NBS CIRCULAR 539

VOLUME III

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

Standard X-ray Diffraction Powder Patterns

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

NBS Circular 539, Volume I, Standard X-ray Diffraction Powder Patterns (Data for 54 inorganic substances)

NBS Circular 539, Volume II, Standard X-ray Diffraction Powder Patterns (Data for 30 inorganic substances)

The price of each volume is 45 cents. Send orders with remittance to: Superintendent of Documents, Government Printing Office, Washington 25, D. C.

UNITED STATES DEPARTMENT OF COMMERCE • Sinclair Weeks, *Secretary*
NATIONAL BUREAU OF STANDARDS • A. V. Astin, *Director*

Standard X-ray Diffraction Powder Patterns

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

National Bureau of Standards Circular 539
Volume III, Issued June 10, 1954

For sale by the Superintendent of Documents, U. S. Government Printing Office, Washington 25, D. C.
Price 45 cents

Contents

ERRATA

Vol. I. Page 64, table 37, Swanson and Tatge pattern. The *a* value for the *d* spacing at 2.680 should read 4.642.

Vol. II. Page 54, column 1. The *a* and *c* values for Bergen should read 4.99003 and 17.0605.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. III—Data for 34 Inorganic Substances

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

Data for thirty-two standard X-ray diffraction powder patterns are presented in revision of the eighty-one corresponding patterns in the American Society for Testing Materials card file, a system for the identification of unknown crystalline materials based on the three strongest reflections of each structurally distinct phase. Patterns for two compounds not represented in the file are also included. A comparison is made between all powder data available for each of the substances reported. The patterns were made with a geiger counter X-ray spectrometer, using samples of exceptionally high purity. The *d*-spacings were assigned Miller indices determined from calculated patterns of theoretical spacings and from space group considerations. The lattice constants and densities were calculated, and the refractive indices were measured whenever possible.

Included in this report is X-ray data for the following thirty-four substances: Ti, As, Rh, Cd, In, Sb, I_2, Hf, Bi, ZnSe, SiO_2 (α-quartz), Sc_2O_3, Y_2O_3, MoO_3 (molybdite), Sb_2O_3 (senarmontite), La_2O_3, HgO (montroydite), α-$Al_2O_3 \cdot H_2O$ (bohmite), β-$Al_2O_3 \cdot H_2O$ (diaspore), $SrTiO_3$, $BaTiO_3$, NaBr, CsBr, $CsICl_2$, $NaClO_3$, $CaCo_3$ (aragonite), $SrCO_3$ (strontianite), KNO_3 (niter), Na_2SO_3, K_2SO_4 (arcanite), $BaSO_4$ (barite), $PbSO_4$ (anglesite), KH_2PO_4, and $(NH_4)_2OsBr_6$

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 a third series[3] of standard powder diffraction patterns for nine elements and twenty-three inorganic compounds. These patterns are recommended to replace eighty-four cards now in the file. Two compounds, scandium oxide and ammonium bromoösmate, not represented in the file, have been added.

Experimental procedures and the general plan of these reports are discussed in the first three papers of this series, two by Swanson and Tatge [1, 2][4] and one by Swanson and Fuyat [3]. The significant changes in procedure and certain basic data discussed below are arranged in the same form as the data for each compound in the body of the report.

ASTM Cards. Each section of this paper, devoted to the discussion of X-ray data for one substance, contains a table listing old and new file card numbers, the ASTM index lines, the radiation used and the literature reference for each card. The old card numbers of these tables refer to the original ASTM card file (1939) and the first supplement (1944). The new card numbers are from

[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, 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 and the Flight Research Laboratory, Wright Air Development Center, Wright-Patterson Air Force Base.

[3] The first paper of this series is Standard X-ray Diffraction Powder Patterns, I. Data for 53 Inorganic Substances by H. E. Swanson and E. Tatge, and the second is Standard X-ray Diffraction Powder Patterns, II. Data for 30 Inorganic Compounds by H. E. Swanson and R. K. Fuyat.

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

the second edition and include the second supplement (1950).

