.344	m	1.344	12
212	1.312	---	1.30	60	1.305	m	1.305	10
205								
107	---	---	1.26	20	1.269	w	1.269	4
116	---	---	1.25	40	1.257	w	1.258	7
213	---	---	1.24	20	1.248	w	1.248	4
300	---	---	---	---	---	---	1.1975	2
301	---	---	1.184	10	---	---	1.1883	3
206								
214	---	---	1.177	20	---	---	1.1787	4
302	---	---	---	---	---	---	1.1614	3
117	---	---	---	---	---	---	1.1358	2
108	---	---	1.130	10	---	---	1.1271	4
303	---	---	1.121	30	---	---	1.1201	4
---	---	---	1.114	20	---	---	---	---
215	---	---	1.100	50	---	---	1.1047	5
207	---	---	1.080	30	---	---	1.0828	2
304	---	---	1.064	20	---	---	1.0693	2
221	---	---	---	---	---	---	1.0309	4
222	---	---	---	---	---	---	1.0132	2
305								
311	---	---	---	---	---	---	0.9910	<1
208								
223	---	---	---	---	---	---	.9859	4
312	---	---	---	---	---	---	.9753	4
217	---	---	---	---	---	---	.9599	3
224	---	---	---	---	---	---	.9503	3
313								
119	---	---	---	---	---	---	.9400	3
314	---	---	---	---	---	---	.9184	3
1·0·10								
225	---	---	---	---	---	---	.9103	<1
209								
400	---	---	---	---	---	---	.8981	1
307								
402	---	---	---	---	---	---	.8821	1
315								
403	---	---	---	---	---	---	.8642	<1
---	---	---	---	---	---	---	---	---
---	---	---	---	---	---	---	---	---
---	---	---	---	---	---	---	---	---

A group of unit-cell data were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
		A	A
1923	Maugin [9]	4. 16	9. 53
1924	Kolkmeijer, Bijvoet, and Karssen [5]	4. 15	9. 48
1925	Buckley and Vernon [1]	4. 168	9. 559
1925	Olshausen [2]	4. 144	9. 491
1925	Ramsdell [6]	4. 16	9. 53
1926	De Jong and Willems [7]	4. 13	9. 45
1927	Gossner and Mussgnug [10]	4. 18	9. 52
1950	Aurivillius [8]	4. 146	9. 497
1953	Swanson, Fuyat, and Ugrinic	4. 149	9.495 at 26° C

The density of hexagonal mercury sulfide calculated from the NBS lattice constants is 8.187 at 26° C.

References

[1] H. E. Buckley and W. S. Vernon, The crystal-structures of the sulfides of mercury, Mineralog. Mag. **20,** 382–392 (1925).

[2] S. v. Olshausen, Strukturuntersuchungen nach der Debye-Scherrer-Methode, Z. Krist. **61,** 463–514 (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] G. A. Harcourt, Tables for the identification of ore minerals by X-ray powder patterns, Am. Mineralogist **27,** 63–113 (1942).

[5] N. H. Kolkmeijer, J. M. Bijvoet, and A. Karssen, The crystal structure of mercuric sulfide, Koninkl. Ned. Akad. Wetenschap., Proc. **27,** 847–850 (1924).

[6] L. S. Ramsdell, The crystal structure of some metallic sulfides, Am. Mineralogist **10,** 281–304 (1925).

[7] W. F. de Jong and H. W. V. Willems, Over de Structuur van Cinnaber, Physica **6,** 129–136 (1926).

[8] K. L. Aurivillius, On the crystal structure of cinnabar, Acta Chem. Scand. **4,** 1413–36 (1950).

[9] C. Maugin, L'arrangement des atomes dans les cristaux de cinabre, Compt. rendus, **176,** 1483–1486 (1923).

[10] B. Gossner and F. Mussgnug, Über die Kristallstruktur von Zinnober und Covellin, Centr. Mineral. Geol. **1927A,** 410–413 (1927).

Mercury (II) Sulfide (metacinnabar), HgS (black) (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
--------	1453	3. 41	Copper	Lehmann [1] 1924.
	3-0398	2. 07		
	3-0396	1. 76		
II–976	1522	3. 38	Copper, 1.53923 A.	Olshausen [2] 1925.
	2-0452	2. 07		
	2-0439	1. 76		
1596	1527	3. 37	Molybdenum	Hanawalt, Rinn, and Frevel [3] 1938.
	1-0649	2. 06		
	1-0643	1. 76		
II–996	1521	3. 36	Copper	Harcourt [4] 1942.
	2-0451	2. 07		
	2-0453	1. 77		

The Lehmann and Harcourt patterns were made by using copper radiation rather than molybdenum, as the ASTM card states. The Lehmann card labeled "hexagonal" should read "cubic."

NBS sample. The cubic mercury sulfide used for the NBS pattern was prepared by A. Perloff of the NBS by precipitation from a solution of $HgCl_2$ in 0.3 N hydrochloric acid with H_2S gas. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, copper, silicon and thallium; 0.001 to 0.01 percent each of silver, magnesium, molybdenum, sodium, lead, and strontium; and 0.0001 to 0.001 percent each of iron, indium, manganese, and tin. The sample was annealed at 300° C for 2 days. The refractive indices could not be determined because cubic mercury sulfide is opaque.

Additional published patterns

Source	Radiation	Wave-length
Kolkmeijer, Bijvoet, and Karssen [5] 1924	Copper	K_α
Buckey and Vernon [6] 1925	Copper	1.5374 A

Interplanar spacings and intensity measurements. The *d*-spacings for the Lehmann, the Olshausen, the Kolkmeijer, Bijvoet, and Karssen, and the Buckley and Vernon patterns were calculated from Bragg angle data, the *d*-spacings for the Hanawalt, Rinn, and Frevel and the Harcourt patterns were converted from kX to angstrom units.

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

	1	2	3
Lehmann	111	220	311
Olshausen	111	220	311
Hanawalt, Rinn, and Frevel	111	220	311
Harcourt	111	220	311
Kolkmeijer, Bijvoet, and Karssen	111	311	220
Buckley and Vernon	111	311	220
Swanson, Fuyat, and Ugrinic	111	220	311

Lattice constant. The structure was determined by Lehmann [1] and by Kolkmeijer, Bijvoet, and Karssen [5] in 1924. The space group is T_d^2-F$\bar{4}$3m with zinc sulfide-type structure and 4(HgS) per unit cell.

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

Lattice constants

		a
		A
1924	Lehmann [1]	5.858
1924	Kolkmeijer, Bijvoet, Karssen [5]	5.86
1925	Olshausen [2]	5.861
1925	Buckley and Vernon [6]	5.866
1926	Hartwig [7]	5.834
1931	Shôji [8]	5.866
1936	Moltzau and Kolthoff [9]	5.85
1953	Swanson, Fuyat, and Ugrinic	5.8517 at 26° C

The density of cubic mercury sulfide calculated from the NBS lattice constant is 7.711 at 26° C.

Mercury (II) Sulfide (meta-cinnabar), HgS (black) (cubic)

hkl	1924 Lehmann Cu, 1.5405 A			1925 Olshausen Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1942 Harcourt Cu, 1.5405 A		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	3. 39	vvs	5. 87	3. 35	s	5. 80	3. 38	100	5. 85	3. 37	100	5. 84
200	2. 94	s	5. 88	2. 91	m	5. 81	2. 93	16	5. 86	2. 93	20	5. 86
220	2. 07	vvs	5. 85	2. 06	s	5. 83	2. 06	30	5. 83	2. 07	50	5. 85
311	1. 76	vvs	5. 85	1. 77	s	5. 86	1. 76	30	5. 84	1. 77	50	5. 87
222	1. 69	w	5. 84	1. 69	w	5. 84	1. 69	4	5. 85	1. 69	10	5. 85
400	1. 46	w	5. 84	1. 47	vd	5. 88	1. 463	2	5. 852	1. 464	5	5. 856
331	1. 34	ms	5. 84	1. 34	m	5. 85	1. 343	8	5. 854	1. 34	20	5. 84
420	1. 30	m	5. 84	1. 31	m	5. 87	1. 308	6	5. 850	1. 31	5	5. 86
422	1. 19	s	5. 84	1. 20	m	5. 85	1. 193	4	5. 844	1. 194	10	5. 849
511	1. 12	s	5. 85	1. 13	m	5. 86	1. 126	4	5. 851	1. 127	10	5. 856
440	1. 030	w	5. 83	1. 035	w	5. 85	-----	-----	-----	-----	-----	-----
531	0. 989	s	5. 85	0. 992	m	5. 87	-----	-----	-----	0. 990	5	5. 857
600	. 975	w	5. 85	-----	-----	-----	-----	-----	-----	-----	-----	-----
620	. 925	m	5. 85	. 929	m	5. 87	-----	-----	-----	. 927	3	5. 863
533	. 890	m	5. 84	-----	-----	-----	-----	-----	-----	-----	-----	-----
622	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
444	. 844	m	5. 85	-----	-----	-----	-----	-----	-----	-----	-----	-----
711	. 818	m	5. 84	-----	-----	-----	-----	-----	-----	-----	-----	-----
Average value of last five lines			5. 85	-----	-----	5. 86	-----	-----	5. 850	-----	-----	5. 857

hkl	1924 Kolkmeijer, Bijvoet, and Karssen Cu, 1.5405 A			1925 Buckley and Vernon Cu, 1.5405 A			1953 Swanson, Fuyat, 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. 35	vs	5. 80	3. 40	100	5. 89	3. 378	100	5. 851
200	2. 98	w	5. 96	2. 92	36	5. 83	2. 926	34	5. 852
220	2. 05	vs	5. 81	2. 07	86	5. 84	2. 068	57	5. 849
311	1. 768	vs	5. 86	1. 756	100	5. 82	1. 7644	45	5. 8519
222	1. 686	vw	5. 84	1. 693	21	5. 87	1. 6891	10	5. 8512
400	1. 464	vw	5. 86	1. 467	28	5. 87	1. 4627	8	5. 8510
331	1. 342	m	5. 85	1. 341	57	5. 85	1. 3424	12	5. 8514
420	1. 307	mw	5. 85	1. 308	57	5. 85	1. 3085	9	5. 8518
422	1. 192	m	5. 84	1. 197	78	5. 86	1. 1945	10	5. 8518
511	1. 125	m	5. 84	1. 131	64	5. 88	1. 1263	8	5. 8524
440	1. 036	w−	5. 86	1. 036	78	5. 86	1. 0344	2	5. 8514
531	0. 993	s	5. 87	0. 992	71	5. 87	0. 9891	5	5. 8516
600	. 975	w	5. 85	. 978	7	5. 87	. 9753	2	5. 8518
620	-----	-----	-----	. 931	43	5. 89	. 9252	4	5. 8515
533	-----	-----	-----	-----	-----	-----	. 8923	1	5. 8512
622	-----	-----	-----	-----	-----	-----	. 8824	1	[a] 5. 8532
444	-----	-----	-----	-----	-----	-----	. 8447	3	5. 8523
711	-----	-----	-----	-----	-----	-----	. 8194	3	5. 8517
Average value of last five lines			5. 85	-----	-----	5. 87	-----	-----	5. 8517

[a] Diffuse line omitted in average of last five.

References

[1] W. Lehmann, Röntgeographische Untersuchungen an natürlichem und synthetischem Metacinnabarit (HgS), Z. Krist. **60**, 379–413 (1924).

[2] S. v. Olshausen, Strukturuntersuchungen nach der Debye-Scherrer-Methode, Z. Krist. **61**, 463–514 (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] G. A. Harcourt, Tables for the identification of ore minerals by X-ray powder patterns, Am. Mineralogist **27**, 63–113 (1942).

[5] N. H. Kolkmeijer, J. M. Bijvoet, and A. Karssen, The crystal structure of mercuric sulphide Koninkl Ned. Akad. Wetenschap., Proc. **27**, 390–392 (1924).

[6] H. E. Buckley and W. S. Vernon, The crystal structures of the sulphides of mercury, Mineralog. Mag. **20**, 382–392 (1925).

[7] W. Hartwig, Die Kristallstruktur einiger Mineralien der regulären HgS–Reihe, Sitzber. deut. Akad. Wiss., Berlin, 79–80 (1926).

[8] H. Shôji, Geometrische Beziehungen unter den Strukturen der Modifikationen einer Substanz, Z. Krist. **77**, 381–410 (1931).

[9] R. Moltzau and J. M. Kolthoff, Mixed crystal formation of ZnS post-precipitated with HgS. The aging of HgS and of ZnS, J. Phys. Chem. **40**, 637–643 (1936).

Bismuth Sulfide (bismuthinite), Bi_2S_3 (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
--------	1257 3–0349 3–0362	3. 50 3. 87 3. 06	Copper------	British Museum.
--------	1258 3–0350 3–0363			Same as preceding card.
II–884	1274 2–0373 2–0391	3. 50 3. 08 1. 94	Copper------	Harcourt [1] 1942.

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

Additional published patterns

Source	Radiation	Wave-length
Garrido and Feo [2] 1938--------	----------	----------

NBS sample. The bismuth sulfide used for the NBS pattern was obtained from the Fisher Scientific Co. The sample was annealed at 500° C for 1 hour in a closed tube with an excess of sulfur. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of gallium, sodium, and silicon; 0.001 to 0.1 percent each of aluminum, calcium, iron, magnesium, and tin; 0.0001 to 0.001 percent of lead; and less than 0.0001 percent each of silver, barium, and copper. Refractive indices could not be determined because the material is opaque.

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

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

	1	2	3
British Museum------------	130, 310	220	230, 211
Harcourt------------------	130, 310	230, 211	151
Garrido and Feo-----------	130, 310	230, 211	152
Swanson, Fuyat, and Ugrinic-	230, 211	130	221

The *d*-spacing of 3.51 A is given as the strongest line in the British Museum, the Harcourt, and the Garrido and Feo patterns because they did not resolve the 130 and the 310 lines, and the sum of the intensities is larger than the intensity of the (230, 211) line, the strongest for NBS pattern.

Lattice constants. The structure was determined by Hofmann [2] in 1933. The space group is D_{2h}^{16}-Pbnm (Pnma) with antimony sulfide-type structure and 4(Bi_2S_3) per unit cell.

Two sets of unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1933--	Hofmann [3]-------	11. 15	11. 29	3. 98
1938--	Garrido and Feo [2]-	11. 15	11. 29	3. 98
1953--	Swanson, Fuyat, and Ugrinic.	11. 150	11. 300	3.981 at 26° C

The density of bismuth sulfide calculated from the NBS lattice constants is 6.808 at 26° C.

Bismuth Sulfide (bismuthinite), Bi_2S_3 (orthorhombic)

hkl	----		1942		1938		1953	
	British Museum		Harcourt		Garrido and Feo		Swanson, Fuyat, and Ugrinic	
	Cu, 1.5405 A		Cu, 1.5405 A		----		Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
020	5. 46	50	5. 56	11	5. 488	w	5. 65	20
120	4. 89	50	4. 96	11	4. 951	w	5. 04	19
220	3. 88	75	3. 93	22	3. 897	mw	3. 97	38
101	--------	-------	--------	-------	3. 679	vw	3. 75	20
130	3. 51	100	3. 51	100	3. 503	s	3. 56	94
310							3. 53	60
021	--------	-------	3. 23	11	3. 198	vw	3. 256	18
230	3. 07	75	3. 09	66	3. 065	ms	3. 118	100
211								
221	2. 80	50	2. 80	44	2. 772	m	2. 811	63
301	--------	-------	2. 70	11	2. 669	w	2. 716	34
311	--------	-------	2. 62	11	2. 597	w	2. 641	24
240	2. 49	75	2. 500	33	2. 488	m	2. 520	35
420	--------	-------	--------	-------	--------	-------	2. 499	13
231	--------	-------	2. 430	11	2. 436	vw	2. 456	15
041	2. 29	50	2. 28	11	2. 272	mw	2. 304	24
141	2. 23	60	2. 23	33	2. 225	m	2. 256	36
241	--------	-------	--------	-------	--------	-------	2. 129	9
421	2. 11	25	2. 11	11	2. 097	w	2. 118	15
250	--------	-------	--------	-------	--------	-------	2. 096	11
520	2. 06	25	2. 06	6	2. 071	w	2. 074	10
002	--------	-------	1. 98	11	1. 966	w	1. 990	33
431	--------	-------	--------	-------	--------	-------	1. 953	55
151	1. 94	75	1. 939	55	1. 935	m	1. 935	20
530	1. 91	75	--------	-------	1. 907	mw	1. 919	20
060	--------	-------	1. 874	11	1. 872	mw	1. 884	14
251	1. 86	60	1. 844	11	1. 842	vw	1. 854	17
610	1. 83	50	--------	-------	--------	-------	1. 834	7
222	1. 77	25	--------	-------	1. 766	m	1. 779	13
620	--------	-------	--------	-------	--------	-------	1. 765	5
351	--------	-------	--------	-------	--------	-------	1. 737	7
312	1. 72	75	1. 728	55	1. 721	mw	1. 734	35
061	1. 69	50	1. 693	11	1. 693	vw	1. 703	10
161	--------	-------	--------	-------	1. 671	vw	1. 682	7
360	1. 67	25	1. 673	11	--------	-------	1. 679	8
611	1. 63	25	--------	-------	--------	-------	1. 665	2
412	1. 59	25	1. 598	2	--------	-------	1. 604	4
242	--------	-------	--------	-------	--------	-------	1. 562	15
640	1. 55	50	1. 553	33	1. 550	mw	1. 552	11
720	1. 52	50	1. 524	6	1. 530	w	1. 533	8
342	--------	-------	--------	-------	--------	-------	1. 490	6
152	1. 47	75	1. 478	22	1. 484	ms	1. 481	11
271	1. 44	50	--------	-------	--------	-------	1. 444	10
252								
522	--------	-------	1. 433	22	--------	-------	1. 436	9
650								
721	1. 43	50	--------	-------	1. 428	w	1. 431	12
442	--------	-------	--------	-------	1. 408	w	1. 405	5
470	1. 39	25	1. 393	11	1. 394	w	1. 397	6
352	--------	-------	--------	-------	--------	-------	1. 386	8
532	1. 38	25	1. 378	11	1. 377	w	1. 3816	10
280	--------	-------	--------	-------	1. 362	w	1. 3679	7
062								
162	--------	-------	--------	-------	--------	-------	1. 3573	7
561	1. 35	50	1. 350	22	1. 347	w	1. 3527	10
660	--------	-------	1. 318	11	1. 320	w	1. 3216	8
181								
410	[a] 1. 31	50B	[b] 1. 305	22	[c] 1. 308	w	1. 3100	17

[a] Thirteen additional lines have been omitted.
[b] Nineteen additional lines have been omitted.
[c] Twenty-three additional lines have been omitted.

References

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

[2] J. Garrido and R. Feo, Sur les sulfotellurures de Bismuth, Bull. Soc. franc. Mineral. **61,** 196–204 (1938).

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

4. OXIDES

Alpha-**Gallium Oxide,** α–Ga_2O_3 **(hexagonal)**

ASTM cards. None.
Additional published patterns

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

NBS sample. The gallium oxide used for the NBS pattern was prepared by A. Perloff of the NBS by igniting at 425° C gallium hydroxide precipitated from the hydrochloric-acid solution of pure gallium metal. Spectrographic analysis of the oxide at the NBS showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, copper, iron, sodium, lead, silicon, and tin; 0.001 to 0.01 percent of barium, magnesium, and manganese; 0.0001 to 0.001 percent each of chromium, indium, and nickel; and less than 0.0001 percent of silver. The sample was too finely divided for determination of the refractive indices.

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

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

	1	2	3
Zachariasen	116	124	300
Swanson, Fuyat, and Ugrinic	014	110	116

Lattice constants. The structure was determined by Zachariasen [1] in 1928. The space group is D_{3d}^6-R$\bar{3}$c with alpha-aluminum-oxide-type structure and 6 (Ga_2O_3) per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1928	Zachariasen [1]	4. 99	13. 47
1953	Swanson, Fuyat, and Ugrinic.	4. 9793	13. 429 at 24° C

The density of gallium oxide calculated from NBS lattice constants is 2.158 at 24° C.

Alpha-**Gallium Oxide,** Ga_2O_3 **(hexagonal)**

hkl	1928 Zachariasen Fe, 1.93597 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.54050 A, 24° C	
	d	*I*	*d*	*I*
	A		*A*	
102	3. 61	30	3. 630	26
014	2. 654	60	2. 651	100
110	2. 496	60	2. 491	80
006	-----	---	2. 238	4
113	2. 182	10	2. 177	16
022	-----	---	2. 052	3
204	1. 815	50	1. 814	36
116	1. 667	100	1. 665	45
108	-----	---	1. 565	9
124	1. 467	80	1. 466	33
300	1. 441	80	1. 438	30
028	-----	---	1. 325	4
0·1·10	1. 286	40	1. 282	11
220	1. 247	40	1. 245	9
306	-----	---	1. 209	4
218	-----	---	1. 1696	4
2·0·10	-----	---	1. 1396	6
314	-----	---	1. 1266	8
226	-----	---	1. 0878	6
1·2·10	-----	---	1. 0366	8
044	-----	---	1. 0266	3
138	-----	---	0. 9738	3
234	-----	---	. 9487	7

Reference

[1] W. H. Zachariasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO_3, Skrifter Norske Videnskaps-Akad. Oslo, I. Mat.-Naturv. Klasse 1928 No. 4, 165 pages (1928).

Neodymium Oxide, Nd_2O_3 (hexagonal)

ASTM cards. None.
Additional published patterns

Source	Radiation	Wave-length
Zachariasen [1] 1926	Copper	

NBS sample. The neodymium oxide used for the NBS pattern was obtained from the Johnson, Matthey, & Co., Ltd. Their spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of silicon, copper, indium, magnesium, calcium, sodium, iron, potassium, and lithium. The sample was heated to 1,000° C to insure complete conversion to the hexagonal form. The NBS sample is too finely divided to permit resolution of the refractive indices, but both of them appear to be above 1.915.

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

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

	1	2	3
Zachariasen	101	112	201
Swanson, Fuyat, and Ugrinic	101	100	110

Lattice constants. The structure was determined by Zachariasen [1] in 1926. The space group is D_3^2-P321 with lanthanum-oxide-structure type and 1(Nd_2O_3) per unit cell. A cubic form of neodymium oxide, also stable at room temperature, can be prepared by heating the oxide at 700° C for 3 hours. It can be converted to the hexagonal form by heating at 1,000° C and then converted back to cubic by heating at 700° C, all according to Löhberg [2].

Zachariasen's unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
		A	A
1926	Zachariasen [1]	3.85	6.02
1953	Swanson, Fuyat, and Ugrinic.	3.831	5.999 at 26° C

The density of neodymium oxide calculated from the NBS lattice constants is 7.327 at 26° C.