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

NBS pattern. 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 a spectrographic or chemical analysis. A phase purity check was made on the nonopaque materials during the refractive index determination. Another excellent check on the phase purity was provided by the X-ray pattern itself, since it was indexed by comparison with theoretical *d*-values. However, some uncertainty was possible in the unequivocal isolation of the desired isomorphic forms when their *d*-spacings tended to coincide.

The majority of the samples that were initially too coarse for X-ray analysis could be reduced to the proper size and then annealed to remove the lattice distortion caused by grinding. It was found that powder samples of soluble salts which could not be annealed successfully or which could not be obtained free from the distortion of grinding, could be recrystallized by using a throat aspirator. Particles averaging 15 microns were obtained by using an aspirator or a nebulizer in which a concentrated solution of a salt was atomized to form a fine mist. This mist was confined in a box set over a glass plate on which the crystallites fell as they formed. Sufficient material, fine enough for an intensity pattern, could be collected in a few hours.

The equipment and procedures were essentially the same as those described in Standard X-ray Diffraction Patterns [1] and Standard X-ray Diffraction Powder Patterns I [2] with the exception of the newer X-ray spectrometer equipment described in Standard X-ray Diffraction Powder Patterns II [3].

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 removed. This surface was used for exposure to the X-ray beam. For a few powder samples which did not flow readily or were prone to orient badly, 25 to 50 percent finely ground silica-gel was added as a diluent. The intensity values of each pattern were measured as peak height above background and were expressed as percentages of the strongest line. The *d*-spacing patterns were made with a sample packed into a shallow sample holder, using approximately 5 weight percent of tungsten as an internal standard, whose lattice constant at 25°C is 3.1648 A, as determined by Jette and Foote [4]. All the NBS patterns were made by using copper radiation with a wavelength of 1.5405.

Interplanar spacings and intensity measurements. Interplanar spacing data presented in the tables were converted to angstrom units as internationally defined in 1946 [5], from Bragg angle data, from *d*-spacings in kX units or supposed 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 tables of *d*-spacings and intensities are given in angstroms; 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.

Indexing of the NBS patterns was accomplished by comparison of the experimental data 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 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. Although an attempt was made to reconcile these values with pub-

lished single crystal work when it was available, errors inherent in this method of indexing undoubtedly are present. For the NBS pattern a maximum of 40 lines were generally considered sufficient for any identification problem, and indexing of a cell large enough to have many more lines would become increasingly indefinite beyond that number.

The intensity of the three strongest lines is particularly important as the ASTM card file system of identification depends upon comparing the three strongest lines of the unknown material with those on the file cards, which are arranged according to their first, second, and third strongest lines, respectively. Thus 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 portion of the pattern. The lattice constants 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 recalculated to values corresponding to 25° or 26°C for comparison with the NBS values if the temperature of measurement and the thermal expansion were known. Unless otherwise indicated, the coefficient of linear thermal expansion as used is defined as the change in length per unit length per degree centigrade in the room-temperature range. 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 error generally published with unit-cell data have not been included in the table as the number of determinations, their accuracy and variation were such that a statistical evaluation would be invalid.

The densities calculated from the NBS lattice constants were 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] H. E. Swanson and E. Tatge, Standard X-ray diffraction patterns, NBS J. Research **46**, 318 (1951) RP2202.

[2] H. E. Swanson and E. Tatge, Standard X-ray diffraction powder patterns, NBS Circular 539, Vol. I (1953).

[3] H. E. Swanson and R. K. Fuyat, Standard X-ray diffraction powder patterns, NBS Circular 539, Vol. II (1953).

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

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

2. X-RAY DATA

2.1. Elements

Titanium, Ti (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
3136	3323	2.24	Molybdenum 0.7078	Patterson [1] 1925.
	1-1207	1.34		
	1-1197	2.56		
3148	3291	2.23	Molybdenum_____	Hanawalt, Rinn and Frevel [2] 1938.
	1-1198	2.54		
	1-1198	2.34		

The Patterson pattern is one of four very similar patterns made on titanium, after four different types of physical treatment, in an attempt to determine the existence of any unknown forms.

Additional published patterns. None.

NBS sample. The titanium used for the NBS pattern was a high-purity sample from the New Jersey Zinc Co., prepared by the iodide process. Their spectrographic analysis showed the following impurities: 0.02 percent of aluminum, 0.012 percent each of iron and manganese, 0.006 percent of molybdenum, 0.004 percent of nitrogen, 0.0025 percent of magnesium, and 0.002 percent of copper.

Interplanar spacings and intensity measurements. The Patterson 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:

Pattern	1	2	3
Patterson_____	011	103	010
Hanawalt, Rinn, and Frevel_____	011	010	002
Swanson and Fuyat_____	011	010	002

Lattice constants. The structure was determined by Hull [3] in 1921. The space group is D^4_{6h}-$P6_3/mmc$ with 2(Ti) per unit cell.

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

Lattice constants in angstroms

		a	*c*
1921	Hull [3]_____	2.98	4.73
1925	Patterson [1]_____	2.957	4.701
1930	Hägg [4]_____	2.959	4.739
1936	Burgers and Jacobs [5]_____	2.959	4.739
1949	Clark [6]_____	2.9504	4.6833 at 25°C
1953	Swanson and Fuyat_____	2.950	4.686 at 25°C

The density of titanium calculated from the NBS lattice constants is 4.503 at 25°C.

Titanium, Ti (hexagonal)

hkl	1925 Patterson Mo, 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
010	2.561	40	2.55	27	2.557	30
002	2.346	40	2.34	20	2.342	26
011	2.246	100	2.23	100	2.244	100
012	1.731	40	1.72	13	1.726	19
110	1.480	40	1.473	13	1.475	17
103	1.339	50	1.333	13	1.332	16
200	_____	_____	1.278	1	1.276	2
112	1.252	40	1.251	11	1.247	16
201	1.235	30	1.232	5	1.233	13
004	1.178	10	_____	_____	1.1708	2
202	1.127	10	_____	_____	1.1220	2
014	1.067	20	_____	_____	1.0653	3
203	.991	30	_____	_____	.9895	6
211	.944	30	_____	_____	.9458	11
114	.919	30	_____	_____	.9175	10
212	_____	_____	_____	_____	.8927	4
015	.882	10	_____	_____	.8796	4
204	_____	_____	_____	_____	.8634	2
300	.851	_____	_____	_____	.8514	4
213	.821	_____	_____	_____	.8211	12
302	.802	_____	_____	_____	.8005	9

References

[1] R. A. Patterson, Crystal structure of titanium and chromium, Phys. Rev. **26**, 56-9 (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. W. Hull, The crystal structures of Ti, Zr, Ce, Th, and Os, Phys. Rev. **18**, 88-9 (1921).

[4] G. Hägg, Röntgenuntersuchungen über die Hydride von Titan, Zirkonium, Vanadin und Tantal, Z. physik. Chem. **B11**, 433-454 (1930).

[5] W. G. Burgers and F. M. Jacobs, Crystal structure of beta titanium, Z. Krist. **94**, 299-300 (1936).

[6] H. T. Clark, The lattice parameters of high purity alpha titanium; and the effects of oxygen and nitrogen on them, J. Metals **1**, 588-589 (1949).

Arsenic, As (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1895	1856	3.18	Copper 1.539	Bradley [1] 1924.
	1-0779	1.02		
	1-0760	1.22		
-------	2648	2.78	(a)	Bradley[a] [1] 1924.
	3-0769	1.89		
	3-0757	2.05		
-------	2637	2.78	Copper------	Olshausen [2] 1925.
	3-0765	2.05		
	3-0754	1.88		
-------	2649	2.79	Copper------	British Museum.
	3-0770	1.89		
	3-0749	1.29		
2502	2650	2.76	Molybdenum--	Hanawalt, Rinn, and Frevel [3] 1938.
	1-1024	1.88		
	1-1019	2.04		
II-1825	2734	2.74	Copper------	Harcourt [4] 1942.
	2-0892	1.87		
	2-0872	2.04		

[a] The same d-spacings as above but carrying rhombohedral indices and different intensities

All of the patterns with the exception of the Hanawalt, Rinn, and Frevel pattern contain lines of both arsenic and arsenic trioxide with other possible contaminants. The British Museum and the Harcourt patterns were made on mineral material from Andreasberg, Harz Mountains, Germany, and from the Broken Hill Mines, New South Wales, Australia, respectively. The literature source for the intensities on the second Bradley ASTM card is unknown, but the three strongest lines are in better agreement than the previous set.