Neodymium Oxide, Nd_2O_3 (hexagonal)

hkl	1926 Zachariasen Cu, 1.5405 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C	
	d	I	d	I
	A		A	
100	3.343	40	3.319	35
002	3.011	40	2.998	32
101	2.915	100	2.902	100
102	2.235	40	2.225	33
110	1.924	60	1.916	35
103	1.721	80	1.713	31
200	1.666	20	1.659	6
112	1.620	100	1.614	27
201	1.607	100	1.599	20
004	1.505	15	1.500	4
202	1.458	20	1.452	7
104	1.361	20	1.366	5
203	1.281	50	1.276	12
210	-----	---	1.254	4
211	1.230	70	1.227	14
114	1.183	60	1.1807	8
212	1.160	30	1.1566	5
105	1.131	50	1.1282	8
204	-----	---	1.1125	3
300	1.109	30	1.1058	5
213	1.064	70	1.0623	11
302	1.040	40	1.0375	8
205	-----	---	0.9721	7
214	-----	---	.9621	4
106	-----	---	.9574	5
310	-----	---	.9201	2
222	-----	---	.9124	7
311	-----	---	.9097	10
304	-----	---	.8899	7
116	-----	---	.8861	6
312	-----	---	.8794	4
215	-----	---	.8666	9
313	-----	---	.8358	9
107	-----	---	.8296	5
401	-----	---	.8215	4
224	-----	---	.8070	5

References

[1] W. Zachariasen, Die Kristallstruktur der A-Modification von den Sesquioxyden der seltenen Erdmetalle. (La_2O_3, Ce_2O_3, Pr_2O_3, Nd_2O_3), Z. physik. Chem. **123,** 134–150 (1926).

[2] K. Löhberg, Über die C-Modifikation der Sesquioxyde von Neodym und Lanthan, Z. physik. Chem. **28B,** 402–407 (1935).

Palladium Oxide, PdO (tetragonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-4000	3904 2-1430 2-1432	1. 30 2. 60 1. 65	Copper and Iron.	Levi and Fontana [1] 1926.

Levi and Fontana [1] presented two patterns for PdO, one made with copper and the other iron radiation. The ASTM card pattern appears to be the average of the two.

Additional published patterns

Source	Radiation	Wave-length
Zachariasen [2] 1927	Copper	1. 540 A

NBS sample. The powdered palladium metal used in preparation of the NBS sample was obtained from J. Bishop & Co. Palladium oxide was formed by heating the powdered metal at 600° C for 18 hours in an open porcelain crucible. Spectrographic analysis of the oxide at the NBS showed the following impurities: 0.01 to 0.1 percent of platinum; 0.001 to 0.01 percent each of iron and silicon, 0.0001 to 0.001 percent each of silver, aluminum, calcium, copper, magnesium, and lead.

The refractive indices could not be determined because the sample is opaque.

Interplanar spacings and intensity measurements. The Levi and Fontana and the Zachariasen *d*-spacings were calculated from Bragg angle data. Of the two patterns published by Levi and Fontana, the shorter pattern, made by using iron radiation, agreed better with other work and was used in the table. The copper pattern differed considerably and was not included.

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

	1	2	3
Levi and Fontana	202, 211	002, 101	112
Zachariasen	002, 101	202, 211	112
Swanson, Fuyat, and Ugrinic	101	002	112

Lattice constants. The structure was determined by Moore and Pauling [3] in 1941. The space group is D_{4h}^{9}-$P4_2/mmc$ with 2(PdO) per unit cell. This structure was confirmed by Waser, Levy, and Peterson [4] in 1953. Their calculated X-ray intensities were in good agreement with the experimentally determined values for the NBS pattern.

The first three unit-cell values listed below were converted from kX to angstrom units for comparison with the NBS values. The Waser, Levy, and Peterson were given in angstroms.

Lattice constants

		a	c
		A	*A*
1926	Levi and Fontana [1]	3. 01	5. 21
1927	Zachariasen [2]	3. 035	5. 325
1941	Moore and Pauling [3]	3. 03	5. 32
1953	Waser, Levy, and Peterson [4].	3. 03	5. 33
1953	Swanson, Fuyat, and Ugrinic.	3. 0434	5. 337 at 26° C

The density of palladium oxide calculated from the NBS lattice constants is 8.242 at 26° C.

Palladium Oxide, PdO (tetragonal)

hkl	1926 Levi and Fontana Fe, 1.93597 A		1927 Zachariasen Cu, 1.5405 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
100	------	------	------	------	3. 046	3
002	2. 59	s	2. 64	100	2. 667	33
101					2. 644	100
110	2. 12	w	2. 151	25	2. 153	20
112	1. 65	s	1. 673	60	1. 674	28
103	------	------	1. 536	40	1. 536	18
200	1. 51	ms	1. 520	40	1. 522	11
004	------	------	------	------	1. 335	4
202	1. 31	vs	1. 319	70	1. 322	12
211					1. 319	22
114	1. 13	w	1. 132	15	1. 1334	5
213	1. 08	s	1. 077	40	1. 0806	9
220					1. 0761	3
105	------	------	1. 003	30	1. 0072	5
204					1. 0035	6
222	------	------	0. 995	40	0. 9977	6
301					. 9966	3
310	------	------	. 960	20	. 9623	3
312	------	------	------	------	. 9053	6
303	------	------	------	------	. 8812	3
215	------	------	------	------	. 8400	6
224	------	------	------	------	. 8377	5
321	------	------	------	------	. 8338	4
116	------	------	------	------	. 8219	2

References

[1] G. R. Levi and C. Fontana, Ossidi di palladio, Gazz. chim. ital. **56**, 388–396 (1926).

[2] W. Zachariasen, Über die Kristallstruktur des Palladiumoxyds (PdO), Z. physik. Chem. **128**, 412–416 (1927).

[3] W. J. Moore, Jr. and L. Pauling, The crystal structures of the tetragonal monoxides of lead, tin, palladium and platinum, J. Am. Chem. Soc. **63**, 1392–4 (1941).

[4] J. Waser, H. A. Levy and S. W. Peterson, The structure of PdO, Acta Cryst. **6**, 661–663 (1953).

Tin (II) Oxide, SnO (tetragonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2198	2260 1–0904 1–0902	2.96 1.60 1.48	No data	Weiser and Milligan [1] 1932.
2180	2261 1–0905 1–0891	2.97 1.59 4.81	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.

The Weiser and Milligan pattern is not listed in the 1950 edition of the ASTM index.

Additional published patterns

Source	Radiation	Wavelength
Levi [3] 1924	Copper	

NBS sample. The stannous oxide used for the NBS pattern was obtained from the Baker Chemical Co. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of calcium, copper, iron, magnesium, antimony, and silicon; and 0.0001 to 0.001 percent each of aluminum, barium, nickel, and lead. The refractive indices could not be resolved because the sample was too finely divided, but both of them appeared to be above 2.0.

Interplanar spacings and intensity measurements. The *d*-spacings for the Levi pattern were calculated from Bragg angle data; the *d*-spacings for the Weiser and Milligan and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units.

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

	1	2	3
Weiser and Milligan	101	211	202
Hanawalt, Rinn, and Frevel	101	211	001
Levi	101	112	211
Swanson, Fuyat, and Ugrinic	101	110	112

Lattice constants. Levi and Natta [4] determined the structure in 1926. The space group is D_{4h}^{7}-P4/nmm with red-lead-monoxide-type structure and 2(SnO) per unit cell.

Lattice constants

		a	*c*
		A	*A*
1926	Levi and Natta [4]	3.81	4.82
1932	Weiser and Milligan [1]	3.80	4.80
1933	Straumanis and Strenk [5]	3.801	4.843
1941	Moore and Pauling [6]	3.804	4.826
1953	Swanson, Fuyat, and Ugrinic.	3.802	4.836 at 26° C

The density of tin oxide calculated from the NBS lattice constants is 6.398 at 26° C.

Tin (II) Oxide, SnO (tetragonal)

hkl	1932		1938		1924		1953	
	Weiser and Milligan		Hanawalt, Rinn, and Frevel		Levi		Swanson, Fuyat, and Ugrinic	
	--------------		Mo, 0.709 A		Cu, 1.5405 A		Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
001	4.80	40	4.82	30	-------	-------	4.85	10
101	2.97	100	2.98	100	2.82	s	2.989	100
110	2.69	50	2.67	25	2.55	mw	2.688	37
002	2.40	30	2.39	5	2.31	w	2.418	14
102	-------	-------	-------	-------	-------	-------	2.039	<1
200	1.894	40	1.89	15	1.83	m	1.901	13
112	1.791	70	1.79	30	1.75	s	1.797	27
211	1.598	90	1.59	40	1.56	s	1.604	25
202	1.485	80	1.483	15	1.45	s	1.494	11
103	-------	-------	-------	-------	1.43	mw	1.484	12
113	1.372	10	-------	-------	-------	-------	1.382	3
220	1.339	20	1.335	5	1.32	w	1.344	5
301	1.222	10	1.224	5	1.21	mw	1.225	4
004	-------	-------	-------	-------	-------	-------	1.209	3
310	1.197	10	1.196	5	1.19	mw	1.202	4
222	-------	-------	-------	-------	-------	-------	1.1747	6
213	1.167	30	1.167	10	1.155	s	1.1697	8
104	-------	-------	-------	-------	-------	-------	1.1520	1
114	1.101	10	-------	-------	1.093	w	1.1026	4
312	1.074	20	1.075	5	1.067	ms	1.0766	6
321	1.029	20	1.027	5	1.022	s	1.0303	4
204	1.020	10	-------	-------	1.012	w	1.0201	3
303	0.994	10	-------	-------	0.989	m	0.9965	1
214	-------	-------	-------	-------	-------	-------	.9852	1
005	-------	-------	-------	-------	-------	-------	.9674	<1
400	-------	-------	-------	-------	-------	-------	.9507	3
105	.934	10	-------	-------	.933	w	.9371	3
411	.902	10	-------	-------	.903	m	.9056	4
224	-------	-------	-------	-------	.894	mw	.8988	4
323	.881	10	-------	-------	.881	ms	.8824	5
---------	.874	10	-------	-------	-------	-------	--------	------
314	.852	10	-------	-------	.852	ms	.8524	4
420	-------	-------	-------	-------	-------	-------	.8503	4
215 332	.841	10	-------	-------	.839	ms	.8405	6
006	-------	-------	-------	-------	.803	ms	.8062	1
422	-------	-------	-------	-------	-------	-------	.8020	<1
413	.800	10	-------	-------	-------	-------	.8002	1
---------	.751	10	-------	-------	-------	-------	--------	------
---------	.713	10	-------	-------	-------	-------	--------	------

References

[1] H. B. Weiser and W. O. Milligan, X-ray studies on the hydrous oxides. III. Stannous oxide, J. Phys. Chem. **36,** 3039–3045 (1932).

[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] G. R. Levi, Isomorfismo degli ossidi stannoso e piomboso, Nuovo Cimento **1,** 335–344 (1924).

[4] G. R. Levi and G. Natta, Isomorfismo degli ossidi piomboso e stannoso, Nuovo Cimento **3,** 114–134 (1926).

[5] M. Straumanis and C. Strenk, Über das Zinn (2)-Oxyd, Z. anorg. u. allg. Chem. **213,** 301–9 (1933).

[6] W. J. Moore, Jr. and L. Pauling, The crystal structures of the tetragonal monoxides of lead, tin, palladium and platinum, J. Am. Chem. Soc. **63,** 1392–4 (1941).

5. HALIDES AND HALIDE HYDRATES

Lithium Bromide, LiBr (cubic)

ASTM cards

Card numbers		New index lines	Radiation	Source
Old	New			
1813	1817 1–0766 1–0751	3.19 2.75 1.65	Molybdenum, 0.712.	Davey [1] 1923.
1846	1818 1–0767 1–0764	3.17 2.74 1.94	Molybdenum.	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns

Source	Radiation	Wavelength
Ott [3] 1923	Copper	K.

NBS sample. The lithium bromide used for the NBS pattern was obtained from the Fisher Scientific Co. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of calcium and sodium; 0.001 to 0.01 percent each of aluminum, magnesium, and silicon; 0.0001 to 0.001 percent of copper; and less than 0.0001 percent each of silver, barium, and iron. The sample was heated at 425° C to remove water and then on cooling mounted in petrolatum. The NBS sample is too hygroscopic to permit measurement of the refractive indices by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The *d*-spacings for the Ott pattern were calculated from Bragg angle data; the Hanawalt, Rinn, and Frevel *d*-spacings were converted from kX to angstrom units; and the *d*-spacings for the Davey pattern were converted from molybdenum radiation, 0.712 A, to the weighted Kα radiation having a wavelength of 0.7107 A.

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

	1	2	3
Davey	111	200	311
Hanawalt, Rinn, and Frevel	111	200	220
Ott	111	200	220
Swanson, Fuyat, and Ugrinic	111	200	220

Lattice constant. The structure was determined by R. W. G. Wyckoff [4] in 1921. The space group is O_h^5-Fm3m with sodium-chloride-structure type and 4(LiBr) per unit cell.

Several unit-cell values were converted from kX to angstrom units for comparison with the NBS values. The value determined by Davey was converted from Mo 0.712 to 0.7107 A.

Lattice constants

		a
		A
1921	Wyckoff [4]	5.49
1923	Davey [1]	5.480
1923	Ott [3]	5.500
1936	Finch and Fordham [5]—electron diffraction data.	5.506
1953	Swanson, Fuyat, and Ugrinic	5.5013 at 26° C

The density of lithium bromide calculated from the NBS lattice constant is 3.464 at 26° C.

Lithium Bromide, LiBr (cubic)

hkl	1923 Davey Mo, 0.7107 A			1938 Hanawalt, Rinn and Frevel Mo, 0.709 A			1923 Ott Cu, 1.5418 A			1953 Swanson, Fuyat 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. 18	100	5. 51	3. 18	100	5. 51	3. 17	s	5. 49	3. 177	100	5. 503
200	2. 74	100	5. 48	2. 75	75	5. 50	2. 76	s	5. 52	2. 751	78	5. 502
220	1. 935	40	5. 473	1. 94	75	5. 49	1. 94	s	5. 49	1. 945	58	5. 501
311	1. 651	100	5. 476	1. 65	75	5. 47	1. 65	s	5. 49	1. 659	43	5. 502
222	1. 581	20	5. 477	1. 58	25	5. 47	1. 58	m	5. 48	1. 588	17	5. 501
400	1. 370	15	5. 480	1. 375	13	5. 500	1. 369	vw	5. 48	1. 376	7	5. 504
331	1. 258	40	5. 483	1. 262	38	5. 501	1. 260	s	5. 49	1. 262	17	5. 501
420	1. 226	20	5. 483	1. 229	25	5. 496	1. 231	s	5. 51	1. 231	15	5. 505
422	1. 122	20	5. 497	1. 123	13	5. 502	1. 120	s	5. 49	1. 1227	12	5. 5001
511	1. 055	20	5. 482	1. 058	13	5. 498	1. 057	s	5. 492	1. 0585	10	5. 5001
440	-----	-----	-----	-----	-----	-----	0. 9718	m–w	5. 498	0. 9724	3	5. 5007
531	0. 926	15	5. 478	-----	-----	-----	. 9288	s	5. 495	. 9298	8	5. 5008
600	. 912	15	5. 472	-----	-----	-----	. 9162	s	5. 497	. 9169	6	5. 5014
620	. 866	10	5. 477	-----	-----	-----	. 8699	s	5. 502	. 8698	5	5. 5011
533	-----	-----	-----	-----	-----	-----	. 8375	s	5. 492	. 8390	5	5. 5017
622	-----	-----	-----	-----	-----	-----	. 8283	s	5. 495	. 8294	4	5. 5016
Average unit cell value for last five lines-----			5. 481	-----	-----	5. 499	------	-----	5. 496	------	-----	5. 5013

References

[1] W. P. Davey, Precision measurements of crystals of the alkali halides, Phys. Rev. **21,** 143–61 (1923).

[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] H. Ott, Die Raumgitter der Lithiumhalogenide, Phys. Z. **24,** 209–212 (1923).

[4] R. W. G. Wyckoff, The crystal structures of the alkali halides, J. Wash. Acad. Sci. **11,** 429–434 (1921).

[5] G. I. Finch and S. Fordham, The effect of crystal size on lattice dimensions, Proc. Phys. Soc. (London) **48,** 85–94 (1936).

Sodium Iodide, NaI (cubic)

ASTM cards

Old card number	New card number	New index lines	Radiation	Source
1738----	1754 1–0740 1–0715	3. 24 2. 29 3. 74	Molybdenum, 0.712.	Davey [1] 1923.
1760----	1700 1–0715 1–0724	3. 22 3. 74 2. 29	Molybdenum-	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns. None.

NBS sample. The sodium iodide used for the NBS pattern was obtained from the Merck Chemical Co., Inc. Spectrographic analysis at the NBS showed the following impurities: 0.0001 to 0.001 percent each of aluminum, calcium, magnesium, and silicon; and less than 0.0001 percent of copper. The refractive index of the NBS sample is 1.774.

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

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

	1	2	3
Davey----------------------------------	200	220	111
Hanawalt, Rinn, and Frevel------------	200	111	220
Swanson, Fuyat, and Ugrinic-----------	200	111	220

Lattice constant. The structure was determined by Posnjak and Wyckoff [3] in 1922. The space group is O_h^5-Fm3m with sodium-chloride-structure type and 4(NaI) per unit cell.

Sodium Iodide, NaI (cubic)

hkl	1923 Davey Mo, 0.709 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1953 Swanson, Fuyat, 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. 75	67	6. 50	3. 75	83	6. 50	3. 74	82	6. 475
200	3. 25	100	6. 50	3. 23	100	6. 46	3. 236	100	6. 472
220	2. 29	83	6. 48	2. 29	83	6. 48	2. 289	63	6. 475
311	1. 957	67	6. 49	1. 95	58	6. 47	1. 951	41	6. 472
222	1. 868	33	6. 47	1. 87	42	6. 48	1. 868	23	6. 471
400	1. 618	25	6. 47	1. 61	17	6. 44	1. 618	14	6. 472
331	1. 489	33	6. 49	1. 484	23	6. 47	1. 485	14	6. 471
420	1. 451	50	6. 49	1. 448	42	6. 48	1. 447	23	6. 472
422	1. 322	41	6. 48	1. 323	23	6. 48	1. 321	19	6. 472
511	1. 248	25	6. 48	1. 247	13	6. 48	1. 246	13	6. 473
440	1. 147	16	6. 49	1. 146	7	6. 48	1. 1444	5	6. 4737
531	1. 098	16	6. 50	1. 096	7	6. 48	1. 0941	8	6. 4727
600	1. 079	16	6. 47	1. 081	7	6. 49	1. 0788	10	. 64728
620	1. 024	16	6. 48	1. 022	3	6. 46	1. 0233	7	6. 4719
533	0. 989	8	6. 48	--------	--------	--------	0. 9872	4	6. 4735
622	. 975	12	6. 47	0. 976	3	6. 47	. 9759	6	6. 4734
444	--------	--------	--------	--------	--------	--------	. 9343	2	6. 4730
711	. 907	8	6. 48	--------	--------	--------	. 9064	6	6. 4730
640	. 899	8	6. 48	--------	--------	--------	. 8975	4	6. 4720
642	. 866	8	6. 48	--------	--------	--------	. 8650	7	6. 4731
731	. 843	8	6. 48	--------	--------	--------	. 8427	8	6. 4729
--------	. 784	8	6. 46	--------	--------	--------	--------	--------	--------
--------	. 763	8	6. 47	--------	--------	--------	--------	--------	--------
Average of last five lines------			6. 48	--------	--------	6. 48	--------	--------	6. 4728

A group of unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a
		A
1922--	Posnjak and Wyckoff [3]------	6.48
1923--	Davey [1]------------------	6.479
1948--	Mehmel [4]-----------------	6.47
1953--	Swanson, Fuyat, and Ugrinic--	6.4728 at 26° C

The density of sodium iodide calculated from the NBS lattice constant is 3.671 at 26° C.

References

[1] W. P. Davey, Precision measurements of crystals of the alkali halides, Phys. Rev. **21,** 143–161 (1923).

[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] E. Posnjak and R. W. G. Wyckoff, The crystal structures of the alkali halides, J. Wash. Acad. Sci. **12.** 248–251 (1922).

[4] M. Mehmel, Kristallchemische Betrachtungen zur I. und VII. Gruppe des periodischen Systems der Elemente, Optik **3,** 41–46 (1948).

Magnesium Fluoride (sellaite), MgF_2 (tetragonal)

ASTM cards

Old card number	New card number	New index lines	Radiation	Source
3792	3858 1–1297 1–1297	1. 47 1. 00 2. 57	Copper, Kα	Buckley and Vernon [1] 1925.
3141	3308 1–1206 1–1196	2. 24 1. 72 3. 29	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns

Date	Source	Radiation	Wave-length
1925	Van Arkel [3]	Copper	Kα
1925	Ferrari [4]	No data	

NBS sample. The magnesium fluoride used for the NBS pattern was obtained from the Mallinckrodt Chemical Works. The sample was annealed by heating in a hydrothermal bomb at 700° C under a pressure of 16,000 psi for 15 hours.

Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of calcium, sodium, and silicon; 0.001 to 0.01 percent each of aluminum and iron; 0.0001 to 0.001 percent of copper; and less than 0.0001 percent of silver. The refractive indices are too low to be measured by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The *d*-spacings for the Buckley and Vernon, the Van Arkel, and the Ferrari patterns were calculated from Bragg angle data, and the Hanawalt Rinn, and Frevel *d*-spacings were converted from kX to angstrom units.

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

	1	2	3
Buckley and Vernon	301	111	211
Hanawalt, Rinn, and Frevel	111	211	110
Van Arkel	110	111	211
Ferrari	111	211	301
Swanson, Fuyat, and Ugrinic	110	111	211

To form a basis for comparison, the Buckley and Vernon intensities, listed in descending order of rank, were converted to percentages, with the strongest line being 100 and the weakest 4, assuming each step between ranks to be of equal size.

The Hanawalt, Rinn, and Frevel, the Van Arkel, and the Ferrari patterns contain extra lines not permissible in the magnesium-fluoride pattern, and not otherwise identified. A pattern published by Bruni and Levi [5] in 1924 was retracted in 1925.

Lattice constants. The structure was determined by Van Arkel [3] and by Buckley and Vernon [1] in 1925. The space group is D_{4h}^{14}—$P4_2/mnm$ with titanium dioxide (rutile) type structure and $2(MgF_2)$ per unit cell.

Two sets of lattice constants were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1925	Ferrari [4]	4. 65	3. 07
1925	Buckley and Vernon [1]	4. 669	3. 084
1953	Swanson, Fuyat, and Ugrinic.	4. 623	3. 052 at 27° C

The density of magnesium fluoride calculated from the NBS lattice constants is 3.172 at 27° C.

References

[1] H. E. Buckley and W. S. Vernon, The crystal structure of magnesium fluoride, Phil. Mag. **49,** 945–951 (1925).

[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] A. E. van Arkel, Kristalstructuur van Magnesiumfluoride en andere Verbindingen van Hetzelfde Kristaltype, Physica **5,** 162–171 (1925).

[4] A. Ferrari, I reticoli cristallini dei fluoruri di litio e magnesio e il loro isomorphismo, Atti accad. nazl. Lincei, Rend., Classe Sci. fis. mat. e nat. **1,** 664–671 (1925).

[5] G. Bruni and G. R. Levi, Soluzioni solide fra composti di elementi a valenza diversa, Rend. Accad. Atti accad. nazl. Lincei, Rend., Classe sci. fis. mat. e nat. Lincei **33,** 377–384 (1924).

Magnesium Fluoride (sellaite), MgF_2 (tetragonal)

hkl	1925		1938		1925		1925		1953	
	Buckley and Vernon		Hanawalt, Rinn, and Frevel		Van Arkel		Ferrari		Swanson, Fuyat, and Ugrinic	
	Cu, 1.5405 A		Mo, 0.709 A		Cu, 1.5405 A		--------------		Cu, 1.5405 A, 27° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
110	3. 315	90	3. 30	80	3. 317	vs	3. 218	s	3. 265	100
-------	------	---	3. 15	5	------	----	------	----	------	-----
101	2. 573	11	2. 57	20	2. 584	vw	2. 471	mw	2. 545	22
200	------	---	-----	---	------	----	2. 289	mw	2. 310	<1
111	2. 262	97	2. 24	100	2. 254	vs	2. 212	vs	2. 231	96
210	2. 083	86	2. 07	32	2. 106	s	2. 058	m	2. 067	34
-------	------	---	1. 93	12	------	----	------	----	------	-----
-------	------	---	-----	---	------	----	1. 829	w	------	-----
211	1. 729	97	1. 72	100	1. 745	vs	1. 708	vs	1. 711	73
220	1. 643	75	1. 64	32	1. 666	s	1. 640	ms	1. 635	31
002	1. 541	72	1. 53	20	1. 544	s	------	----	1. 526	19
-------	------	---	-----	---	------	----	1. 486	s	------	-----
310	1. 469	4	1. 463	5	1. 483	vw	1. 465	w	1. 462	6
221	------	---	1. 440	1	------	----	------	----	1. 441	4
-------	------	---	1. 411	1	------	----	------	----	------	-----
112	1. 427	36	-----	---	------	----	------	----	1. 382	14
301	1. 386	100	1. 381	60	1. 400	vs	1. 386	vs	1. 375	35
-------	------	---	1. 343	1	1. 342	vw	------	----	------	-----
311	1. 329	36	1. 322	8	1. 303	vvw	1. 323	w	1. 318	7
320	1. 284	18	-----	---	------	----	1. 289	vw	1. 282	1
212	1. 232	68	1. 229	6	1. 247	m	------	----	1. 228	6
-------	1. 191	11	-----	---	1. 185	w	------	----	------	-----
400	1. 164	25	1. 157	2	1. 138	s	1. 160	w	1. 1556	4
410	------	---	-----	---	------	----	------	----	1. 1217	6
222	1. 125	86	1. 118	16	1. 114	w	1. 121	ms	1. 1154	10
330	1. 097	58	1. 092	5	------	----	1. 095	mw	1. 0893	6
312	------	---	-----	---	------	----	------	----	1. 0555	4
411	1. 063	58	1. 054	6	1. 073	m	1. 058	ms	1. 0524	6
420	1. 042	43	-----	---	1. 045	vw	1. 039	mw	1. 0333	2
103	------	---	-----	---	------	----	------	----	0. 9937	1
322	0. 9994	4	-----	---	0. 9952	w	------	----	. 9812	2
421	. 9864	50	-----	---	------	----	0. 9759	w	. 9790	3
113	. 9773	18	-----	---	------	----	------	----	. 9715	2
500 430	------	---	-----	---	------	----	------	----	. 9249	1
402	. 9274	36	-----	---	. 9228	m	. 9259	mw	. 9216	4
213	. 9185	58	-----	---	------	----	. 9159	m	. 9128	7
510	. 9108	68	-----	---	------	----	. 9083	m	. 9068	4
412	------	---	-----	---	. 9011	m	------	----	. 9039	5
332	. 8925	79	-----	---	------	----	. 8866	vs	. 8867	6
431 501	------	---	-----	---	------	----	------	----	. 8849	8
223	. 8614	40	-----	---	------	----	. 8659	vw	. 8634	<1
422	. 8522	68	-----	---	. 8581	w	. 8575	mw	. 8559	4
303	. 8433	25	-----	---	. 8411	w	. 8503	m	. 8486	5
-------	------	---	-----	---	------	----	[a]. 8371	vw	------	-----

[a] Five additional lines have been omitted.

Copper (I) Chloride (nantokite), CuCl (cubic)

ASTM cards

Card number Old	Card number New	New index lines	Radiation	Source
1834	1845 1–0776 1–0759	3. 18 1. 93 1. 65	Molybdenum, 0.712.	Wyckoff and Posnjak [1] 1922.
1912	1931 1–0801 1–0793	3. 12 1. 91 1. 63	Molybdenum.	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns

Source	Radiation	Wave-length
Barth and Lunde [3] 1922	Copper	1. 539A

NBS sample. The cuprous-chloride sample used for the NBS pattern was obtained from the Baker Chemical Co. The sample was washed with glacial acetic acid to remove cupric chloride and dried with ether. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of silver, aluminum, calcium, magnesium, silicon, and tin; and 0.0001 to 0.001 percent each of barium, iron, and nickel. The refractive index of the NBS sample is above 1.93, but the exact value could not be resolved.

Interplanar spacings and intensity measurements. The *d*-spacings for the Wyckoff and Posnjak patterns were reduced to angstroms, and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units. The *d*-spacings for the Barth and Lunde pattern were calculated from Bragg angle data.

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

	1	2	3
Wyckoff and Posnjak	111	220	311
Hanawalt, Rinn, and Frevel	111	220	311
Barth and Lunde	111	220	311
Swanson, Fuyat, and Ugrinic	111	220	311

Lattice constant. Wyckoff and Posnjak [1] determined the structure in 1922. The space group is T_d^2–$F\bar{4}3m$ with zinc-sulfide-type structure and 4(CuCl) per unit cell.

Several unit-cell values were converted from

Copper(I) Chloride (nantokite), CuCl (cubic)

hkl	1922			1938			1925			1953		
	Wyckoff and Posnjak			Hanawalt, Rinn, and Frevel			Barth and Lunde			Swanson, Fuyat, and Ugrinic		
	Mo, 0.709 A			Mo, 0.709 A			Cu, 1.5405 A			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. 17	100	5. 49	3. 13	100	5. 42	3. 123	100	5. 409	3. 127	100	5. 416
200	----	---	----	2. 71	8	5. 42	----	---	---	2. 710	8	5. 420
220	1. 92	80	5. 43	1. 91	60	5. 40	1. 913	100	5. 411	1. 915	55	5. 416
311	1. 64	70	5. 44	1. 63	30	5. 41	[a] 1. 628	80	5. 399	1. 633	32	5. 416
400	----	---	----	1. 356	6	5. 424	1. 355	30	5. 420	1. 354	6	5. 416
331	1. 26	3	5. 49	1. 243	8	5. 418	1. 243	40	5. 418	1. 243	9	5. 418
422	1. 14	1	5. 58	1. 106	6	5. 418	1. 104	60	5. 408	1. 1054	8	5. 415
511	----	---	----	1. 045	4	5. 430	1. 042	40	5. 414	1. 0422	5	5. 415
440	----	---	----	---	---	---	0. 957	20	5. 414	0. 9574	2	5. 416
531	----	---	----	---	---	---	. 914	60	5. 407	. 9154	4	5. 416
620	----	---	----	---	---	---	----	---	---	. 8564	3	5. 416
Average of last five lines			5. 49	---	---	5. 420	----	---	5. 412	----	---	5. 416

[a] This line is from a second pattern not containing NaCl standard.

kX to angstrom units for comparison with the NBS values.

Lattice constants

		A
1922	Wyckoff and Posnjak [1]	5.50
1925	Barth and Lunde [3]	5.418
1942	Vegard and Skofteland [4]	5.4166
1953	Swanson, Fuyat, and Ugrinic	5.416 at 25° C

The thermal expansion in the room-temperature range is approximately 30×10^{-6}, according to Klemm, Tilk, and Müllenheim [5]. The density of cuprous chloride calculated from the NBS lattice constant is 4.138 at 25° C.

References

[1] R. W. G. Wyckoff and E. Posnjak, The crystal structures of the cuprous halides, J. Am. Chem. Soc. **44,** 30–36 (1922).

[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] T. Barth and G. Lunde, Lattice constants of the cuprous and silver halides, Norsk. Geol. Tidsskr. **8,** 281–292 (1925).

[4] L. Vegard and G. Skoftland, Röntgenometrische Untersuchungen der aus den substanzen CuCl, CuBr, und CuI gebildeten binären Mischkrystallsysteme, Chem. Zentr. 1943 I, 1243–4 (1943) as abstracted from Arch. Math. Naturvidenskab. **45,** 163–88 (1942).

[5] W. Klemm, W. Tilk, and S. V. Müllenheim, Dilatometrische Messung der Wärmeausdehnung zersetzlicher kristallisierter Salze, Z. anorg. u. allgem. Chem. **176,** 1–22 (1928).

Copper (I) Bromide, CuBr (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1598	1529	3.37	Molybdenum, 0.712A.	Wyckoff and Posnjak [1] 1922.
	1-0651	2.04		
	1-0645	1.75		
1680	1671	3.29	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.
	1-0707	2.01		
	1-0683	1.71		

Additional published patterns

Source	Radiation	Wavelength
Barth and Lunde [3] 1925	Copper Kα.	1.539 A

NBS sample. The cupric bromide used to prepare the NBS sample was obtained from the W. M. Welch Scientific Co. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of aluminum; 0.001 to 0.01 percent each of silver, calcium, chromium, iron, and titanium; 0.0001 to 0.001 percent each of barium, magnesium, nickel, and silicon; and less than 0.0001 percent each of manganese and lead. The cupric bromide was heated at 200° C to produce cuprous bromide. Another sample produced by the action of a water solution of cupric bromide on copper gave an identical diffraction pattern. The refractive index of cuprous bromide is too high to be measured by the usual grain-oil immersion methods.

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

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

	1	2	3
Wyckoff and Posnjak	111	220	311
Hanawalt, Rinn, and Frevel	111	220	311
Barth and Lunde	111	220	311
Swanson, Fuyat, and Ugrinic	111	220	311

Lattice constant. The structure was determined by Davey [4] and by Wyckoff and Posnjak [1] both in 1922. The space group is T_d^2-F$\bar{4}$3m with zinc-sulfide-type structure and 4(CuBr) per unit cell. An investigation of cuprous bromide by Hoshino [5] in 1952 disclosed three phases as follows: The gamma phase discussed in this report, which is stable at room temperature, converted to a hexagonal beta phase at 430° C and a body-centered cubic alpha phase at 480° C.

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

Lattice constants

		a
		A
1922--	Wyckoff and Posnjak [1]-----	5.83
1925--	Barth and Lunde [3]---------	5.692
1942--	Vegard and Skofteland [6]----	5.6921
1952--	Hoshino [5]------------------	5.6909
1953--	Swanson, Fuyat, and Ugrinic--	5.6905 at 26° C

The density of cuprous bromide calculated from the NBS lattice constant is 5.170 at 26° C.

Copper (I) Bromide, CuBr (cubic)

hkl	1922 Wyckoff and Posnjak Mo, 0.712 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1925 Barth and Lunde Cu, 1.5405 A			1953 Swanson, Fuyat, 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. 37	100	5. 84	3. 30	100	5. 72	3. 26	100	5. 65	3. 285	100	5. 690
200	----	---	----	-----	---	-----	------	---	-----	2. 846	3	5. 692
220	2. 04	80	5. 77	2. 01	67	5. 69	2. 016	90	5. 701	2. 012	59	5. 691
311	1. 75	60	5. 80	1. 71	50	5. 67	1. 719	70	5. 703	1. 716	36	5. 691
222	----	---	----	-----	---	-----	------	---	-----	1. 643	1	5. 692
400	----	---	----	1. 423	7	5. 692	1. 428	20	5. 713	1. 423	7	5. 692
331	1. 31	20	5. 71	1. 308	13	5. 701	1. 308	40	5. 702	1. 306	9	5. 693
420	----	---	----	-----	---	-----	------	---	-----	1. 272	2	5. 689
422	1. 18	10	5. 78	1. 162	13	5. 693	1. 163	50	5. 698	1. 1615	10	5. 6902
511	----	---	----	1. 096	7	5. 695	1. 096	40	5. 695	1. 0951	6	5. 6903
440	----	---	----	1. 010	3	5. 713	1. 009	20	5. 707	1. 0059	3	5. 6902
531	----	---	----	0. 964	3	5. 703	0. 9626	50	5. 695	0. 9619	4	5. 6907
600	----	---	----	-----	---	-----	------	---	-----	. 9484	2	5. 6904
620	----	---	----	-----	---	-----	. 9013	40	5. 700	. 8998	3	5. 6908
533	----	---	----	-----	---	-----	------	---	-----	. 8678	1	5. 6905
622	----	---	----	-----	---	-----	------	---	-----	. 8579	<1	5. 6907
444	----	---	----	-----	---	-----	------	---	-----	. 8214	<1	5. 6908
711	----	---	----	-----	---	-----	------	---	-----	. 7968	2	5. 6903
640	----	---	----	-----	---	-----	------	---	-----	. 7891	<1	5. 6903
Average unit cell value for last five lines-----			5. 80	-----	---	5. 701	------	---	5. 699	------	-----	5. 6905

References

[1] R. W. G. Wyckoff and E. Posnjak, The crystal structures of the cuprous halides, J. Am. Chem. Soc. **44**, 30–36 (1922).

[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] T. Barth and G. Lunde, Lattice constants of the cuprous and silver halides, Norsk Geol. Tidsskr. **8**, 281–292 (1925).

[4] W. P. Davey, The absolute sizes of certain monovalent and bivalent ions, Phys. Rev. **19**, 248–251 (1922).

[5] S. Hoshino, Crystal structure and phase transition of some metallic halides. II. On the phase transition and the crystal structures of cuprous bromide, J. Phys. Soc. Japan **7**, 560–4 (1952).

[6] L. Vegard and G. Skofteland, Röntgenometrische Untersuchungen der aus den Substanzen CuCl, CuBr, und CuJ gebildeten binären mischkristallsysteme, Arch. Math. Naturvidenskab. **45**, 163–188 (1942).

Copper (I) Iodide (marshite), CuI (cubic)

ASTM cards

Old card number	New card number	New index lines	Radiation	Source
1405	1315 1-0566 1-0561	3. 52 2. 15 1. 84	Molybdenum, 0.712 A.	Wyckoff and Posnjak [1] 1922.
II-869	1316 2-0389 2-0384	3. 52 2. 15 1. 83	Calculated pattern.	Waldo [2] 1935.
1449	1384 1-0599 1-0581	3. 49 2. 14 1. 82	Molybdenum	Hanawalt, Rinn, and Frevel [3] 1938.

The Waldo pattern was calculated from unit-cell data by Barth and Lunde [4]. No intensities were given in the original reference, although a set of intensity data appears on the ASTM cards.

Additional published patterns

Date	Source	Radiation	Wavelength
1922	Aminoff [5]	Iron	
1925	Barth and Lunde [4]	Copper	K_α 1.539 A.

NBS sample. The cuprous iodide used for the NBS pattern was obtained from the Fisher Scientific Co. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of aluminum and mercury; 0.001 to 0.01 percent each of barim, calcium, iron, magnesium lead, and silicon; and 0.0001 to 0.001 percent each of silver and tin. The refractive index of cuprous iodide is too high to be measured by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The *d*-spacings for the Aminoff and the Barth and Lunde patterns were calculated from Bragg angle data, and those for the Wyckoff, the Waldo, and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units. The *d*-spacing of 2.001 A in the Aminoff pattern is not possible in the cuprous-iodide structure and does not belong in the pattern.

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

	1	2	3
Wyckoff and Posnjak	111	220	311
Waldo	----	----	----
Hanawalt, Rinn, and Frevel	111	220	311
Aminoff	220	311	422
Barth and Lunde	220	422	531
Swanson, Fuyat, and Ugrinic	111	220	311

Lattice constant. The structure was determined by Wyckoff and Posnjak [1] in 1922. The space group is T_d^2-$F\bar{4}3m$ with sphalerite-type structure and 4(CuI) per unit cell. This gamma form is converted to the hexagonal beta form at 369° C, and to a cubic alpha form at 407° C, according to Miyake, Hoshino, and Takenaka [6].

A group of unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a
		A
1922	Aminoff [5]	6.03
1922	Wyckoff and Posnjak [1]	6.07
1925	Barth and Lunde [4]	6.059
1942	Vegard and Skoftland [7]	6.0549
1948	Mehmel [8]	6.06
1952	Miyake, Hoshino, and Takenaka [6]	6.0527 at 20° C
1953	Swanson, Fuyat, and Ugrinic	6.0507 at 26° C

The density of cuprous iodide calculated from the NBS lattice constant is 5.710 at 26° C.

Copper (I) Iodide (marshite), CuI (cubic)

hkl	1922 Wycoff and Posnjak Mo, 0.712 A			1935 Waldo Calculated Pattern			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1922 Aminoff Fe, 1.93597 A			1925 Barth and Lunde Cu, 1.5405 A			1953 Swanson, Fuyat, 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*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	3. 51	100	6. 11	3. 50	---	6. 06	3. 50	100	6. 06	3. 431	m	5. 94	3. 506	50	6. 073	3. 493	100	6. 050
200	---	---	---	3. 03	---	6. 06	3. 02	6	6. 04	---	---	---	(a)	10	---	3. 025	12	6. 050
220	2. 14	90	6. 08	2. 14	---	6. 05	2. 14	80	6. 05	2. 128	s	6. 02	2. 139	100	6. 050	2. 139	56	6. 050
---	---	---	---	---	---	---	---	---	---	2. 001	w	---	---	---	---	---	---	---
311	1. 83	80	6. 10	1. 828	---	6. 063	1. 82	60	6. 04	1. 817	s	6. 03	1. 827	90	6. 059	1. 824	32	6. 050
222	---	---	---	1. 750	---	6. 062	---	---	---	---	---	---	(a)	10	---	1. 747	5	6. 052
400	---	---	---	1. 515	---	6. 060	1. 51	12	6. 04	1. 508	w	6. 03	1. 511	30	6. 044	1. 5127	7	6. 051
331	1. 37	20	6. 02	1. 385	---	6. 037	1. 389	20	6. 055	1. 387	ms	6. 046	1. 390	50	6. 059	1. 3881	11	6. 0505
420	---	---	---	1. 356	---	6. 064	1. 353	4	6. 051	1. 354	w	6. 055	(a)	30	---	1. 3529	4	6. 0504
422	1. 24	10	6. 07	1. 236	---	6. 055	1. 235	25	6. 050	1. 234	s	6. 045	1. 235	100	6. 050	1. 2351	10	6. 0507
511	---	---	---	1. 166	---	6. 059	1. 164	12	6. 048	1. 163	ms	6. 043	1. 164	80	6. 048	1. 1644	7	6. 0504
440	---	---	---	1. 071	---	6. 058	1. 072	2	6. 064	1. 068	s	6. 042	1. 069	50	6. 047	1. 0696	3	6. 0506
531	---	---	---	1. 024	---	6. 058	1. 022	8	6. 046	1. 021	s	6. 040	1. 022	100	6. 046	1. 0228	6	6. 0510
600	---	---	---	1. 010	---	6. 060	---	---	---	---	---	---	1. 009	46	6. 054	1. 0084	1	6. 0504
620	---	---	---	0. 959	---	6. 065	0. 958	6	6. 059	---	---	---	0. 9567	80	6. 051	0. 9568	3	6. 0513
533	---	---	---	. 925	---	6. 066	. 923	2	6. 053	---	---	---	. 9230	60	6. 053	. 9228	2	6. 0512
622	---	---	---	. 914	---	6. 063	---	---	---	---	---	---	. 9122	30	6. 051	. 9121	<1	6. 0502
444	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	. 8733	1	6. 0504
711	---	---	---	---	---	---	. 849	2	6. 063	---	---	---	---	---	---	. 8473	3	6. 0509
640	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	. 8391	<1	6. 0508
642	---	---	---	---	---	---	. 811	2	6. 069	---	---	---	---	---	---	. 8086	4	6. 0510
---	---	---	---	---	---	---	. 789	2	---	---	---	---	---	---	---	---	---	---
Average of last five lines	---		6. 07	---	---	6. 062	---	---	6. 058	---	---	6. 045	---	---	6. 051	---	---	6. 0507

[a] These lines covered by NaCl standards.

References

[1] R. W. G. Wyckoff and E. Posnjak, The crystal structures of the cuprous halides, J. Am. Chem. Soc. **44,** 30–36 (1922).

[2] A. W. Waldo Identification of the copper ore minerals by means of X-ray powder diffraction patterns, Am. Mineralogist **20,** 590 (1935).

[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] T. Barth and G. Lunde, Lattice constants of the cuprous and silver halides, Norsk Geol. Tidsskr. **8,** 281–292 (1925).

[5] G. Aminoff, Über die Kristallstruktur von Jodsilber, Marshit (CuJ) und Miersit (4AgJ·CuJ), Geol. Fören. i Stockholm Förh. **44,** 444–481 (1922).

[6] S. Miyake, S. Hoshino, and T. Takenaka, On the phase transition in cuprous iodide, J. Phys. Soc. Japan **7,** 19–24 (1952).

[7] L. Vegard and G. Skoftland, Röntgenometric investigation of the series of binary solid solutions formed from the substances CuCl, CuBr, and CuI, Arch. Math. Naturvidenskab. **45,** 163–88 (1942).

[8] M. Mehmel, Kristallchemische Betrachtungen zur I. und VII. Gruppe des periodischen Systems der Elemente, Optik **3,** 41–6 (1948).

Strontium Chloride, $SrCl_2$ (cubic)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wave-length
Mark and Tolksdorf [1] 1925	Copper	Kα

NBS sample. The strontium chloride used for the NBS pattern was obtained from the Fisher Scientific Co. as the hexahydrate. Spectrographic analysis of the hexahydrate at the NBS showed the following impurities: 0.01 to 0.1 percent of calcium; 0.001 to 0.01 percent of magnesium; 0.0001 to 0.001 percent each of aluminum, barium, manganese, and silicon; and less than 0.0001 percent each of silver, copper, and iron.

The anhydrous salt, prepared by dehydrating the hexahydrate at 300° C, hydrated so readily that it was necessary to make the pattern in two sections, using a freshly dehydrated sample mounted in petrolatum for each part. The refractive index of the NBS sample was not determined because of this rapid hydration.

Interplanar spacings and intensity measurements. The *d*-spacings for the Mark and Tolksdorf pattern were calculated from Bragg angle data.

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

	1	2	3
Mark and Tolksdorf	220	642	822
Swanson, Fuyat, and Ugrinic	220	111	311

The Mark and Tolksdorf pattern contains a *d*-spacing of 2.260 angstrom units, which is not permissible in the strontium-chloride structure. Two *d*-spacings of 3.466 and 2.054 angstrom units are possible in the structure but are not present in the NBS pattern.

Lattice constant. The structure was determined by Mark and Tolksdorf [1] in 1925. The space group is O_h^5-Fm3m with calcium-fluoride-type structure and 4($SrCl_2$) per unit cell.

Two unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a
		A
1925	Mark and Tolksdorf [1]	7.01
1926	Ott [2]	6.979 at 20° C.
1953	Swanson, Fuyat, and Ugrinic	6.9767 at 26° C

The density of strontium chloride calculated from the NBS lattice constant is 3.101 at 26° C.

Strontium Chloride, $SrCl_2$ (cubic)

hkl	1925 Mark and Tolksdorf Cu, 1.5418 A			1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	4. 1	w	7. 1	4. 03	59	6. 98
---	3. 47	vw	----	------	--	------
220	2. 39	s	6. 75	2. 467	100	6. 978
---	2. 26	vvw	----	------	--	------
311	2. 15	w	7. 12	2. 104	44	6. 978
---	2. 05	w	----	------	--	------
400	1. 72	ms	6. 87	1. 745	20	6. 980
331	1. 57	ms	6. 84	1. 600	17	6. 974
422	1. 41	ms	6. 91	1. 424	28	6. 976
511	1. 32	w	6. 88	1. 343	12	6. 978
440	1. 22	ms	6. 92	1. 233	10	6. 975
531	1. 17	w	6. 92	1. 1794	11	6. 9774
620	1. 09	ms	6. 91	1. 1032	12	6. 9772
533	-----	---	----	1. 0640	4	6. 9771
444	-----	---	----	1. 0070	4	6. 9767
711	0. 978	w	6. 98	0. 9769	7	6. 9765
642	. 932	s	6. 97	. 9323	14	6. 9767
731	. 911	ms	6. 99	. 9083	7	6. 9768
800	-----	---	----	. 8721	3	6. 9768
733	. 845	vvw	6. 92	. 8523	2	6. 9764
822	. 824	s	6. 99	. 8222	10	6. 9766
751	-----	---	----	. 8056	6	6. 9767
Average of last five lines			6. 97	------	--	6. 9767

References

[1] H. Mark and S. Tolksdorf, Über das Beugungsvermögen der Atome für Röntgenstrahlen, Z. Physik. **33,** 681–687 (1925).

[2] H. Ott, Die Strukturen von MnO, MnS, AgF, NiS, SnJ_4, $SrCl_2$, BaF_2; Präzisionsmessungen einiger Alkalihalogenide, Z. Krist. **63,** 222–230 (1926)

Rubidium Chloride, RbCl (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1721	1622	3.25	Molybdenum, 0.712 A.	Davey [1] 1923.
	1-0684	3.77		
	1-0707	2.29		
--------	1660	3.29	Copper, 1.53923A	Olhausen [2] 1925.
	3-0476	2.34		
	3-0458	3.69		
1677	1662	3.29	Molybdenum	Hanawalt, Rinn, and Frevel [3] 1938.
	1-0702	2.32		
	1-0681	3.80		

The following pattern made at −190° C is the same sodium-chloride-type structure as the room-temperature patterns listed above, but differs considerably due to contraction of the lattice.

--------	3691	1.85	Copper	Wagner and Lippert [4] 1936.
	3-1097	3.21		
	3-1097	2.27		

Additional published patterns

Source	Radiation	Wave-length
		A
Ott [5] 1924	Copper	----------
Wasastjerna [6] 1944	Copper	Kα

NBS sample. The rubidium chloride used for the NBS pattern was obtained from the Fairmount Chemical Co. Spectrographic analysis at the NBS showed the following impurities: 0.1 to 1.0 percent of potassium; 0.01 to 0.1 percent of calcium; 0.001 to 0.01 percent each of barium, cesium, sodium, and silicon; 0.0001 to 0.001 percent each of aluminum, chromium, copper, magnesium, molybdenum, and strontium; and less than 0.0001 percent each of silver and iron. The refractive index of the NBS sample is 1.494.

Interplanar spacings and intensity measurements. The *d*-spacings for the Davey and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units; the *d*-spacings for the Olshausen, the Ott, and the Wasastjerna patterns were calculated from Bragg angle data.

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

	1	2	3
Davey	200	111	220
Olshausen	200	220	111
Hanawalt, Rinn, and Frevel	200	220	111
Ott	200	220	222
Swanson, Fuyat, and Ugrinic	200	220	111

The Wasastjerna pattern did not include intensity data.

Lattice constant. The structure was determined by Wyckoff [7] in 1921. The space group is O_h^5-Fm3m with sodium-chloride-type structure and 4(RbCl) per unit cell.

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

Lattice constants

		a
		A
1921	Wyckoff [7]	6.61
1923	Davey [1]	6.548
1923	Spangenberg [8]	6.591
1924	Havighurst, Mack, and Blake [9].	6.584
1925	Olshausen [2]	6.587
1926	Ott [10]	6.548 at 20° C
1953	Swanson, Fuyat, and Ugrinic	6.5810 at 27° C

The density of rubidium chloride calculated from the NBS lattice constant is 2.818 at 27° C

Rubidium Chloride, RbCl (cubic)

hkl	1923			1925			1938			1924			1944		1953		
	Davey			Olshausen			Hanawalt, Rinn, and Frevel			Ott			Wasastjerna		Swanson, Fuyat, and Ugrinic		
	Mo, 0.709 A			Cu, 1.5405 A			Mo. 0.709 A			Cu, 1.5405 A			Cu, 1.5405 A		Cu, 1.5405 A, 27° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*	*A*	*A*		*A*
111	3. 76	67	6. 51	3. 68	md	6. 37	3. 81	17	6. 60	-----	----	-----	3. 80	6. 58	3. 80	29	6. 58
200	3. 24	100	6. 48	3. 29	s	6. 58	3. 30	100	6. 60	3. 292	s	6. 584	3. 29	6. 58	3. 291	100	6. 582
220	2. 28	67	6. 45	2. 334	s	6. 60	2. 32	57	6. 56	2. 325	s	6. 576	2. 325	6. 576	2. 327	65	6. 582
311	1. 967	17	6. 52	1. 982	m	6. 57	1. 98	11	6. 57	2. 000	w	6. 633	1. 983	6. 577	1. 984	13	6. 580
222	1. 886	33	6. 53	1. 904	m	6. 60	1. 89	17	6. 55	1. 900	s	6. 582	1. 898	6. 575	1. 900	20	6. 582
400	1. 630	25	6. 52	1. 644	md	6. 58	1. 64	11	6. 56	1. 636	m	6. 544	1. 644	6. 576	1. 645	9	6. 580
331	1. 494	17	6. 51	1. 503	w	6. 55	1. 50	6	6. 54	-----	----	-----	1. 509	6. 578	1. 510	4	6. 582
420	1. 460	33	6. 53	1. 474	m	8. 59	1. 471	17	6. 578	1. 469	s	6. 570	1. 471	6. 578	1. 472	20	6. 583
422	1. 330	25	6. 52	1. 341	m	6. 57	1. 343	11	6. 579	1. 342	s	6. 574	1. 342	6. 574	1. 343	14	6. 579
511	-----	----	-----	1. 263	vw	6. 56	-----	----	-----	1. 265	s	6. 573	1. 266	6. 578	1. 266	4	6. 578
440	-----	----	-----	1. 161	w	6. 57	-----	----	-----	1. 160	s	6. 562	1. 1624	6. 5755	1. 1637	3	6. 583
531	-----	----	-----	1. 112	w	6. 58	-----	----	-----	-----	----	-----	1. 1116	6. 5763	1. 1123	2	6. 580
600	-----	----	-----	1. 097	m	6. 58	1. 097	6	6. 582	1. 095	s	6. 570	1. 0960	6. 5760	1. 0968	5	6. 581
620	-----	----	-----	1. 042	m	6. 59	-----	----	-----	1. 038	s	6. 565	1. 0397	6. 5757	1. 0404	5	6. 580
533	-----	----	-----	-----	----	-----	-----	----	-----	-----	----	-----	1. 0028	6. 5758	1. 0034	1	6. 580
622	-----	----	-----	0. 992	m	6. 58	-----	----	-----	0. 989	s	6. 560	0. 9913	6. 5755	0. 9920	3	6. 580
444	-----	----	-----	. 952	w	6. 60	-----	----	-----	-----	----	-----	. 9490	6. 5749	. 9497	2	6. 580
711	-----	----	-----	. 918	m	6. 55	-----	----	-----	-----	----	-----	. 9207	6. 5751	. 9215	1	6. 5808
640	-----	----	-----	-----	----	-----	-----	----	-----	. 911	s	6. 569	. 9118	6. 5751	. 9126	3	6. 5809
642	-----	----	-----	. 885	m	6. 62	-----	----	-----	. 878	s	6. 570	. 8787	6. 5756	. 8794	5	6. 5808
731	-----	----	-----	-----	----	-----	-----	----	-----	-----	----	-----	. 8562	6. 5766	. 8568	2	6. 5812
800	-----	----	-----	-----	----	-----	-----	----	-----	-----	----	-----	. 8220	6. 5760	. 8227	2	6. 5816
733	-----	----	-----	-----	----	-----	-----	----	-----	-----	----	-----	------	------	. 8040	1	6. 5810
820	-----	----	-----	-----	----	-----	-----	----	-----	-----	----	-----	------	------	. 7980	4	6. 5805
Average of the last five lines--------			6. 52	-----	----	6. 59	-----	----	6. 568	-----	----	6. 567	------	6. 5757	------	---	6. 5810

References

[1] W. P. Davey, Precision measurements of crystals of the alkali halides, Phys. Rev. **21**, 143–161 (1923).

[2] S. v. Olshausen, Strukturuntersuchungen nach der Debye-Scherrer-Methode, Z. Krist. **61**, 463–514 (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] G. Wagner and L. Lippert, Über polymorphe Umwandlungen bei einfachen Ionengittern. I. Versuche zur Umwandlung; NaCl→CsCl→Gitter, Z. physik. Chem. **B33**, 297–303 (1936)

[5] H. Ott, Über eine Verwendung der Pulvermethode zur röntgenometrischen Präzisionsbestimmung von Gitterkonstanten, Sitzungsberichte der mathematisch-physikalischen Klasse der Bayerischen Akademie der Wissenschaften zu München 31–37 (1924).

[6] J. A. Wasastjerna, Eine röntgenometrische Untersuchung von Kaliumbromid und Rubidiumchlorid, Acta Soc. Sci. Fennicae n. s. A, **3**, no. 6 (1944).

[7] R. W. G. Wyckoff, The crystal structures of the alkali halides, J. Wash. Acad. Sci. **11**, 429–434 (1921).

[8] K. Spangenberg, Dichte und Lichtbrechung der Alkalihalogenide Z. Krist. **57**, 494–534 (1923).

[9] R. J. Havighurst, E. Mack, and F. C. Blake, Precision crystal measurements on some alkali and ammonium halides, J. Am. Chem. Soc. **46**, 2368–2374 (1924).

[10] H. Ott, Die Strukturen von MnO, MnS, AgF, NiS, SnJ_4, $SrCl_2$, BaF_2; Präzisionsmessungen einiger Alkalihalogenide, Z. Krist. **63**, 222–230 (1926).

Rubidium Iodide, RbI (cubic)

ASTM cards

Card number		New Index lines	Radiation	Source
Old	New			
1272	1211 1–0521 1–0513	3.66 2.58 1.63	Molybdenum	Hanawalt Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wave-length
Davey [2] 1923	Molybdenum	0.712A

NBS sample. The rubidium iodide used for the NBS pattern was obtained from the Fairmount Chemical Co. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of calcium, potassium, sodium, and phosphorous; 0.001 to 0.01 percent each of barium, cesium, magnesium, and silicon; 0.0001 to 0.001 percent each of silver, aluminum, and strontium; and less than 0.0001 percent each of beryllium, chromium, copper, iron, manganese, and lead. The refractive index of the NBS sample could not be measured because the rubidium iodide reacted with the index liquids.

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

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

	1	2	3
Hanawalt, Rinn, and Frevel	200	220	420
Davey	200	220	111
Swanson, Fuyat, and Ugrinic	200	220	222

Lattice constant. The structure was determined by Wyckoff [3] in 1921. The space group is O_h^5-Fm3m with sodium-chloride-type structure and 4(RbI) per unit cell.

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

Lattice constants

		a
		A
1921	Wyckoff [3]	7.37
1923	Davey [2]	7.324
1923	Spangenberg [4]	7.348
1924	Havighurst, Mack, and Blake [5].	7.340
1953	Swanson, Fuyat, and Ugrinic	7.342 at 27° C

The density of rubidium iodide calculated from the NBS lattice constant is 3.564 at 27° 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. P. Davey, Precision measurements of crystals of the alkali halides, Phys. Rev. **21,** 143–161 (1923).

[3] R. W. G. Wyckoff, The crystal structures of the alkali halides, J. Wash. Acad. Sci. **11,** 429–434 (1921).

[4] K. Spangenberg, Dichte und Lichtbrechung der Alkalihalogenide, Z. Krist. **57,** 494–534 (1923).

[5] R. J. Havighurst, E. Mack, and F. C. Blake, Precision crystal measurements on some alkali and ammonium halides, J. Am. Chem. Soc. **46,** 2368–2374 (1924).

Rubidium Iodide, RbI (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1923 Davey Mo, 0.709 A			1953 Swanson, Fuyat and Ugrinic Cu, 1.5405 A, 27° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	4.25	4	7.36	4.22	14	7.31	4.24	8	7.34
200	3.67	100	7.34	3.68	100	7.36	3.67	100	7.34
220	2.58	80	7.30	2.58	28	7.30	2.595	60	7.340
311	2.20	4	7.30	2.20	7	7.30	2.214	4	7.343
222	2.11	20	7.31	2.11	14	7.31	2.119	19	7.340
400	1.83	15	7.32	1.821	7	7.284	1.835	9	7.340
331	-----	-----	-----	-----	-----	-----	1.684	2	7.340
420	1.63	32	7.29	1.629	14	7.285	1.642	18	7.343
422	1.496	16	7.329	1.487	14	7.285	1.498	11	7.339
440	1.294	4	7.320	1.287	7	7.280	1.298	4	7.342
600	1.222	8	7.332	1.213	7	7.278	1.224	6	7.344
620	1.159	4	7.330	1.151	7	7.280	1.1610	5	7.343
622	1.105	4	7.330	1.097	7	7.277	1.1068	3	7.342
640	-----	-----	-----	1.010	7	7.283	1.0181	2	7.342
642	-----	-----	-----	0.972	7	7.274	0.9808	2	7.340
820	-----	-----	-----	-----	-----	-----	.8903	3	7.342
Average of last five lines			7.328	-----	-----	7.278	------	-----	7.342

Silver Chloride (cerargyrite), AgCl (cubic)

ASTM cards

Old card number	New card number	New index lines	Radiation	Source
2487	2644 1–1021 1–1013	2.77 1.96 3.20	Molybdenum	Hanawalt, Rinn and Frevel [1] 1938.
11–1777	2641 2–0855 2–0848	2.77 1.97 3.20	Copper	Harcourt [2] 1942.

The Harcourt pattern was made by using copper radiation rather than molybdenum, as the ASTM card states.

Additional published patterns

Source	Radiation	Wavelength
Barth and Lunde [3] 1926	Copper	1.539 A

NBS sample. The silver chloride was prepared at the NBS by precipitation from a solution of silver nitrate by the addition of potassium chloride. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of aluminum and iron; 0.001 to 0.01 percent each of magnesium and silicon; 0.0001 to 0.001 percent each of calcium, copper, and lead; and less than 0.0001 percent of manganese. The refractive index is too high to be measured by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The *d*-spacings for the Barth and Lunde pattern were calculated from Bragg angle data; the Hanawalt, Rinn, and Frevel, and the Harcourt *d*-spacings were converted from kX to angstrom units. The Harcourt pattern contains a *d*-spacing at 2.81 A, which is not possible in the silver-chloride structure.

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

	1	2	3
Hanawalt, Rinn, and Frevel	200	220	111
Harcourt	-----	200	220
Barth and Lunde	200	600	220
Swanson, Fuyat, and Ugrinic	200	220	111

Lattice constant. The structure was investigated by Davey [4] in 1922. The space group is O_h^5-Fm3m with sodium-chloride-type structure and 4(AgCl) per unit cell.

A group of unit-cell values were converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		a
		A
1922	Davey [4]	5.53
1923	Wilsey [5]	5.551
1925	Broomé [6]	5.545
1926	Barth and Lunde [3]	5.556
1940	Wilman [7] (electron diffraction data).	5.558
1953	Swanson, Fuyat, and Ugrinic	5.5491 at 26° C

The coefficient of expansion in the room-temperature range is 31.0×10^{-6}, according to Sharma [8].

The density of silver chloride calculated from the NBS lattice constant is 5.571 at 26° C.

Silver Chloride (cerargyrite), AgCl (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1942 Harcourt Cu, 1.5405 A			1926 Barth and Lunde Cu, 1.5405 A			1953 Swanson, Fuyat, 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. 21	40	5. 56	3. 21	40	5. 56	3. 22	20	5. 58	3. 203	49	5. 548
------	-----	-----	-----	2. 81	100	----	-----	-----	-----	------	-----	------
200	2. 78	100	5. 56	2. 76	100	5. 52	2. 78	100	5. 57	2. 774	100	5. 548
220	1. 96	75	5. 54	1. 97	70	5. 57	1. 95	80	5. 55	1. 962	50	5. 549
311	1. 67	20	5. 54	1. 67	30	5. 54	1. 67	60	5. 54	1. 673	15	5. 549
222	1. 60	25	5. 54	1. 61	40	5. 58	1. 60	60	5. 55	1. 602	15	5. 549
400	1. 388	9	5. 552	1. 398	20	5. 59	1. 389	60	5. 56	1. 387	6	5. 548
331	1. 273	6	5. 549	1. 277	20	5. 57	1. 270	20	5. 54	1. 273	3	5. 549
420	1. 243	20	5. 559	1. 248	40	5. 58	1. 243	80	5. 56	1. 241	11	5. 550
422	1. 133	13	5. 551	-----	-----	----	1. 133	70	5. 55	1. 1326	7	5. 5486
511	1. 067	1	5. 544	-----	-----	----	1. 068	40	5. 549	1. 0680	3	5. 5495
440	0. 982	1	5. 555	0. 989	20	5. 60	0. 982	40	5. 555	0. 9810	2	5. 5494
531	. 939	1	5. 555	-----	-----	----	. 938	40	5. 553	. 9380	2	5. 5493
600	. 926	4	5. 556	. 932	20	5. 51	. 926	100	5. 558	. 9248	3	5. 5488
620	. 879	1	5. 559	. 885	20	5. 60	. 878	-----	5. 556	. 8774	3	5. 5492
533	-----	-----	-----	. 845	20	5. 54	-----	-----	-----	. 8462	2	5. 5489
622	. 838	1	5. 559	-----	-----	----	-----	-----	-----	. 8366	3	5. 5494
Average unit cell value for last five lines			5. 544	-----	-----	5. 56	-----	-----	5. 554	------	-----	5. 5491

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. Mineralogist **27,** 63–113 (1942).

[3] T. Barth and G. Lunde, Beiträge zur Kenntnis der Mischkristalle, Z. physik. Chem. **122,** 293–334 (1926).

[4] W. P. Davey, The absolute sizes of certain monovalent and bivalent ions, Phys. Rev. **19,** 248–251 (1922).

[5] R. B. Wilsey, The crystalline structures of silver iodide, Phil. Mag. **46,** 487–496 (1923).

[6] B. H. Broomé, Röntgenographische Untersuchung einiger Mischkristalle der Systeme (Na, Ag) Cl und K(Cl, Br), Z. anorg. u. allgem. Chem. **143,** 60–75 (1925).

[7] H. Wilman, The structure and orientation of silver halides, Proc. Phys. Soc. (London) **52,** 323–347 (1940).

[8] S. S. Sharma, Thermal expansion of crystals; IV, Silver chloride, lithium fluoride, and magnesium oxide, Proc. Indian Acad. Sci. **32A,** 268–274 (1950).

Silver Bromide (bromyrite), AgBr (cubic)

ASTM cards

Old card numbers	New card numbers	New index lines	Radiation	Source
II-2970	3583 2-1265 2-1269	2. 00 1. 28 1. 17	Iron	Natta and Vecchia [1] 1933.
2315	2455 1-0972 1-0950	2. 88 2. 03 1. 66	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns

Source	Radiation	Wave-length
Barth and Lunde [3] 1925	Copper	1.539A

NBS sample. The silver bromide was prepared at the NBS by precipitation from a solution of silver nitrate by the addition of potassium bromide. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of aluminum and silicon; 0.001 to 0.01 percent each of iron, indium, and zirconium; and 0.0001 to 0.001 percent each of calcium, copper, and magnesium. The refractive index of silver bromide is too high to be measured by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The *d*-spacings for the Natta and Vecchia and the Barth and Lunde patterns were calculated from Bragg angle data; the Hanawalt, Rinn, and Frevel *d*-spacings were converted from kX to angstrom units. The first three lines of the Natta and Vecchia pattern are in poor agreement with the calculated pattern and could cause confusion in the identification of an unknown.

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

	1	2	3
Natta and Vecchia	220	420	422
Hanawalt, Rinn, and Frevel	200	220	222
Barth and Lunde	200	220	420
Swanson, Fuyat, and Ugrinic	200	220	222

Lattice constants. The structure was determined by Wilsey [4] in 1923. The space group is O_h^5–Fm3m with sodium-chloride-type structure, 4(AgBr) per unit cell.

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

Lattice constants

		a
		A
1922	Davey [5]	5.79
1923	Wilsey [4]	5.780
1925	Barth and Lunde [3]	5.767
1940	Wilman [6] (electron diffraction data).	5.776
1951	Berry [7]	5.7745 at 25° C
1953	Swanson, Fuyat, and Ugrinic	5.7745 at 26° C

The density of silver bromide calculated from the NBS lattice constant is 6.477 at 26° C.

References

[1] G. Natta and O. Vecchia, Struttura e polimorfismo del cianuro di argento, Gazz. chim. ital. **63,** 439–448 (1933).

[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] T. Barth and G. Lunde, Lattice constants of the cuprous and silver halides, Norsk Geol. Tidsskr. **8,** 281 (1925).

[4] R. B. Wilsey, The crystalline structures of silver bromide, Phil. Mag. **46,** 487–96 (1923).

[5] W. P. Davey, The absolute sizes of certain monovalent and bivalent ions, Phys. Rev. **19,** 248–51 (1922).

[6] H. Wilman, The structure and orientation of silver halides, Proc. Phys. Soc. (London) **52,** 323 (1940).

[7] C. R. Berry, Lattice defects in silver bromide, Phys. Rev. **82,** 422–3 (1951).

Silver Bromide (bromyrite), AgBr (cubic)

hkl	1933 Natta and Vecchia Fe, 1.93597 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1925 Barth and Lunde Cu, 1.5405 A			1953 Swanson, Fuyat, 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. 333	7	5. 773
200	2. 80	s	5. 60	2. 89	100	5. 78	2. 875	100	5. 751	2. 886	100	5. 772
---	2. 20	m	------	-----	-----	-----	-----	-----	-----	------	-----	-------
220	2. 00	vs	6. 62	2. 03	60	5. 74	2. 041	100	5. 772	2. 041	56	5. 773
311	-----	-----	------	-----	-----	-----	-----	<10	-----	1. 742	2	5. 778
222	1. 64	ms	5. 68	1. 66	20	5. 75	1. 661	50	5. 755	1. 667	15	5. 775
400	1. 427	m	5. 71	1. 444	8	5. 776	1. 440	30	5. 761	1. 444	7	5. 776
331	-----	-----	------	1. 323	2	5. 767	-----	-----	-----	1. 325	7	5. 776
420	1. 280	vs	5. 72	1. 292	20	5. 778	1. 290	70	5. 770	1. 291	13	5. 774
422	1. 171	vs	5. 74	1. 180	12	5. 781	1. 176	60	5. 761	1. 1787	9	5. 7744
440	1. 018	ms	5. 76	1. 021	2	5. 776	1. 019	20	5. 764	1. 0207	3	5. 7740
600	-----	-----	------	0. 965	2	5. 790	0. 961	60	5. 765	0. 9624	4	5. 7744
620	-----	-----	------	. 915	2	5. 787	. 912	50	5. 767	. 9131	3	5. 7750
622	-----	-----	------	. 873	2	5. 791	. 870	-----	5. 769	. 8705	3	5. 7742
444	-----	-----	------	-----	-----	-----	-----	-----	-----	. 8336	2	5. 7750
640	-----	-----	------	-----	-----	-----	-----	-----	-----	. 8007	3	5. 7741
Average unit cell value for last five lines-----			[a] 5. 74	-----	-----	5. 785	-----	-----	5. 765	------	-----	5. 7745

[a] Average of last three lines.

Cesium Iodide, CsI (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1753	1768 1–0743 1–0722	3. 23 1. 86 2. 28	Molybdenum 0.712.	Davey [1] 1923.
1768	1769 1–0744 1–0730	3. 22 1. 86 2. 27	Molybdenum.	Hanawalt, Rinn and Frevel [2] 1938.

Additional published patterns

Source	Radiation	Wave-length
Wasastjerna [3] 1944------------	Copper---	K_α

NBS sample. The cesium iodide used for the NBS pattern was obtained from the Harshaw Chemical Co. Chemical analysis at the NBS showed the following impurities: 0.0025 percent of potassium; 0.001 percent each of sodium, bromine, and chlorine; and less than 0.001 percent each of calcium and magnesium. The refractive index of the NBS sample could not be measured because the cesium iodide reacted with the index liquids.

Interplanar spacings and intensity measurements. The *d*-spacings for the Davey and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units; the Wasastjerna pattern was calculated from Bragg angle data.

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

	1	2	3
Davey------------------------------	110	211	200
Hanawalt, Rinn, and Frevel------------	110	211	200
Swanson, Fuyat, and Ugrinic----------	110	211	200

The Wasastjerna pattern did not include intensity data.

Lattice constant. The structure was determined by Wyckoff [4] in 1921. The space group is O_h^1-Pm3m with cesium chloride-type structure and 1(CsI) per unit cell.

Several unit-cell values were converted from kX to angstrom units, and the Rymer and Hambling value published in angstroms was converted from 20° to 26° C for comparison with the NBS values, using their value for the coefficient of expansion, 4.86×10^{-5} [5].

Lattice constants

		a
		A
1921	Wyckoff [4]	4.56
1923	Clark and Duane [6]	4.571
1923	Davey [1]	4.567
1923	Spangenberg [7]	4.532
1951	Rymer and Hambling [5]	4.5680
1953	Swanson, Fuyat, and Ugrinic	4.5679 at 26° C

The density of cesium iodide calculated from the NBS lattice constant is 4.525 at 26° C.

Cesium Iodide, CsI (cubic)

hkl	1923 Davey Mo, 0.709 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1944 Wasastjerna Cu, 1.5418 A			1953 Swanson, Fuyat, 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*
110	3. 22	100	4. 55	3. 23	100	4. 57	3. 23	---	4. 57	3. 230	100	4. 568
200	2. 27	40	4. 54	2. 27	15	4. 54	2. 29	---	4. 58	2. 284	20	4. 568
211	1. 857	80	4. 549	1. 86	38	4. 56	1. 86	---	4. 56	1. 865	33	4. 568
220	1. 609	25	4. 551	1. 61	10	4. 55	1. 62	---	4. 58	1. 615	18	4. 569
310	1. 439	30	4. 551	1. 438	13	4. 547	1. 44	---	4. 55	1. 445	8	4. 569
222	1. 314	6	4. 552	---	---	----	1. 32	---	4. 57	1. 319	4	4. 568
321	1. 216	25	4. 550	1. 220	10	4. 565	1. 22	---	4. 56	1. 221	10	4. 568
400	1. 137	3	4. 548	---	---	----	1. 14	---	4. 56	1. 1421	2	4. 5684
411	1. 073	6	4. 552	1. 076	4	4. 565	1. 08	---	4. 58	1. 0766	6	4. 5676
420	1. 016	4	4. 544	---	---	----	1. 02	---	4. 56	1. 0215	3	4. 5683
332	0. 969	4	4. 545	---	---	----	0. 975	---	4. 573	0. 9740	2	4. 5685
422	. 928	3	4. 546	---	---	----	. 933	---	4. 571	. 9323	2	4. 5675
510	. 892	6	4. 548	---	---	----	. 896	---	4. 569	. 8957	4	4. 5674
521	. 828	3	4. 535	---	---	----	. 834	---	4. 568	. 8340	2	4. 5679
440	---	---	---	---	---	----	---	---	---	. 8075	1	4. 5679
530	. 778	3	4. 536	---	---	----	---	---	---	----	---	------
611	. 737	2	4. 543	---	---	----	---	---	---	----	---	------
Average of last five lines			4. 542	---	---	[a] 4. 559	---	---	4. 568	----	---	4. 5679

[a] Average of last three lines.

References

[1] W. P. Davey, Precision measurements of crystals of the alkali halides, Phys. Rev. **21**, 143–161 (1923).

[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] J. A. Wasastjerna, Eine röntgenometrische Untersuchung von Natriumfluorid, Kaliumjodid und Caesiumjodid, Acta Soc. Sci. Fennicae n. s. A, **3**, no. 7 (1944).

[4] R. W. G. Wyckoff, The crystal structures of the alkali halides, J. Wash. Acad. Sci. **11**, 429–434 (1921).

[5] T. B. Rymer and P. G. Hambling, The lattice constant of cesium iodide, Acta Cryst. **4**, 565 (1951).

[6] G. L. Clark and W. Duane, A new method of crystal analysis and the reflection of characteristic X-rays, J. Opt. Soc. Amer. **7**, 455–482 (1923).

[7] K. Spangenberg, Dichte und Lichtbrechung der Alkalihalogenide, Z. Krist. **57**, 494–534 (1923).

Mercury (I) Iodide, HgI (tetragonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1450	1380 1-0597 1-0591	3.48 2.23 2.90	Molybdenum, 0.710 A.	Havighurst [1] 1925.
--------	1395 3-0383 3-0376	3.48 1.11 2.22	Iron, 1.9323 A.	Hylleraas [2] 1926.
1447	1381 1-0598 1-0580	3.49 2.23 2.90	Molybdenum	Hanawalt, Rinn, and Frevel [3] 1938.

Additional published patterns. None.

NBS sample. The mercurous iodide used for the NBS pattern was obtained from the Fisher Scientific Co. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, and sodium; and 0.0001 to 0.0001 percent each of silver, copper, iron, magnesium, lead, silicon, and tin. The refractive indices of mercurous iodide are too high to be determined by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The *d*-spacings for the Hylleraas pattern were calculated from Bragg angle data; *d*-spacings for the Havighurst pattern were converted from Mo K_α, 0.710 A, to Mo $K_{\alpha 1}$, 0.709 A; and 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:

	1	2	3
Havighurst	110	114	004
Hylleraas	110	219	114
Hanawalt, Rinn, and Frevel	110	114	004
Swanson, Fuyat, and Ugrinic	110	114	200

Lattice constants. The structure was first investigated by Hylleraas [2] in 1925. The space group is D_{4h}^{17}-I4/mmm with mercurous-chloride-type structure and 4(HgI) per unit cell.

A group of unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1925	Havighurst [1]	4.93	11.63
1925	Hylleraas [4]	4.92	11.59
1927	Huggins and Magill [5]	4.93	11.66
1953	Swanson, Fuyat, and Ugrinic.	4.933	11.633 at 26° C

The density of mercurous iodide calculated from the NBS lattice constants is 7.683 at 26° C.

Mercury (I) Iodide, HgI (tetragonal)

hkl	1925 Havighurst Mo, 0.709 A		1926 Hylleraas Fe, 1.9373 A		1938 Hanawalt, Rinn and Frevel Mo, 0.709 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
101	4. 561	15	-----	-----	4. 55	20	4. 54	23
110	3. 480	100	3. 479	100	3. 50	100	3. 489	100
103	-----	-----	-----	-----	-----	-----	3. 048	1
004	2. 901	30	2. 899	30	2. 91	25	2. 909	28
200	2. 464	25	2. 459	60	2. 46	25	2. 467	30
114	2. 230	55	2. 225	80	2. 23	50	2. 234	45
211	2. 158	6	2. 156	10	-----	-----	2. 168	5
105	2. 098	30	2. 100	50	2. 10	20	2. 104	20
204	1. 876	30	1. 872	50	1. 88	20	1. 881	20
220	1. 736	20	1. 738	30	1. 74	12	1. 744	9
215	1. 592	20	1. 596	50	1. 60	12	1. 600	12
310	1. 557	15	1. 558	40	1. 56	6	1. 560	7
224	1. 491	20	1. 493	40	1. 493	10	1. 495	8
008	1. 449	4	-----	-----	-----	-----	1. 454	<1
314	1. 370	20	1. 373	60	1. 376	6	1. 374	9
118	1. 336	10	1. 340	40	1. 336	4	1. 342	5
217	-----	-----	-----	-----	-----	-----	1. 327	2
109	1. 251	20	1. 250	80	1. 250	10	1. 250	5
400	-----	-----	1. 228	30	-----	-----	1. 233	1
325	1. 178	7	1. 1786	30	-----	-----	1. 1794	2
330	1. 158	4	1. 1610	20	-----	-----	1. 1624	1
404	1. 136	4	-----	-----	-----	-----	1. 1351	1
219	1. 113	15	1. 1155	100	1. 116	6	1. 1152	6
420	-----	-----	-----	-----	-----	-----	1. 1029	2
334	1. 077	4	-----	-----	-----	-----	1. 0794	1
318	1. 062	4	-----	-----	-----	-----	1. 0636	2
309	1. 012	6	-----	-----	-----	-----	1. 0163	2
329	-----	-----	-----	-----	-----	-----	0. 9398	2
1·0·13	-----	-----	-----	-----	-----	-----	. 8804	1
419	-----	-----	-----	-----	-----	-----	. 8781	<1
2·1·13	-----	-----	-----	-----	-----	-----	. 8291	5

References

[1] R. J. Havighurst, Crystal structure of the mercurous halides, Am. J. Sci. **10,** 15–28 (1925).

[2] E. Hylleraas, Die Anordnung der Atome in den tetragonalen Kristallen der einwertigen Quecksilberhalogenide Hg_2Cl_2, Hg_2Br_2, Hg_2I_2. Berechnung der optischen Doppelbrechung von Hg_2Cl_2, Z. Physik. **36,** 859–897 (1926).

[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] E. Hylleraas, Die Anordnung der Atome in den tetragonalen Kristallen Hg_2Cl_2, Hg_2Br_2, Hg_2I_2 und Berechnung der optischen Doppelbrechung von Hg_2Cl_2, Physik. Z. **26,** 811 (1925).

[5] M. L. Huggins and P. L. Magill, The crystal structures of mercuric and mercurous iodides, J. Am. Chem. Soc. **49,** 2357–2367 (1927).

Thallium Chloride, TlCl (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2577	2677	2.71	Molybdenum	Hanawalt, Rinn and Frevel [1] 1938.
	1-1030	3.82		
	1-1046	1.56		

The following two indexed patterns made at −190° and 380° C are the same simple-cubic, cesium-chloride-type structure as the room-temperature form presented in this report, but differ considerably because of contraction and expansion of the lattices.

--------	--------	2.78	Iron, 1.9373A.	Wagner and Lippert [2] 1936.
	4-0709	1.60		
	4-0703	1.24		
--------	--------	2.66	Copper, 1.5418A.	Wagner and Lippert [2] 1936.
	4-0729	1.68		
	4-0729	1.53		

Additional published patterns

Source	Radiation	Wave-length
Lunde [3] 1925	Copper Kα	1.539 A

NBS sample. The thallium chloride was obtained from the Fairmount Chemical Co. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of aluminum; 0.001 to 0.01 percent each of barium, calcium, magnesium, sodium, and silicon; 0.0001 to 0.001 percent each of copper, iron, and strontium; and less than 0.0001 percent each of silver, manganese, lead, and tin. The refractive index of thallium chloride is too high to be measured by the usual grain-oil immersion methods.

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

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

	1	2	3
Hannawalt, Rinn, and Frevel	110	100	211
Lunde	211	310	321
Swanson, Fuyat, and Ugrinic	110	100	211

Lattice constant. The structure was determined by Davey and Wick [4] in 1921. The space group is O_h^1-Pm3m with cesium-chloride-type structure and 1(TlCl) per unit cell.

Several unit-cell values were converted from kX to angstrom units and to 26° C, from the temperatures indicated in parentheses, for comparison with the NBS values. The coefficient of expansion in this temperature range, is 54.57×10^{-6}, according to Straumanis, Ieviņš, and Karlsons [5].

Lattice constants

		a
		A
1921	Davey and Wick [4]	3.86
1925	Lunde [3]	3.847 (18° C)
1937	Moeller [6]	3.8419 (25° C)
1939	Straumanis, Ieviņš, and Karlsons [5]	3.84256 (25° C)
1953	Hambling [7]	3.84270
1953	Swanson, Fuyat, and Ugrinic	3.8421 at 26° C

The density of thallium chloride calculated from the NBS lattice constant is 7.021 at 26° C.

Thallium Chloride, TlCl (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1925 Lunde Cu, 1.5405 A			1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
100	3. 83	40	3. 83	3. 84	m	3. 84	3. 84	60	3. 84
110	2. 72	100	3. 85	2. 714	vs	3. 84	2. 717	100	3. 842
111	2. 21	20	3. 83	2. 225	w	3. 853	2. 218	22	3. 842
200	1. 91	20	3. 82	1. 924	s	3. 847	1. 921	18	3. 842
210	1. 71	20	3. 82	1. 721	vs	3. 849	1. 718	25	3. 841
211	1. 56	30	3. 82	1. 569	vvs	3. 844	1. 568	35	3. 841
220	1. 358	20	3. 841	1. 364	vs	3. 858	1. 358	9	3. 841
300	-----	-----	-----	1. 282	vs	3. 846	1. 281	9	3. 843
310	-----	-----	-----	1. 217	vvs	3. 848	1. 215	12	3. 842
311	-----	-----	-----	1. 161	m	3. 851	1. 1583	7	3. 8416
222	-----	-----	-----	1. 111	w	3. 850	1. 1091	5	3. 8420
320	-----	-----	-----	1. 065	w	3. 841	1. 0656	3	3. 8421
321	-----	-----	-----	1. 028	vvs	3. 847	1. 0268	12	3. 8419
400	-----	-----	-----	0. 962	vw	3. 851	0. 9606	<1	3. 8424
410	-----	-----	-----	. 932	m	3. 844	. 9318	5	3. 8419
411	-----	-----	-----	. 906	vs	3. 845	. 9056	6	3. 8420
331	-----	-----	-----	. 883	w	3. 849	. 8814	3	3. 8419
420	-----	-----	-----	-----	-----	-----	. 8591	4	3. 8420
421	-----	-----	-----	-----	-----	-----	. 8384	3	3. 8420
332	-----	-----	-----	-----	-----	-----	. 8192	3	3. 8424
422	-----	-----	-----	-----	-----	-----	. 7843	4	3. 8423
Average of last five lines----			3. 83	-----	-----	3. 847	------	---	3. 8421

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. Wagner and L. Lippert, Über polymorphe Umwandlung bei einfachen Ionengittern. I. Versuche zur Umwandlung von CsCl- in NaCl-Gitter durch Erhitzen, Z. physik. Chem **B31,** 263–274 (1936).

[3] G. Lunde, Bemerkungen über die Kristallstruktur von Thalliumchlorür und Thalliumbromür, Z. physik. Chem. **117,** 51–56 (1925); Norsk Geol. Tidsskr. **8,** 217–219 (1925).

[4] W. P. Davey and F. G. Wick, The crystal structure of two rare halogen salts, Phys. Rev. **17,** 403–404 (1921).

[5] M. Straumanis, A. Ieviņš, and K. Karlsons, Hängt die Gitterkonstante von der Wellenlänge ab? Präzisions-bestimmungen von Gitterkonstanten des LiF, NaF, As_2O_3, TlCl, und TlBr, Z. physik. Chem. **B42,** 143–152 (1939).

[6] K. Moeller, Über Präzisionsbestimmungen von Gitterkonstanten nach der Methode von Debye-Scherrer, Z. Krist. **A97,** 170–196 (1937).

[7] P. G. Hambling, The lattice constants and expansion coefficients of some halides, Acta Cryst. **6,** 98 (1953).

Thallium Iodide, TlI (orthorhombic)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wave-length
Barth and Lunde [1] 1926--------	Copper---	----------

NBS sample. The thallium iodide used for the NBS pattern was prepared by F. P. Phelps of the NBS by precipitation from solutions of thallium sulfate and potassium iodide. Spectrographic analysis at the NBS of the thallium sulfate used is as follows: 0.0001 to 0.001 percent each of calcium, silicon, and tin, and less than 0.0001 percent each of magnesium and lead. The precipitate was washed until free of sulfate, and all of the impurities except silicon should have been removed. The refractive indices of thallium iodide are too high to be measured by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The Barth and Lunde data were converted from Bragg angles to *d*-spacings in angstroms.

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

	1	2	3
Barth and Lunde---------------------	313	311	----
Swanson, Fuyat, and Ugrinic----------	111	113	004

Lattice constants. The structure was determined by Helmholz [2] in 1936. The space group is D_{2h}^{17}-Amma (Cmcm) with 4(TlI) per unit cell.

The Helmholz unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1936--	Helmholz [2]---------	5. 25	4. 58	12.95
1953--	Swanson, Fuyat, and Ugrinic.	5. 251	4. 582	12.92 at 25° C

The density of thallium iodide calculated from the NBS lattice constants is 7.078 at 25° C.

Thallium Iodide, TlI (orthorhombic)

hkl	1926 Barth and Lunde Cu, 1.5405A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
002	-----	---	6. 45	2
011	-----	---	4. 32	11
102	-----	---	4. 07	9
111	3. 559	40	3. 332	100
004	3. 152	20	3. 228	52
104	-----	---	2. 749	13
113	2. 719	50	2. 692	73
200	2. 647	10	2. 624	28
020	2. 308	30	2. 291	17
015	2. 264	20	2. 248	8
006	-----	---	2. 153	2
115	2. 077	40	2. 069	17
204	2. 051	50	2. 036	33
122	-----	---	1. 998	2
024	1. 876	30	1. 869	17
124	-----	---	1. 7602	4
220	1. 718	50	1. 7259	12
215	1. 690	10	1. 7083	7
117	-----	---	1. 6271	20
311	1. 624	80	1. 6218	10
008	-----	---	1. 6148	19
108	-----	---	1. 5431	5
313	1. 527	100	1. 5285	12
224	-----	---	1. 5221	18
131	1. 463	50	1. 4574	7
217	1. 431	10	1. 4341	2
133	1. 390	40	1. 3886	8
315	-----	---	1. 3817	5
208	1. 376	10	1. 3753	4
--------	1. 316	40	----	-------
--------	1. 291	40	----	-------
--------	1. 219	50	----	-------
--------	1. 180	40	----	-------
--------	1. 148	60	----	-------
--------	1. 115	40	----	-------
--------	1. 078	60	----	-------
--------	1. 055	60	----	-------
--------	1. 020	30	----	-------
--------	0. 997	50	----	-------

References

[1] T. Barth and G. Lunde, Beiträge zur Kenntnis der Mischkristalle, Z. Physik. Chem. **122,** 293–334 (1926).

[2] L. Helmholz, The crystal structure of the low temperature modification of thallous iodide, Z. Krist. **95A,** 129–137 (1936).

Bismuth Oxychloride [5] (bismoclite), BiOCl (tetragonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
	3782	1. 66	Iron	British Museum.
	3–1125	2. 67		
	3–1126	2. 46		
	3768	1. 66	Copper	British Museum.
	3–1123	7.		
	3–1125	2. 67		
1486	1371	3. 45	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
	1–0595	2. 67		
	1–0600	7. 4		

Additional published patterns. None.

NBS sample. The bismuth oxychloride was obtained from the Fisher Scientific Co. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of lead and silicon; 0.0001 to 0.001 percent each of aluminum, calcium, iron, and magnesium; and less than 0.0001 percent each of silver and barium. The refractive indices of the NBS sample are too high to be measured by the usual grain-oil immersion methods.

Interplanar spacing and intensity measurements. The *d*-spacing for the three ASTM card patterns were converted from kX to angstrom units. The British Museum pattern obtained from bismoclite, contains a *d*-spacing at 2.96 A, which is not in accord with the bismuth oxychloride structure.

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

	1	2	3
British Museum	104	102	003
British Museum	104	001	102
Hanawalt, Rinn, and Frevel	101	102	001
Swanson, Fuyat, and Ugrinic	101	102	110

Lattice constants. The structure was determined by Bannister and Hey [2] in 1934. The space-group is D_{4h}^{7}-P4/nmm with lead-fluochloride-type structure and 2(BiOCl) per unit cell.

Two groups of unit-cell values were converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	*c*
1935	Bannister and Hey [3]	3. 90	7. 38
1941	Sillén [4]	3. 891	7. 362
1953	Swanson, Fuyat, and Ugrinic.	3. 891	7. 369 at 26° C

The density of bismuth oxychloride calculated from the NBS lattice constants is 7.752 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] F. A. Bannister and M. H. Hey, The crystal structure of BiOCl, BiOBr and BiOI, Nature **134**, 856 (1934).

[3] F. A. Bannister and M. H. Hey, The crystal structure of the bismuth oxyhalides, Mineralog. Mag. **24**, 49–58 (1935).

[4] L. G. Sillén, X-ray studies on BiOCl, BiOBr and BiOI, Svensk Kem. Tidskr. **53**, 39–43 (1941).

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[5] Bismoclite, as defined by the Dana System of Mineralogy, 5th Ed., is bismuth oxychloride or any member of the bismuth oxychloride-oxyhydroxide solid-solution series containing more than 50 percent of bismuth oxychloride. The bismoclite of this report is the end member, BiOCl.

Bismuth Oxychloride (bismoclite), BiOCl (tetragonal)

hkl	British Museum		British Museum		1938 Hanawalt, Rinn, and Frevel		1953 Swanson, Fuyat, and Ugrinic	
	Fe, 1.93597 A		Cu, 1.5405 A		Mo, 0.709 A		Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
001	7. 2	40	7.	80	7. 4	70	7. 38	38
002	3. 68	60	3. 74	70	3. 72	8	3. 69	16
101	3. 44	60	3. 42	60	3. 46	100	3. 442	100
---------	2. 96	20	----	-----	-----	-----	------	-----
110	2. 76	40	2. 76	50	2. 76	40	2. 753	76
102	2. 68	80	2. 68	80	2. 68	80	2. 677	97
111	----	-----	----	-----	-----	-----	2. 577	10
003	2. 46	80	2. 45	80	2. 45	8	2. 457	12
112	2. 20	40	2. 18	40	2. 20	24	2. 205	28
103	2. 02	20	----	-----	-----	-----	2. 076	1
200	1. 94	60	1. 94	40	1. 94	24	1. 946	34
201	----	-----	1. 88	20	1. 87	4	1. 881	9
113	1. 83	80	1. 83	70	1. 83	24	1. 833	25
202	----	-----	1. 72	20	-----	-----	1. 720	8
211	1. 69	40	1. 69	40	1. 69	24	1. 694	25
104	1. 66	100	1. 66	100	1. 66	16	1. 665	17
212	1. 57	60	1. 57	60	1. 57	36	1. 574	31
203	1. 53	50	1. 53	60	1. 52	16	1. 528	11
005	1. 48	80	1. 48	60	-----	-----	1. 473	2
220	1. 38	60	1. 38	80	1. 378	16	1. 376	12
221	1. 36	40	----	-----	-----	-----	1. 352	3
204	----	-----	1. 34	20	-----	-----	1. 338	2
115	1. 30	20	1. 30	40	-----	-----	1. 299	3
222	----	-----	----	-----	-----	-----	1. 289	3
301	----	-----	----	-----	-----	-----	1. 278	6
214	1. 27	60	1. 27	70	1. 266	16	1. 266	14
310	1. 23	80D	1. 23	80	-----	-----	1. 231	8
302	----	-----	----	-----	1. 227	20	1. 224	7
311	----	-----	----	-----	-----	-----	1. 214	2
223	1. 20	40	1. 20	20	1. 202	4	1. 200	5
205	1. 18	40	1. 18	40	-----	-----	1. 1745	3
312	1. 17	40	1. 17	20	1. 167	8	1. 1672	6
215	1. 15	20	----	-----	-----	-----	1. 1246	5
116	1. 13	80	1. 13	80	1. 123	8	1. 1218	7
313	1. 10	60	1. 10	50	1. 097	8	1. 1001	9
321	1. 07	60	1. 07	40	1. 067	8	1. 0678	7
304	1. 06	60	1. 06	40	-----	-----	1. 0606	4
206	1. 04	80	1. 04	80	1. 038	12	1. 0384	6
322	1. 03	40	----	-----	-----	-----	1. 0358	11
314	1. 02	60	1. 02	70	-----	-----	1. 0232	3
107	----	-----	----	-----	-----	-----	1. 0158	3
400	----	-----	----	-----	-----	-----	0. 9728	5
401	----	-----	----	-----	-----	-----	. 9639	<1
315	----	-----	----	-----	-----	-----	. 9446	3
411	----	-----	----	-----	-----	-----	. 9361	5
324	----	-----	----	-----	-----	-----	. 9311	7

Ammonium Iodide, NH_4I (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2820	3020 1–1112 1–1107	2.53 2.17 1.65	Molybdenum 0.712 A.	Bartlett and Langmuir [1] 1921.
927	0952 1–0424 1–0416	4.18 3.62 2.56	Molybdenum 0.710 A.	Havighurst, Mack, and Blake [2] 1924.
931	0950 1–0423 1–0415	4.18 3.62 2.56	Molybdenum	Hanawalt, Rinn, and Frevel [3] 1938.

Additional published patterns. None.

NBS sample. The ammonium iodide was obtained from the Baker Chemical Co. The sample was sublimed in an evacuated tube at 150° C before being used for the NBS pattern. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of calcium, magnesium, and zinc; 0.0001 to 0.001 percent each of aluminum, chromium, copper, iron, and silicon; and less than 0.0001 percent of silver. The refractive index of the NBS sample is 1.703.

Interplanar spacings and intensity measurements. The *d*-spacings for the Havighurst, Mack, and Blake pattern were calculated from Bragg angle data; the *d*-spacings for the Bartlett and Langmuir were reduced to angstrom units and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units.

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

	1	2	3
Bartlett and Langmuir	220	311	331
Havighurst, Mack, and Blake	111	200	220
Hanawalt, Rinn, and Frevel	111	200	220
Swanson, Fuyat, and Ugrinic	111	200	220

Lattice constant. The structure was determined by Bartlett and Langmuir [1] in 1921. The space group is O_h^5-Fm3m with sodium-chloride-type structure and 4(NH_4I) per unit cell. There are two low-temperature forms of ammonium iodide, a cesium-chloride-type structure (simple cubic) at −17° C, according to Simon and Simson [4] and a phosphonium-iodide-type structure (tetragonal) at −100° C, according to Ketelaar [5].

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

Lattice constants

		a
		A
1917	Vegard [6]	7.21
1921	Bartlett and Langmuir [1]	7.214
1924	Havighurst, Mack, and Blake [2].	7.2438
1953	Swanson, Fuyat, and Ugrinic	7.2613 at 26° C

The density of ammonium iodide calculated from the NBS lattice constant is 2.514 at 26° C.

References

[1] G. Bartlett and I. Langmuir, The crystal structures of the ammonium halides above and below the transition temperatures, J. Am. Chem. Soc. **43,** 84–91 (1921).

[2] R. J. Havighurst, E. Mack, and F. C. Blake, Precision crystal measurements on some alkali and ammonium halides, J. Am. Chem. Soc. **46,** 2368–2374 (1924).

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

[4] F. Simon and C. V. Simson, Ein Umwandlungspunkt der Ammoniumsalze zwischen −30 and −40 Grad, Naturwissenschaften **14,** 880 (1926).

[5] J. A. Ketelaar, Crystal structure of the low temperature modification of ammonium bromide, Nature **134,** 250 (1934).

[6] L. Vegard, Results of crystal analysis IV, Phil. Mag. **33,** 395–428 (1917).

Ammonium Iodide, NH_4I (cubic)

hkl	1921 Bartlett and Langmuir Mo, 0.709 A			1924 Habighurst, Mack, and Blake Mo, 0.710 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1953 Swanson, Fuyat, 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	---	---	----	4. 18	100	7. 24	4. 18	100	7. 24	4. 19	100	7. 26
200	---	---	----	3. 62	90	7. 24	3. 62	100	7. 24	3. 63	93	7. 26
220	2. 53	100	7. 16	2. 566	80	7. 258	2. 56	80	7. 24	2. 568	70	7. 263
311	2. 17	100	7. 19	2. 187	50	7. 253	2. 18	48	7. 23	2. 190	44	7. 263
222	2. 09	30	7. 23	2. 092	18	7. 247	2. 08	20	7. 21	2. 098	20	7. 268
400	1. 80	20	7. 19	1. 813	8	7. 252	1. 81	10	7. 24	1. 816	10	7. 264
331	1. 65	80	7. 20	1. 664	15	7. 253	1. 66	16	7. 24	1. 666	18	7. 262
420	1. 61	80	7. 19	---	---	---	1. 62	30	7. 24	1. 624	19	7. 263
422	1. 47	50	7. 21	1. 480	20	7. 251	1. 476	13	7. 231	1. 482	12	7. 260
511	1. 38	40	7. 20	1. 395	8	7. 248	1. 391	13	7. 228	1. 397	10	7. 259
440	1. 27	20	7. 17	1. 284	2	7. 263	1. 278	3	7. 229	1. 283	3	7. 258
531	1. 22	40	7. 24	1. 226	5	7. 253	1. 223	4	7. 235	1. 227	7	7. 259
600	1. 20	40	7. 21	1. 208	2	7. 247	1. 208	4	7. 248	1. 210	5	7. 260
620	1. 14	20	7. 22	---	---	---	1. 144	3	7. 235	1. 1481	4	7. 261
533	1. 10	15	7. 18	1. 106	1	7. 253	---	---	---	1. 1076	2	7. 2630
622	1. 08	15	7. 18	1. 092	2	7. 244	---	---	---	1. 0946	3	7. 2607
444	1. 04	5	7. 21	---	---	---	---	---	---	1. 0478	<1	7. 2594
711	1. 01	15	7. 21	1. 015	4	7. 246	1. 012	2	7. 227	1. 0170	3	7. 2628
640	---	---	----	---	---	---	---	---	---	1. 0069	3	7. 2608
642	0. 966	10	7. 23	0. 968	3	7. 246	---	---	---	0. 9704	3	7. 2618
731	. 936	10	7. 19	---	---	---	---	---	---	. 9454	4	7. 2617
Average of last five lines			7. 20	---	---	7. 247	---	---	7. 235	----	---	7. 2613

Strontium Chloride Hexahydrate, $SrCl_2 \cdot 6H_2O$ (hexagonal)

ASTM cards

Card number		New Index Lines	Radiation	Source
Old	New			
II–660	1080 2–0306 2–0302	3. 88 3. 44 2. 61	Copper, K_α	Herrmann [1] 1931.
200	0325 1–0131 1–0114	6. 9 2. 64 2. 20	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.
--------	1287 3–0357 3–0349	3. 54 2. 64 2. 20	Iron	Jensen [3] 1940.

From the original literature it seems clear that the Jensen ASTM card is a combination of powder-pattern intensities and calculated Bragg angle data. Many d-spacings, not listed on the ASTM card of the original article, have an observed intensity of zero and are not included in the table.

Additional published patterns. None.

NBS sample. The strontium-chloride hexahydrate used for the NBS pattern was obtained from the Fisher Scientific Co. The water content, determined by heating the sample at 300° C, was 99.6 percent of the theoretical loss for the hexahydrate. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of calcium; 0.001 to 0.01 percent of magnesium; 0.0001 to 0.001 percent each of aluminum, barium, manganese, and silicon; and less than 0.0001 percent each of silver, copper, and iron. The refractive indices of the NBS sample are as follows: $\epsilon = 1.487$ and $\omega = 1.536$, with negative optical sign.

Interplanar spacings and intensity measurements. The *d*-spacings for the Herrmann and the Jensen patterns were calculated from Bragg angle data; 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:

	1	2	3
Herrmann	110	101	201
Hanawalt, Rinn, and Frevel	100	201	211
Jensen	101	201	211
Swanson, Fuyat, and Ugrinic	100	101	110

The Herrmann and the Hanawalt, Rinn, and Frevel patterns contain a *d*-spacing of 1.44 angstrom units, which is not possible in the structure.

Lattice constants. The most recent structure determination was made by Jensen [3] in 1940. The space group is D_3^2–P321 with 1($SrCl_2 \cdot 6H_2O$) per unit cell. This compound is a prototype for other similar structures.

Two sets of unit-cell data were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
		A	A
1930	Herrmann [4]	7. 922	4.08
1940	Jensen [3]	7. 956	4.116
1953	Swanson, Fuyat, and Ugrinic.	7. 963	4.125 at 26° C

The density of strontium chloride hexahydrate calculated from the NBS lattice constants is 1.954 at 26° C.

References

[1] Z. Herrmann, Über die Strukturen der Bariumjodid- und Calciumjodid-hexahydrate. Vollständige struktur der Erdalkalihalogenid-hexahydrate: Typus $SrCl_2$ $6H_2O$, Z. anorg. u. allgem. Chem. **197,** 339–349 (1931).

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

[3] A. Tovbarg Jensen, On the structure of $SrCl_2 \cdot 6H_2O$, Kgl. Danske Videnskab selskab. Mat. fys. Medd. **17,** no. 9, 27 pp. (1940).

[4] Z. Herrmann, Über die Struktur des Strontium chlorid-Hexahydrates, Z. anorg. u. allgem. Chem. **187,** 231–236 (1930).

Strontium Chloride Hexahydrate, $SrCl_2 \cdot 6H_2O$ (hexagonal)

hkl	1931 Herrmann Cu, 1.5418 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1940 Jensen Fe, 1.93597 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
100	-----	-----	6. 9	100	6. 90	ms	6. 89	100
110	3. 89	s	3. 98	88	3. 98	ms	3. 98	87
101	3. 448	s	3. 55	88	3. 536	s	3. 539	89
200	-----	-----	-----	-----	-----	-----	3. 446	5
111	2. 826	w	2. 86	40	2. 860	m	2. 865	31
201	2. 611	s	2. 65	100	2. 642	s	2. 647	70
210	-----	-----	-----	-----	2. 604	vw	2. 606	10
300	2. 274	m	2. 29	75	2. 297	ms	2. 298	50
211	2. 189	s	2. 20	100	2. 201	s	2. 204	78
002	-----	-----	2. 06	20	2. 058	mw	2. 062	12
301	-----	-----	-----	-----	2. 006	w	2. 008	7
220	1. 971	m	1. 98	40	1. 990	w	1. 992	12
102					1. 973	mw	1. 976	15
310	1. 910	w	1. 91	10	1. 912	w	1. 912	6
112	1. 818	s	1. 83	20	1. 828	w	1. 831	9
202	-----	-----	-----	-----	1. 767	mw	1. 770	5
311	1. 728	w	1. 73	45	1. 734	m	1. 735	21
212	1. 621	m	1. 62	20	1. 615	mw	1. 617	8
401	-----	-----	1. 59	15	1. 589	w	1. 590	5
302	-----	-----	1. 53	20	1. 533	m	1. 535	14
410	-----	-----	1. 50	20	1. 504	m	1. 505	11
321	1. 497	s	1. 478	20	1. 476	m	1. 477	13
-------	1. 444	m	1. 445	5	-----	-----	------	-----
222	1. 431	w	1. 431	5	1. 430	w	1. 432	5
312	1. 376	w	1. 408	10	1. 401	mw	1. 403	7
103	-----	-----	-----	-----	1. 346	w	1. 349	4
330	-----	-----	1. 328	10	1. 326	w	1. 327	6
402	-----	-----	-----	-----	1. 321	w	1. 323	6
501	-----	-----	-----	-----	1. 307	vw	1. 308	1
113	1. 301	m	-----	-----	-----	-----	1. 299	4
203	-----	-----	1. 275	5	1. 275	vw	1. 277	4
331	-----	-----	-----	-----	1. 262	vw	1. 263	1
322	-----	-----	-----	-----	1. 254	vw	1. 255	5
421	1. 247	m	-----	-----	1. 242	mw	1. 242	8
213	1. 217	m	-----	-----	-----	-----	1. 216	11
412								
511	1. 181	m	-----	-----	-----	-----	1. 1854	6
502	-----	-----	-----	-----	-----	-----	1. 1467	3
223	-----	-----	-----	-----	-----	-----	1. 1308	1
313	-----	-----	-----	-----	-----	-----	1. 1161	5
332								
520	-----	-----	-----	-----	-----	-----	1. 1038	2
431	-----	-----	-----	-----	-----	-----	1. 0927	7
403	-----	-----	-----	-----	-----	-----	1. 0744	2
521	-----	-----	-----	-----	-----	-----	1. 0659	1
512	-----	-----	-----	-----	-----	-----	1. 0612	1
104	-----	-----	-----	-----	-----	-----	1. 0190	2
611								

Strontium Bromide Hexahydrate, $SrBr_2 \cdot 6H_2O$ (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-620	0986 2-0281 2-0288	4.01 3.53 2.66	Copper, $K\alpha$	Herrmann [1] 1931.
964	0953 1-0425 1-0427	4.11 3.60 2.70	Molybdenum	Hangwalt, Rinn gnd Frevel [2] 1938.

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

Additional published patterns. None.

NBS sample.—The strontium-bromide hexahydrate used for the NBS pattern was obtained from the Mallinckrodt Chemical Works. The water content, determined by heating the sample at 200° C for 3 days, was 100.5 percent of the theoretical loss for the hexahydrate. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of calcium and sodium; 0.001 to 0.01 percent of barium; 0.0001 to 0.001 percent each of aluminum, iron, magnesium, and silicon; and less than 0.0001 percent of copper. The refractive indices of the NBS sample are as follows: $\epsilon=1.540$ and $\omega=1.576$, with negative optical sign.

Interplanar spacings and intensity measurements. The *d*-spacings for the Herrmann pattern were calculated from Bragg angle data to copper $K\alpha$, 1.5418 A. 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:

	1	2	3
Herrmann	110	101	201
Hangwalt, Rinn, and Frevel	110	101	201
Swanson, Fuyat, and Ugrinic	110	101	211

Strontium Bromide Hexahydrate, $SrBr_2 \cdot 6H_2O$ (hexagonal)

hkl	1931 Herrmann Cu, 1.5418 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson, Fuyat, and Urginic Cu, 1.5405 A, 26° C	
	d	I	*d*	I	*d*	I
	A		*A*		*A*	
100	-----	---	-----	---	7.13	14
001	-----	---	-----	---	4.16	30
110	4.01	s	4.12	100	4.12	100
101	3.54	s	3.61	57	3.60	84
111	2.87	m	2.92	17	2.928	31
201	2.66	s	2.71	46	2.707	57
300	2.34	m	3.36	34	2.377	48
211	2.24	s	2.25	46	2.263	66
002	-----	---	-----	---	2.082	13
220	2.05	m	2.04	11	2.058	19
102	1.971	m	-----	---	1.999	8
112	1.838	s	1.85	11	1.858	15
202	-----	---	-----	---	1.797	6
311	1.768	m	1.79	23	1.785	22
212	-----	---	-----	---	1.647	6
401	1.636	m	1.63	6	1.637	6
302	-----	---	-----	---	1.566	13
410	1.548	s	1.56	23	1.555	14
321	1.512	m	1.51	11	1.522	11
222	1.451	w	1.487	6	1.4633	6
411	-----	---	1.465	6	1.4570	2
312	1.421	w	-----	---	1.4334	3
330	-----	---	-----	---	1.3710	5
103	1.350	m	-----	---	1.3620	3
113	-----	---	-----	---	1.3152	2
421	1.276	m	-----	---	1.2811	6
412	1.239	m	-----	---	1.2454	7
213			-----	---	1.2335	5
511	1.225	m	-----	---	1.2230	5
600	-----	---	-----	---	1.1875	2
332	1.168	w	-----	---	1.1450	3
520	-----	---	-----	---	1.1410	3
313	1.137	w	-----	---	1.1357	3
431	1.127	s	-----	---	1.1275	4
403	-----	---	-----	---	1.0953	2
512	1.087	w	-----	---	1.0902	1
323	-----	---	-----	---	1.0580	1
611	1.050	m	-----	---	1.0516	3
602	-----	---	-----	---	1.0316	2
522	-----	---	-----	---	1.0005	3
531 701	-----	---	-----	---	0.9890	2

Lattice constants. The most recent structure determination made on the group of isomorphous compounds, including strontium-bromide hexahydrate, was made on strontium-chloride hexahydrate by Jensen [3] in 1940. Therefore, the space group should be D_3^2-P321 with 1 ($SrBr_2 \cdot 6H_2O$) per unit cell.

Two sets of unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1931	Herrmann [4]	8. 229	4. 154
1940	Jensen [3]	8. 222	4. 154
1953	Swanson, Fuyat, and Ugrinic	8. 228	4. 164

The density of strontium bromide hexahydrate calculated from the NBS lattice constants is 2.418 at 26° C.

References

[1] Z. Herrmann, Über die Strukturen der Strontiumjodid-, Calciumchlorid-, und Calciumbromid-Hexahydrats, Z. anorg. u. allgem. Chem. **197,** 223–218 (1931).

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

[3] A. T. Jensen, On the structure of $SrCl_2 \cdot 6H_2O$, Kgl. Danske Videnskab. Selskab. Mat.-fys. Medd. **17,** No. 9 (1940).

[4] Z. Herrmann, Über die Struktur des Strontiumbromid-Hexahydrats, Z. anorg. u. allgem. Chem. Chem. **196,** 79–84 (1931).

6. NITRATES AND NITRITES

Silver (II) oxynitrate[6], $Ag_7O_8NO_3$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The argentic oxynitrate [6] used for the NBS pattern was prepared by R. E. Wood at the NBS by the electrolysis of silver nitrate between platinum electrodes. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of aluminum, magnesium, and silicon; and 0.0001 to 0.001 percent each of calcium, copper, and iron. The refractive index of the NBS sample could not be determined because the sample is opaque.

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

	1	2	3
Swanson, Fuyat, and Ugrinic	222	400	440

Lattice constant. The existence of this compound, resulting from the electrolytic oxidation of argentous silver dissolved in dilute acid, was known early in the nineteenth century. Investigations by Poggendorf [1] confirmed this, and Sulc [2] and Mulder and Heringa [3] found the structural formula to be $Ag_7O_8NO_3$. A more recent investigation by Noyes, DeVault, Coryell, and Deahl [4] also showed the oxynitrate character of the structure and found that it could be produced by the equilibration of argentic oxide, AgO, with dilute nitric acid containing silver nitrate, as well as by electrolysis. Their empirical formula, $AgO_{1.148}(NO_3)_{0.153}$, compares favorably with the $AgO_{1.143}(NO_3)_{0.143}$ or $Ag_7O_8NO_3$ given earlier found by Sulc.

Bräkken [5] established the cubic symmetry and determined the unit-cell size by means of single-crystal rotation photographs. The structure appears to be face-centered with 4 ($Ag_7O_8NO_3$) per unit cell.

The unit-cell value was converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

	A
Bräkken [5]	9.89
Swanson, Fuyat, and Ugrinic	9.893 at 26° C

The density of argentic oxynitrate calculated from the NBS lattice constant is 6.483 at 26° C.

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[6] Argentic oxynitrate is the name given to this compound by Noyes, DeVault, Coryell, and Deahl [4].

Silver (II) Oxynitrate, $Ag_7O_8NO_3$ (cubic)

hkl	1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C			*hkl*	1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C		
	d	*I*	*a*		*d*	*I*	*a*
	A		*A*		*A*		*A*
111	5. 73	10	9. 92	731	1. 288	3	9. 892
200	4. 96	6	9. 92	800	1. 237	7	9. 896
220	3. 498	4	9. 894	733	1. 209	2	9. 896
311	2. 980	2	9. 884	751	1. 1425	1	9. 894
222	2. 856	100	9. 893	662	1. 1348	14	9. 893
400	2. 474	45	9. 896				
331	2. 270	12	9. 895	840	1. 1062	9	9. 894
420	2. 213	4	9. 897	911	1. 0858	<1	9. 892
422	2. 019	3	9. 891	842	1. 0795	<1	9. 894
511	1. 903	2	9. 888	664	1. 0545	1	9. 892
440	1. 749	42	9. 894	844	1. 0097	9	9. 893
531	1. 672	4	9. 892				
600	1. 649	4	9. 894	933	0. 9942	1	9. 892
620	1. 564	1	9. 892	951	. 9563	<1	9. 892
533	1. 508	<1	9. 892	10·2·2	. 9520	11	9. 893
				10·4·0	. 9186	1	9. 894
622	1. 491	37	9. 890	880	. 8744	5	9. 893
444	1. 428	15	9. 893				
711	1. 385	2	9. 891	11·3·1	. 8644	2	9. 894
640	1. 372	2	9. 894	10·6·2	. 8361	14	9. 893
642	1. 322	1	9. 893	12·0·0	. 8244	9	9. 893
Average unit cell value for last five lines-----							9. 893

References

[1] J. C. Poggendorff, Ueber die angeblichen Hydrüre des Silbers und einiger anderen Metalle, Ann. Physik. **75,** 337–350 (1848).

[2] O. Sulc, Über das sogenannte elektrolytische Silbersuperoxyd, Z. anorg. Chem. **12,** 89 (1896).

[3] E. Mulder and J. Heringa, Sur un peroxy-azotate d'argent, Rec. trav. chim. **15,** 1, 235 (1896).

[4] A. A. Noyes, D. DeVault, C. D. Coryell and T. J. Deahl, Argentic salts in acid solution. V. Oxidation potentials, equilibria with higher silver oxides, and formation of nitrate complexes, J. Am. Chem. Soc., **59,** 1326–1337 (1937).

[5] K. Bräkken, Zur Krystallstruktur des Silberperoxyds, Ag_2O_3, Norske Vidensk. Selskabs, Forh. **7,** 143–6 (1935) as abstracted in Chem. Zentr. **106,** 1, 3634 (1935).

Sodium Nitrite, $NaNO_2$ (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
--------	2193 3–0628 3–0628	2. 97 2. 79 2. 04	Molybdenum-	Ziegler [1] 1931.
2169----	2195 1–0886 1–0883	2. 97 2. 78 2. 02	Molybdenum-	Hanawalt, Rinn and Frevel [2] 1938.

The powder pattern that appears in Ziegler's paper was used there primarily to compare observed and calculated intensities as part of a crystal-structure determination and apparently consisted of a combination of data from single-crystal and powder patterns. The absence of brackets around unresolved lines apparently led the compiler of the ASTM card to believe that each *d*-spacing should be treated singly and, therefore, dashes were filled in for a number of intensities. It appears, however, that the author intended to bracket the *d*-spacings as follows: 3.00 (110) and 2.97 (101) with I of 100, 1.41 (132), 1.39 (040), and 1.39 (123) with I of 20, 1.23 (042), 1.23 (213), and 1.23 (114) with I of 33, and 1.16 (310) and 1.16 (301) with I of 13.

Additional published patterns. None.

NBS sample. The sodium nitrite used for the NBS pattern was obtained from the Fisher Scientific Co. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of aluminum and calcium; and less than 0.0001 percent each of silver, barium, copper, and magnesium. The sample was heated at 120° C to remove water. The grain size of the NBS sample was too small for a refractive-index determination.

Interplanar spacings and intensity measurements. Ziegler's Bragg angle data was converted to *d*-spacings and the Hanawalt, Rinn, and Frevel *d*-spacings were converted from kX to angstrom units.

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

	1	2	3
Ziegler	110, 101	020	121
Hanawalt, Rinn, and Frevel	110, 101	020	121
Swanson, Fuyat, and Ugrinic	101	020	121

The Ziegler pattern contains *d*-spacings at 1.619 and 1.227 angstroms, which are possible in the sodium-nitrite structure, but which were not present in the NBS pattern. Ziegler assigned indices 040 and 123 to the *d*-spacings at 1.391 A, and 310 and 301 to those at 1.159 A, as shown on the ASTM card. Only one value for each of these reflections has been included in the comparison table because identical *d*-spacings would obviously coincide on a powder pattern. The total intensity of the pair was given in each case.

Lattice constants. The structure was determined by Ziegler [1] in 1931. The space group is C_{2v}^{20}-Im2m (Imm2) with 2($NaNO_2$) per unit cell. Sodium nitrite is a prototype for other similar structures.

Ziegler's unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1931	Ziegler [1]	3. 56	5. 57	5.39
1952	Carpenter [3]	3. 55	5. 56	5.38
1953	Swanson, Fuyat, and Ugrinic.	3. 570	5. 578	5.390 at 26° C

The density of sodium nitrite calculated from the NBS lattice constants is 2.135 at 26° C.

Sodium Nitrite, $NaNO_2$ (orthorhombic)

hkl	1931 Ziegler Mo, 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
011	3. 89	7	-------	-----	3. 88	2
110	3. 004	100	2. 98	100	3. 006	32
101	2. 982				2. 976	100
020	2. 791	47	2. 79	40	2. 789	56
002	2. 685	7	-----	---	2. 695	5
121	2. 038	47	2. 02	40	2. 035	37
112	2. 003	40	2. 00	23	2. 007	29
022	1. 939	27	1. 93	11	1. 938	13
200	1. 782	33	1. 78	12	1. 784	14
031	1. 756	7	-----	---	1. 757	3
013	1. 704	27	1. 70	8	1. 710	8
130	1. 642	20	1. 64	3	1. 650	4
---	1. 619	0	-----	---	------	----
103	1. 604	0	-----	---	1. 605	<1
220	1. 503	27	1. 500	5	1. 504	7
202	1. 484	0	-----	---	1. 488	<1
132	1. 407	20	1. 401	1	1. 406	5
123	1. 391		1. 392	4	1. 391	6
004	1. 348	7	1. 346	2	1. 348	2
222	1. 309	20	1. 313	2	1. 313	5
033	1. 290	7	1. 293	1	1. 292	2
141	1. 262	13	1. 261	1	1. 263	2
231	1. 249	0	-----	---	1. 253	<1
042	1. 236	33	-----	---	1. 238	5
213	1. 231		1. 235	4	1. 235	4
---	1. 227		-----	---	------	---
024	1. 214	7	1. 213	1	1. 213	1
301	1. 159	13	1. 162	1	1. 1623	1
321	-----	---	-----	---	1. 0728	2
312	-----	---	1. 068	1	1. 0687	2
143	-----	---	1. 050	1	1. 0525	3
233	-----	---	-----	---	1. 0466	<1
105	-----	---	1. 032	1	1. 0321	1
242	-----	---	1. 017	1	1. 0175	1
224	-----	---	-----	---	1. 0027	1
330						
044	-----	---	-----	---	0. 9689	2
125	-----	---	-----	---	. 9676	1
332	-----	---	-----	---	. 9392	<1
323	-----	---	-----	---	. 9345	<1

References

[1] G. E. Ziegler, The crystal structure of sodium nitrite, $NaNO_2$, Phys. Rev. **38,** 1040–1047 (1931).

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

[3] G. B. Carpenter, The crystal structure of sodium nitrite, Acta Cryst. **5,** 132–135 (1952).

7. PHOSPHATES

Ammonium Dihydrogen Phosphate, $(NH_4)H_2PO_4$ (tetragonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1979	1953 1–0807 1–0817	3. 07 5. 3 3. 76	Molybdenum	Hanawalt, Rinn and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The ammonium dihydrogenphosphate used for the NBS pattern was obtained from F. P. Phelps of the NBS. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of aluminum and silicon; 0.001 to 0.01 percent each of barium and calcium; 0.0001 to 0.001 percent each of magnesium and nickel; and less than 0.0001 percent each of silver, copper, and lead. The refractive indices of the NBS sample are as follows: $\epsilon=1.480$ and $\omega=1.529$, with negative optical sign.

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:

	1	2	3
Hanawalt, Rinn, and Frevel	112, 211	101	200
Swanson, Fuyat, and Ugrinic	101	112	211

Lattice constants. The structure was determined by Hassel [2] in 1925. The space group is D_{2d}^{12}-$I\bar{4}2d$ with potassium dihydrogen phosphate-type structure and $4((NH_4)H_2PO_4)$ per unit cell.

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

Lattice constants

		a	*c*
		A	A
1925	Hassel [2]	7. 50	7. 58
1927	Hendricks [3]	7. 53	7. 55
1948	Ueda [4]	7. 494	7. 531
1953	Swanson, Fuyat, and Ugrinic.	7. 499	7. 548 at 26° C

The density of ammonium dihydrogen phosphate calculated from the NBS lattice constants is 1.800 at 26° C.

Ammonium Dihydrogen Phosphate, $(NH_4)H_2PO_4$ (tetragonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*
	A		A	
101	5. 3	83	5. 32	100
200	3. 77	53	3. 75	64
112	3. 08	100	3. 075	89
211			3. 065	75
202	2. 66	9	2. 659	18
220	-----	---	2. 651	15
301	2. 37	5	2. 373	8
312	2. 00	27	2. 009	29
321			2. 004	22
303	1. 77	3	1. 773	5
204	1. 68	3	1. 686	5
420	-----	---	1. 677	4
332	1. 60	5	1. 602	9
224	1. 54	3	1. 537	4
413	-----	---	1. 473	4
431	1. 476	4	1. 470	5
501				
510				
215	1. 376	3	1. 376	3
512	-----	---	1. 370	4
521				
404	1. 331	4	1. 330	5
433	1. 294	1	1. 289	3
503				
424	1. 257	3	1. 254	3
116	1. 222	3	1. 224	3
532	-----	---	1. 218	4
620	1. 190	1	1. 1857	2
415	1. 163	1	1. 1613	1
316	1. 110	1	1. 1113	2
613	-----	---	1. 1078	1
631	-----	---	1. 1062	2
543	-----	---	1. 0620	2
604	-----	---	1. 0416	<1
217	-----	---	1. 0264	2

References

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

[2] O. Hassel, Über die Kristallstruktur des primären Kaliumphosphats KH_2PO_4 und isomorpher salze, Z. Elektrochem. **31,** 523–529 (1925).

[3] S. B. Hendricks, The crystal structure of potassium dihydrogen-phosphate, Am. J. Sci. **14,** 269–287 (1927).

[4] R. Ueda, The crystal structure of ammonium dihydrogen phosphate, $NH_4H_2PO_4$, J. Phys. Soc. Japan **3,** 328–333 (1948).

8. SULFATES

Calcium Sulfate (anhydrite), $CaSO_4$ (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
-----	0675 3-0164 3-0162	4. 63 3. 86 3. 48	Molybdenum Kα.	Dickson and Binks [1] 1926.
-----	0676 3-0165 3-0163			A continuation of the preceding card.
-----	1365 3-0372 3-0368	3. 49 2. 79 1. 85	Copper Kα	Hill and Hendricks [2] 1936.
1444	1362 1-0591 1-0578	3. 49 2. 85 2. 32	Molybdenum.	Hanawalt, Rinn, and Frevel [3] 1938.
-----	1396 3-0384 3-0377	3. 48 1. 10 3. 87	Copper	British Museum.

The intensities listed on the ASTM card for the Dickson and Binks pattern do not represent the authors' observed intensities, but, rather, the result of a series of calculations made by using the observed intensities. Therefore, the three strongest lines on this ASTM card are not those indicated by the authors. The date of the reference for the Hill and Hendricks ASTM card should be 1936 rather than 1938, and the pattern should be described as orthorhombic rather than monoclinic as indicated.

Additional published patterns

Source	Radiation	Wavelength
Wasastjerna [4] 1925	Copper	Kα.
Jung [5] 1925	Copper	----------

NBS sample. The calcium sulfate used for the NBS pattern was prepared at the NBS by the reaction between potassium-sulfate and calcium-chloride solutions. The product was heated at 700° C for 16 hours. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of bismuth, strontium, and titanium; 0.001 to 0.01 percent each of silver, aluminum, iron, magnesium, nickel, and tin; 0.0001 to 0.001 percent each of barium, chromium, copper, and lead; and less than 0.0001 percent of manganese. The refractive indices of the NBS sample are as follows: $\alpha=1.570$, $\beta=1.575$, $\gamma=1.614$ with 2V of 40° and positive optical sign.

Interplanar; spacings and intensity measurements. The *d*-spacings for the Dickson and Binks, the Wasastjerna, and the Jung patterns were calculated from Bragg angle data; the *d*-spacings for the Hanawalt, Rinn, and Frevel and the British Museum patterns were converted from kX to angstrom units. The Hill and Hendricks *d*-spacing data were calculated from lattice constants determined from single crystals. The Dickson and Binks pattern was made with an ionization spectrometer, using single crystals. Reflections were measured from faces ground to correspond to the desired *hkl's* accounting for those *d*-spacings that fall extremely close together. The intensities, listed in the table as percentages of the strongest line, are those observed for the reflections from each crystal face. The intensities shown on the ASTM card, which decrease in order from 100 to 1, were the result of applying several rather specialized corrections for the purpose of testing the corrections of the authors' postulated structure and are quite useless for identification purposes.

The British Museum pattern contains a *d*-spacing at 4.25 A, and the Hanawalt, Rinn, and Frevel pattern, a *d*-spacing at 2.26 A, neither of which are permissible in the calcium-sulfate structure. The Wasastjerna pattern contains a *d*-spacing at 4.60 A, which is a permissible anhydrite line, but which is not present in the NBS pattern. The Dickson and Binks pattern contains a *d*-spacing at 1.157 A, which might be an anhydrite line, but which is not present in the NBS pattern.

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

	1	2	3
Dickson and Binks	002, 020	210	220
Hill and Hendricks	002, 020	210	230
Hanawalt, Rinn, and Frevel	002, 020	210	202, 220
British Museum	002, 020	424, 442	111
Wasastjerna	002, 020	210	202, 220
Jung	002, 020	103	123
Swanson, Fuyat, and Ugrinic	002, 020	210	202, 220

Lattice constants. The structure was determined simultaneously by Rinne, Hentschel and Schiebold [6], by Wasastjerna [4], and by Mark, Basche, and Pohland [7] in 1925. The space group is D_{2h}^{17}-Bbmm (Cmcm) with $4(CaSO_4)$ per unit cell. Calcium sulfate is a prototype for other similar structures.

Calcium Sulfate (anhydrite), $CaSO_4$ (orthorhombic)

hkl	1926		1936		1938		----		1925		1925		1953	
	Dickson and Binks		Hill and Hendricks		Hanawalt, Rinn, and Frevel		British Museum		Wasastjerna		Jung		Swanson, Fuyat and Ugrinic	
	Mo, 0.709 A		Cu, 1.5405 A		Mo, 0.709 A		Cu, 1.5405 A		Cu, 1.5405 A		Cu, 1.5405 A		Cu, 1.5405 A, 26° C	
	[a] *d*	*I*	*d* (calc.)	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*		*A*	
---	4.62	---	----	----	-----	---	4.25	25	4.60	w	------	-----	------	---
111	3.854	2	3.84	w	3.89	3	3.88	75	3.90	mw	------	-----	3.87	6
002	3.473	100	3.50	vs	3.50	100	3.49	100	3.51	vs	3.416	vs	3.498	100
020														
200	3.104	10	3.13	m	3.12	3	3.17	50	3.14	w	------	-----	3.118	3
210	2.833	61	2.80	ms	2.86	67	2.84	75	2.85	s	------	-----	2.849	33
121	2.776	3	----	----	-----	---	----	---	----	----	2.783	w-ms	2.797	4
022	2.454	12	2.47	w	2.46	7	2.46	50	2.45	w	------	-----	2.473	8
202	2.315	4	2.33	m	2.32	33	2.32	75	2.31	s	2.304	ms	2.328	22
220	2.313	36												
---	------	---	----	----	2.26	1	----	---	----	----	------	-----	------	---
212	------	---	2.20	m	2.20	33	2.19	75	2.20	s	------	-----	2.208	20
103	------	---	----	----	-----	---	----	---	----	----	2.177	s	2.183	8
113	------	---	2.08	mw	2.08	11	2.07	50	2.07	mw	------	-----	2.086	9
301	------	---	1.99	w	1.99	11	2.01	25	1.99	w	1.998	vw	1.993	6
222	1.926	5	1.92	w	1.93	4	1.93	25	1.93	w	------	-----	1.938	4
230	------	---	1.85	ms	1.86	27	1.86	75	1.86	m	------	-----	1.869	15
123	------	---	----	----	-----	---	----	---	----	----	1.847	s	1.852	4
004	1.737	32	1.74	m	1.74	20	1.75	75	1.74	m	1.734	s	1.749	11
040													1.748	10
232	------	---	----	----	1.64	27	1.64	75	1.64	m	1.642	s	1.648	14
133	1.552	3	----	----	1.59	3	----	---	1.59	vw	------	-----	1.594	3
024	1.543	---	----	----	1.56	5	1.57	50	----	----	1.566	w	1.564	5
042														
204	------	---	----	----	1.52	7	1.52	50	----	----	------	-----	1.525	4
240														
313	------	---	----	----	-----	---	----	---	----	----	1.519	w	1.515	1
331														
214	------	---	----	----	1.490	8	1.49	50	----	----	1.478	ms	1.490	5
402	------	---	----	----	1.423	8	1.42	50	----	----	1.425	w	1.424	3
420														
323	1.417 1.416	6 11	----	----	-----	---	----	---	----	----	------	-----	1.418	1
242	------	---	----	----	1.398	7	1.40	50	----	----	------	-----	1.398	3
412	1.388	3	----	----	-----	---	----	---	----	----	------	-----	1.396	2
143	------	---	----	----	1.363	1	----	---	----	----	------	-----	1.365	1
422	------	---	----	----	1.321	9	1.32	50	----	----	1.314	w	1.319	4
430	1.285	2	----	----	1.299	3	----	---	----	----	------	-----	1.296	2
234	------	---	----	----	1.278	9	1.28	25	----	----	1.271	s	1.277	5
044	1.227	6	----	----	-----	---	----	---	----	----	------	-----	1.237	2
432	------	---	----	----	1.217	5	1.22	50	----	----	------	-----	1.216	4
252	------	---	----	----	1.199	1	1.20	25	----	----	------	-----	1.1993	2
135	------	---	----	----	-----	---	----	---	----	----	------	-----	1.1781	<1
006	1.158	19	----	----	1.165	7	1.17	75	----	----	1.163	s	1.1663	4
060	1.1576	3											1.1651	1
---	1.157	8	----	----	-----	---	----	---	----	----	------	-----	------	---
414	------	---	----	----	-----	---	----	---	----	----	------	-----	1.1483	1
026	------	---	----	----	-----	---	----	---	----	----	------	-----	1.1062	5
424	1.098	10	----	----	1.105	9	1.10	85	----	----	1.100	s	1.1044	4
442														
216	------	---	----	----	-----	---	1.08	25	----	----	1.076	ms	1.0785	2

Calcium Sulfate (anhydrite), $CaSO_4$ (orthorhombic)—Continued

hkl	1926		1936		1938		----		1925		1925		1953	
	Dickson and Binks		Hill and Hendricks		Hanawalt, Rinn, and Frevel		British Museum		Wasastjerna		Jung		Swanson, Fuyat and Ugrinic	
	Mo, 0.709 A		Cu, 1.5405 A		Mo, 0.709 A		Cu, 1.5405 A		Cu, 1.5405 A		Cu, 1.5405 A		Cu, 1.5405 A, 26° C	
	[a] d	I	d (calc.)	I	d	I	d	I	d	I	d	I	d	I
	A		A		A		A		A		A		A	
226	------	---	----	----	-----	---	----	---	----	----	------	-----	1. 0429	2
434	1. 034	11	----	----	-----	---	1. 04	50	----	----	1. 041	ms	1. 0414	3
254	------	---	----	----	-----	---	1. 03	25	----	----	------	-----	1. 0312	2
602 620	------	---	----	----	-----	---	----	---	----	----	0. 9964	w	0. 9968	3
236	------	---	----	----	-----	---	----	---	----	----	. 9886	s	. 9886	3
046	0. 965	9	----	----	-----	---	----	---	----	----	------	-----	. 9701	3
064	. 964	3	----	----	-----	---	----	---	----	----	. 9680	s	. 9695	2
622	------	---	----	----	-----	---	----	---	----	----	------	-----	. 9585	1
270	. 945	---	----	----	-----	---	----	---	----	----	------	-----	. 9521	1
246	. 9259	---	----	----	-----	---	----	---	----	----	------	-----	. 9264	<1
416	. 9255	---	----	----	-----	---	----	---	----	----	------	-----	. 9252	<1
272	------	---	----	----	-----	---	----	---	----	----	------	-----	. 9187	2
426	------	---	----	----	-----	---	----	---	----	----	------	-----	. 9024	1
454	------	---	----	----	-----	---	----	---	----	----	------	-----	. 8948	<1
604 317 640	------	---	----	----	-----	---	----	---	----	----	. 8937	w	. 8937	1
614 165	------	---	----	----	-----	---	----	---	----	----	------	-----	. 8863	<1
008	------	---	----	----	-----	---	----	---	----	----	. 8763	w	. 8747	<1
080	------	---	----	----	-----	---	----	---	----	----	------	-----	. 8737	<1
436	. 8685	5	----	----	-----	---	----	---	----	----	------	-----	. 8665	2
624 642	------	---	----	----	-----	---	----	---	----	----	. 8659	s	. 8659	2
256	(b)	---	----	----	-----	---	----	---	----	----	(c)	-----	. 8607	1

[a] Single crystal reflections measured on an ionization spectrometer. [b] Eleven additional lines have been omitted. [c] Three additional lines have been omitted.

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

Lattice constants

		a	b	c
		A	A	A
1925--	Rinne, Hentschel, and Schiebold [6].	6. 22	6. 96	6.97
1925--	Wasastjerna [4]-------	6. 25	6. 99	6. 99
1926--	Dickson and Binks [1]-	6. 20	6. 95	6. 95.
1926--	Basche and Mark [8]--	6. 21	6. 95	6. 98.
1953--	Swanson, Fuyat, and Ugrinic.	6. 238	6. 991	6. 996 at 26° C

The density of calcium sulfate calculated from the NBS lattice constants is 2.963 at 26° C.

References

[1] E. C. S. Dickson and W. Binks, The crystalline structure of anhydrite, Phil. Mag. **2,** 114–128 (1926).

[2] W. L. Hill and S. B. Hendricks, Composition and properties of superphosphate. Calcium phosphate and calcium sulfate constituents as shown by chemical and X-ray diffraction analysis, Ind. Eng. Chem. **28,** 441–447 (1936).

[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] J. A. Wasastjerna, Die Struktur des Anhydrits. Der Bau der Sulfatgruppe, Soc. Sci. Fennica, Commentationes Phys.-Math. **2,** 26 (1925).

[5] H. Jung, Röntgenographische Untersuchungen an den Entwässerungsprodukten des Gipses, Z. anorg. u. allgem. Chem. **142,** 73–79 (1925).

[6] F. Rinne, H. Hentschel, and E. Schiebold, Zum Feinbau von Anhydrit und Schwerspat, Z. Krist. **61,** 164–176 (1925).

[7] H. Mark, W. Basche and E. Pohland, Über die Ermittlung der Struktur einiger einfacher anorganischer Körper, Z. Elektrochem. **31,** 523 (1925).

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

9. SILICATES

Zirconium Silicate (zircon), $ZrSiO_4$ (tetragonal)

ASTM cards

Old card number	New card number	New index lines	Radiation	Source
--------	1681 3–0482 3–0459	3. 29 1. 71 2. 52	Copper	Binks [1] 1926.
--------	1682 3–0483 3–0460	------	-------------	A continuation of the preceding card.
--------	1599 3–0451 3–0443	3. 32 1. 72 2. 53	Molybdenum	Wyckoff and Hendricks [2] 1927.
--------	2244 3–0640 3–0630	2. 97 1. 81 1. 55	Copper	Stackelberg and Chudoba [3] 1937.
1675	1657 1–0698 1–0679	3. 29 2. 51 1. 71	Molybdenum	Hanawalt, Rinn, and Frevel [4] 1938.
II–1044	1586 2–0469 2–0474	3. 30 2. 52 1. 71	Iron	Kovalev [5] 1938.
--------	1600 3–0452 3–0456	3. 30 1. 71 2. 52	Copper, 1.5418 A.	United Steel Companies, Sheffield, England.
--------	1601 3–0453 3–0457	------	-------------	A continuation of the preceding card.
II–1123	1771 2–0524 2–0517	3. 21 1. 70 1. 37	Copper	British Museum.

The Stackelberg and Chudoba ASTM card pattern listed below carrying the title "Zirconium silicate, Zircon" is largely ZrO_2 in an amorphous matrix according to the note on the card. Except for the three largest *d*-spacings, it gives a pattern similar to true zirconium silicate. It was not included in the table and should be removed from the file or retained only with a more descriptive title such as "Low density zirconium silicate" or "Zirconium silicate and zirconium oxide."

II–1455	2245 2-0704 2-0701	2. 96 1. 81 1. 55	Copper	Stackelberg and Chudoba [3] 1937.

An earlier Chudoba and Stackelberg pattern made from normal-density zircon is included in the table.

The Binks pattern was obtained by using molybdenum, rather than copper, radiation, and the Kovalev pattern was made by using iron, not molybdenum, radiation, as their ASTM cards indicate.

Additional published patterns

Date	Source	Radiation	Wave-length
1936	Chudoba and Stackelberg [6]	Copper	K_α
1926	Vegard [7]	Copper	----------

NBS sample. The zirconium silicate used for the NBS pattern was a natural mineral sample obtained from the U. S. Geological Survey, Naval Gun Factory. Spectrographic analysis at the NBS showed the following impurities: 1.0 to 3.0 percent of hafnium; 0.1 to 1.0 percent of aluminum; 0.001 to 0.01 percent each of calcium, iron, and magnesium; 0.0001 to 0.001 percent of manganese; and less than 0.0001 percent of copper. The NBS sample is optically positive with the following refractive indices: ω=1.923 and ϵ=1.963.

Interplanar spacings and intensity measurements. The *d*-spacings for the Binks, the Stackelberg and Chudoba, the Chudoba and Stackelberg, and the Vegard patterns were calculated from their Bragg angle data; the *d*-spacings for the Wyckoff and Hendricks, the Hanawalt, Rinn, and Frevel, the Boldyrev, the United Steel, and the British Museum patterns were converted from kX to angstrom units.

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

	1	2	3
Binks	200	312	112
Wyckoff and Hendricks	200	312	112
Stackelberg and Chudoba	-----	321	411
Hanawalt, Rinn, and Frevel	200	112	312
Boldyrev	200	112	312
United Steel	200	312	112
British Museum	200	312	332
Chudoba and Stackelberg	312	200	112
Vegard	312	200	332
Swanson, Fuyat, and Ugrinic	200	101	112

A number of cubic and monoclinic zirconium oxide lines are present in the Stackelberg and Chudoba, the Hanawalt, Rinn, and Frevel, and the British Museum patterns, as indicated in the table. The index satisfying the *d*-spacing of 6.61 A in the British Museum pattern is not allowed by the space group, and like the 0.902 A spacing of the United Steel pattern, is not present in the NBS pattern.

Lattice constants. The structure was determined by Vegard [8] in 1916. The space group is D_{4h}^{19}-$I4_1/amd$ 4($ZrSiO_4$) per unit cell. Zirconium silicate is a prototype for other similar structures.

A group of unit-cell values were converted from kX to angstrom units for comparison with the NBS values. The Binks and the Vegard values for *a*, based on the larger cell caused by a 45° rotation of the *a*-axis about *c*, have been converted to the smaller cell for comparison with the other values.

Lattice constants

		a	*c*
		A	A
1926	Vegard [7]	6. 67	6. 02
1926	Binks [1]	6. 59	5. 94
1926	Hassel [9]	6. 59	5. 94
1927	Wyckoff and Hendricks [2]	6. 61	5. 89
1953	Swanson, Fuyat, and Ugrinic.	6. 604	5. 979 at 25° C

The density of zirconium silicate calculated from the NBS lattice constants is 4.668 at 25° C.

References

[1] W. Binks, The crystalline structure of zircon, Mineralog. Mag. **21,** 176–87 (1926).

[2] R. W. G. Wyckoff and S. B. Hendricks, Die Kristallstruktur von Zirkon und die Kriterien für spezielle Lagen in tetragonalen Raumgruppen, Z. Krist. **66,** 73–102 (1927).

[3] M. v. Stackelberg and K. Chudoba, Dichte und Struktur des Zirkons II, Z. Krist. **97,** 252–262 (1937).

[4] 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).

[5] J. A. Kovalev, Debye diffraction diagrams of some oxide and borate minerals, Materiali Tsentr. Nauchno-Issl. Geol.-Razv. Inst. Geokhimiya 1938 as taken from A. K. Boldyrev, X-ray determinative tables for minerals, Annales de l'Institut des Minès à Léningrad, Vol. **XI,** liv. 1 (1938).

[6] K. Chudoba and M. V. Stackelberg, Dichte und Struktur des Zirkons, Z. Krist. **95,** 230–246 (1936).

[7] L. Vegard, Results of crystal analysis, Phil. Mag. **1,** 1151–93 (1926).

[8] L. Vegard, Results of crystal analysis, Phil. Mag. **32,** 65–96 (1916).

[9] O. Hassel, Die Kristallstruktur einiger Verbindungen von der Zusammensetzung MRO_4, I. Zirkon $ZrSiO_4$, Z. Krist. **63,** 247–254 (1926).

Zirconium Silicate, $ZrSiO_4$ (tetragonal)

hkl	1926 Binks Cu, 1.5405 A		1927 Wyckoff and Hendricks Mo, 0.709 A		1937 Stackelberg and Chudoba Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1938 Boldyrev Fe, 1.93597 A	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
------	------	-----	-----	-----	------	----	------	-----	-----	---
101	4. 41	33	4. 438	25	------	----	4. 44	50	4. 448	40
200	3. 292	100	3. 323	100+	3. 30	mw	3. 30	100	3. 305	100
------	------	-----	-----	-----	[a]2. 967	vs	------	-----	-----	---
211	2. 632	8	-----	-----	------	----	2. 65	4	-----	---
112	2. 517	58	2. 531	70	2. 549	ms	2. 52	100	2. 530	80
220	2. 339	13	2. 338	5+	------	----	2. 33	13	2. 343	40
------	------	-----	-----	-----	------	----	------	-----	2. 292	10
202	2. 207	8	2. 213	4+	------	----	2. 21	15	2. 223	20
301	2. 070	21	2. 083	30	2. 076	vw	2. 05	30	2. 067	60
103	1. 913	17	1. 906	20	------	----	1. 90	25	-----	---
------	------	-----	-----	-----	------	----	------	-----	-----	---
321	1. 750	8	-----	-----	1. 811	vs	1. 74	15	1. 754	40
312	1. 711	83	1. 718	100	1. 721	vw	1. 71	75	1. 716	80
400	1. 645	33	1. 652	30	1. 653	vvw	1. 64	25	1. 658	60
411	1. 549	8	-----	-----	1. 551	vs	1. 54	3	-----	---
004	------	-----	-----	-----	------	----	------	-----	-----	---
420	1. 473	25	1. 480	20	1. 484	w	1. 482	15	1. 479	40
332	1. 378	25	1. 377	40	1. 382	vvw	1. 383	20	1. 386	40
204	1. 366	17	-----	-----	------	----	1. 363	15	-----	---
431 501	1. 288	8	1. 287	5	1. 281	w	1. 288	6	1. 298	40
------	------	-----	-----	-----	------	----	------	-----	-----	---
224	1. 258	17	1. 257	15	------	----	1. 258	20	1. 268	20
413	------	-----	-----	-----	------	----	------	-----	-----	---
------	------	-----	-----	-----	------	----	[b]1. 212	2	-----	---
512	1. 185	21	1. 187	15	1. 177	m	1. 187	18	1. 196	40
440	1. 166	8	-----	-----	1. 151	w	1. 163	3	-----	---
404	1. 105	17	-----	-----	1. 101	vvw	1. 100	15	-----	---
600	1. 098	12	-----	-----	------	----	------	-----	-----	---
611	------	-----	-----	-----	------	----	------	-----	-----	---
532	1. 056	21	-----	-----	------	----	1. 059	8	-----	---
424	1. 050	21	-----	-----	------	----	1. 048	13	-----	---
523 620	1. 043	8	-----	-----	1. 047	ms	------	-----	-----	---
325	1. 000	4	-----	-----	------	----	1. 001	4	-----	---
116	------	-----	-----	-----	0. 9838	m	------	-----	-----	---
631	0. 9682	8	-----	-----	------	----	0. 974	10	-----	---
415	------	-----	-----	-----	------	----	------	-----	-----	---
613	. 9517	4	-----	-----	------	----	------	-----	-----	---
701	------	-----	-----	-----	------	----	------	-----	-----	---
444	------	-----	-----	-----	------	----	------	-----	-----	---
543 640	. 9156	17	-----	-----	------	----	------	-----	-----	---
------	------	-----	-----	-----	------	----	------	-----	-----	---
316	. 8945	17	-----	-----	. 9073	m	------	-----	-----	---
552 712	. 8898	21	-----	-----	------	----	------	-----	-----	---
604	. 8826	8	-----	-----	------	----	------	-----	-----	---
525 624	. 8552	21	-----	-----	. 8646	s	------	-----	-----	---
703	. 8344	12	-----	-----	------	----	------	-----	-----	---
732	. 8310	21	-----	-----	------	----	------	-----	-----	---
723 800	------	-----	-----	-----	------	----	------	-----	-----	---
741 811	------	-----	-----	-----	------	----	------	-----	-----	---
------	------	-----	-----	-----	------	----	------	-----	-----	---
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[a] Cubic zirconium-oxide line.

[b] Monoclinic zirconium-oxide (baddelcyite) line.

Zirconium Silicate, $ZrSiO_4$ (tetragonal)—Continued

hkl	United Steel Companies Cu, 1.5405 A		British Museum Cu, 1.5405 A		1936 Chudoba and Stackelberg Cu, 1.5405 A		1926 Vegard Cu, 1.5405 A		1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 25° C	
	d	I	d	I	d	I	d	I	d	I
	A		A		A		A		A	
-----	-----	-----	6. 61	20B	------	---	------	---	------	-----
101	4. 45	70	4. 33	70	4. 405	m	------	---	4. 434	45
200	3. 31	100	3. 22	100	3. 295	s	3. 278	70	3. 302	100
-----	-----	-----	[b] 2. 76	50	------	---	------	---	------	-----
211	2. 66	50	2. 63	20	------	---	------	---	2. 650	7
112	2. 53	85	2. 50	70	2. 519	s	2. 524	50	2. 518	45
220	2. 34	60	2. 31	50	2. 330	mw	2. 339	10	2. 336	10
-----	-----	-----	------	-----	------	---	------	---	------	-----
202	2. 22	50	2. 19	20	2. 212	w	2. 217	5	2. 217	8
301	2. 07	70	2. 05	70	2. 059	ms	2. 075	30	2. 066	20
103	1. 91	60	1. 892	70	1. 897	mw	1. 919	30	1. 908	14
-----	-----	-----	[a] 1. 815	20	------	---	------	-----	------	-----
321	1. 75	70	1. 738	50	1. 744	m	1. 756	20	1. 751	11
312	1. 71	100	1. 704	100	1. 701	vs	1. 720	100	1. 712	40
400	1. 65	70	1. 641	70	1. 641	ms	1. 658	40	1. 651	14
411	1. 55	50	1. 534	20	1. 538	w	1. 553	10	1. 547	4
004	1. 51	30	------	-----	------	---	------	---	1. 495	3
420	1. 48	70	1. 471	70	1. 468	m	1. 485	35	1. 477	8
332	1. 38	70	1. 375	90	1. 375	ms	1. 390	60	1. 381	10
204	1. 36	60	1. 359	70	1. 357	m	1. 373	30	1. 362	7
431 501	1. 29	60	1. 305	20	1. 285	m	1. 290	15	1. 290	5
-----	-----	-----	[a] 1. 285	50	------	---	------	---	------	-----
224	1. 26	60	1. 257	50	1. 254	m	1. 266	20	1. 259	8
413	1. 25	30	1. 250	20	1. 247	vw	------	---	1. 248	3
-----	-----	-----	[b] 1. 217	20D	------	---	------	---	------	-----
512	1. 19	70	1. 184	60	1. 183	ms	1. 198	25	1. 1883	11
440	1. 17	50	1. 161	50	1. 163	w	1. 177	10	1. 1672	2
404	1. 11	60	1. 108	70	1. 106	m	1. 115	30	1. 1079	5
600	1. 10	60	1. 096	70	1. 097	ms	1. 108	40	1. 1006	5
611	1. 07	30	------	-----	------	---	1. 068	50	1. 0682	1
532	1. 06	60	1. 058	70	1. 059	ms	1. 060	50	1. 0590	7
424	1. 05	60	1. 050	70	1. 048	ms	1. 051	40	1. 0506	7
523 620	1. 04	60	1. 039	70	1. 043	ms	------	---	1. 0442	5
325	1. 00	30	------	-----	1. 014	vw	------	---	1. 0015	1
116	0. 977	50	------	-----	0. 9976	w	0. 9811	30	0. 9745	5
631	. 974	50	------	-----	------	---	. 9621	10	. 9713	5
415	. 956	50	------	-----	------	---	------	---	. 9582	1
613	-----	-----	------	-----	------	---	------	---	. 9532	1
701	. 934	30	------	-----	------	---	. 9378	20	. 9321	1
444	. 923	50	------	-----	------	---	. 9217	30	. 9201	2
543 640	. 918	60	------	-----	------	---	------	---	. 9157	4
-----	. 902	50	------	-----	------	---	------	---	------	-----
316	. 899	20	------	-----	------	---	. 9057	25	. 8994	5
552 712	. 894	60	------	-----	------	---	. 8972	50	. 8915	5
604	. 889	50	------	-----	------	---	. 8943	20	. 8863	7
525 624	. 859	70	------	-----	------	---	. 8620	50	. 8561	5
703	. 842	30	------	-----	------	---	------	---	. 8527	2
732	. 835	70	------	-----	------	---	. 8378	60	. 8329	4
723 800	. 828	60	------	-----	------	---	------	---	. 8256	1
741 811	. 814	60	------	-----	------	---	------	---	. 8116	3
-----	. 803	60	------	-----	------	---	------	---	------	-----
-----	. 793	70	------	-----	------	---	------	---	------	-----
-----	. 783	85	------	-----	------	---	------	---	------	-----
-----	. 781	70	------	-----	------	---	------	---	------	-----

Aluminum Antimony, AlSb (cubic)

ASTM cards. None.
Additional published patterns

Source	Radiation	Wave-length
Owen and Preston [1] 1924	Molybdenum	--------

NBS sample. The AlSb used for the NBS pattern was prepared by W. R. Hosler of the NBS. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of bismuth, gallium, indium, and silicon; 0.001 to 0.01 percent of silver; and 0.0001 to 0.001 percent each of calcium, copper, iron, magnesium, and manganese. The refractive indices could not be determined because the material is opaque. The compound was found to be unstable on exposure to the atmosphere over a period of months.

Interplanar spacings and intensity measurements. The Owen and Preston pattern was calculated from Bragg angle data.

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

	1	2	3
Owen and Preston	111	311	220
Swanson, Fuyat, and Ugrinic	111	220	200

Lattice constant. The structure was determined by Owen and Preston [1] in 1924. The space group is T_d^2–F$\bar{4}$3m with zinc-sulfide-structure type and 4(AlSb) per unit cell.

Two unit-cell values were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a
		A
1924	Owen and Preston [1]	6.138
1927	Goldschmidt [2]	6.103
1953	Swanson, Fuyat, and Ugrinic	6.1347 at 26° C

The density of AlSb calculated from the NBS lattice constant is 4.279 at 26° C.

Aluminum Antimony, AlSb (cubic)

hkl	1924 Owen and Preston Mo, 0.709 A			1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405 A, 26° C		
	d	I	a	d	I	a
	A		A	A		A
111	3. 54	100	6. 13	3. 54	100	6. 13
200	3. 08	34	6. 16	3. 067	34	6. 134
220	2. 13	56	6. 02	2. 169	74	6. 135
311	1. 85	68	6. 14	1. 850	31	6. 136
222	1. 75	36	6. 06	1. 771	5	6. 135
400	1. 53	23	6. 12	1. 534	5	6. 136
331	1. 40	48	6. 10	1. 407	15	6. 133
420	1. 36	18	6. 08	1. 372	10	6. 136
422	1. 24	26	6. 07	1. 252	21	6. 134
511	1. 17	34	6. 08	1. 1808	10	6. 1356
440	1. 08	15	6. 11	1. 0845	3	6. 1349
531	1. 04	36	6. 15	1. 0371	14	6. 1356
600	1. 02	11	6. 12	1. 0226	7	6. 1356
620	0. 959	12	6. 07	0. 9700	9	6. 1348
533	-------	-----	------	. 9355	3	6. 1345
622	. 927	29	6. 15	. 9248	2	6. 1344
444	. 879	15	6. 09	. 8855	3	6. 1349
711	-----	---	----	. 8590	11	6. 1345
640	-----	---	----	. 8507	3	6. 1345
642	-----	---	----	. 8198	16	6. 1348
731	-----	---	----	. 7987	20	6. 1349
Average unit cell value for last five lines			6. 12	------	--	6. 1347

References

[1] E. A. Owen and G. D. Preston, The atomic structure of two intermetallic compounds, Proc. Phys. Soc. (London) **36,** 341-348 (1924).

[2] V. M. Goldschmidt, Geochemische Verteilungsgesetze VIII, Skrifter Norske Videnskaps-Akad. Oslo, I. Mat.-Naturv. Kl. 1927.

Indium Antimony, InSb (cubic)

ASTM cards. None.

Additional published patterns

Date	Source	Radiation	Wave-length
1941	Iandelli [1]	Copper	K_a

NBS sample. The InSb sample used for the NBS pattern was prepared by J. Becker at the NBS. Spectrographic analysis at the NBS showed the following impurities: Approximately 0.1 percent each of aluminum and hafnium; 0.01 to 0.1 percent each of arsenic, calcium, iron, magnesium, sodium, lead, silicon, thallium, tungsten, and zirconium; 0.001 to 0.01 percent each of silver, cobalt, copper, manganese, nickel, tin, and zinc; and 0.0001 to 0.001 percent of chromium.

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

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

	1	2	3
Iandelli	111	642	731
Swanson, Fuyat, and Ugrinic	111	220	311

Lattice constant. The structure was investigated by Goldschmidt [2] in 1926. The space group is T_d^2-F$\bar{4}$3m with sphalerite-type structure and 4(InSb) per unit cell.

Lattice constants

		a
		A
1941	Iandelli [1]	6.474
1951	Liu and Peretti [3]	6.4760 at 25° C
1953	Swanson, Fuyat, and Ugrinic	6.4782 at 25° C

The density of InSb calculated from the NBS lattice constant is 5.777 at 25° C.

Indium Antimony, InSb (cubic)

hkl	1941 Iandelli Cu, 1.5405A			1953 Swanson, Fuyat, and Ugrinic Cu, 1.5405A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
111	3.779	es [a]	6.546	3.74	100	6.477
220	2.287	vs	6.468	2.290	80	6.477
311	1.951	s	6.469	1.953	55	6.477
400	1.619	m	6.477	1.620	15	6.479
331	1.485	ms	6.474	1.486	22	6.477
422	1.322	vs	6.477	1.323	25	6.479
511	1.246	ms	6.474	1.247	12	6.479
440	1.146	ms	6.482	1.1453	9	6.4788
531	1.095	vs	6.477	1.0950	12	6.4781
620	1.024	s	6.475	1.0243	9	6.4782
533	0.9873	ms	6.474	0.9880	6	6.4787
444	.9338	m	6.469	.9349	7	6.4779
711	.9063	vs	6.472	.9071	8	6.4780
642	.8653	vvs	6.475	.8657	12	6.4783
731	.8427	vvs	6.473	.8434	9	6.4783
800	-----	---	-----	.8098	3	6.4784
Average of last five lines			6.473	------	--	6.4782

[a] Extremely strong (strgonste).

References

[1] A. Iandelli, Sulla struttura dei composti InP, InAs e InSb, Gazz. Chim. Ital. **71,** 58–62 (1941).

[2] V. M. Goldschmidt, Die Gesetze der Krystallochemie, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Klasse **1926** No. 2 (1926), Naturwissenschaften **14,** 477 (1926).

[3] T. S. Liu and E. A. Peretti, Lattice parameter of InSb, J. Metals **3,** No. 9, Trans. 791 (1951).

11. CUMULATIVE INDEX TO VOLUMES I, II, III, AND IV[7]

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[7] 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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