Additional published patterns

Source	Radiation	Wavelength
Willott and Evans [5] 1934----	Copper------	----------

NBS sample. The arsenic used for the NBS pattern was obtained from the Baker Chemical Co. and was purified at the NBS by J. Osmalov by sublimation in a nitrogen atmosphere. The sample was kept in nitrogen until mixed with petrolatum for grinding and mounting. (The presence of even a minute amount of water in air or oxygen catalyzes the oxidation of arsenic to a black powder giving an arsenic trioxide pattern, according to Stohr [6].) Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of bismuth and antimony; 0.001 to 0.01 percent each of iron and silicon; and 0.0001 to 0.001 percent each of silver, aluminum, calcium, magnesium, and lead.

Interplanar spacings and intensity measurements. The d-spacings for the Bradley and Olshausen patterns were converted to angstroms from Bragg angle data, whereas the British Museum, the Hanawalt, Rinn, and Frevel, the Harcourt, and the Willott and Evans d-spacings were converted from kX to angstrom units.

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

Patterns	1	2	3
Bradley----------	-------	-------	121,108
Olshausen----------	102	014	110
British Museum----------	102	110	025
Hanawalt, Rinn, and Frevel-----	102	110	014
Harcourt----------	102	110	014
Willott and Evans----------	102	014	110
Swanson and Fuyat----------	102	003	110

The first and second strongest lines of the Bradley pattern are possible arsenic oxide lines, and therefore are not included in this table.

The previous arsenic patterns, except for the Hanawalt, Rinn, and Frevel pattern, contain such large percentages of arsenic trioxide and other impurities that they are essentially useless for identification. Of the lines present that cannot be indexed as arsenic, those that might be due to arsenic trioxide are denoted by an (a) in the *hkl* column.

Lattice constants. The structure was determined by Bradley [1] in 1924, who showed that arsenic is isomorphous with antimony and bismuth. The space group is D_{3d}^5-$R\bar{3}m$ with 6(As) per unit cell. Arsenic is a prototype for other similar structures.

Rhombohedral unit cell values were converted to their hexagonal equivalents and from kX to angstrom units. In addition, the Jung and the Willott and Evans a-values based on a cell twice the accepted value for that direction were divided by two for comparison with the NBS results.

Lattice constants in angstroms

		a	*c*
1925	Olshausen [2]	3.758	10.646
1926	Jung [7]	3.765	10.638
1934	Willott and Evans [5]	3.770	10.575
1935	Hägg and Hybinette [8]	3.758	10.547
1939	Stohr [6]	3.762	10.543
1953	Swanson and Fuyat	3.760	10.548 at 26°C

The density of arsenic calculated from the NBS lattice constants is 5.778 at 26°C.

Arsenic, As (hexagonal)

hkl	1924 Bradley Cu, 1.5405 A		1925 Olshausen Cu, 1.5405 A		---- British Museum Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1942 Harcourt Cu, 1.5405 A		1934 Willott and Evans Cu, 1.5405 A		1953 Swanson and Fuyat 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*	
(a)	-----	-----	-----	-----	-----	-----	-----	-----	6.51	3	-----	-----	-----	-----
-----	-----	-----	-----	-----	-----	-----	-----	-----	6.18	25	-----	-----	-----	-----
-----	-----	-----	-----	-----	4.02	20	-----	-----	-----	-----	-----	-----	-----	-----
003	3.56	76	3.537	w	3.58	40	3.52	4	-----	-----	-----	-----	3.52	26
-----	-----	-----	-----	-----	-----	-----	-----	-----	3.46	25	-----	-----	-----	-----
-----	-----	-----	-----	-----	3.28	20	-----	-----	-----	-----	-----	-----	-----	-----
(a)	3.184	100	3.211	w	-----	-----	-----	-----	3.15	50	-----	-----	-----	-----
011	-----	-----	-----	-----	3.12	60	-----	-----	-----	-----	-----	-----	3.112	6
-----	-----	-----	-----	-----	2.97	60	-----	-----	-----	-----	-----	-----	-----	-----
-----	-----	-----	-----	-----	-----	-----	-----	-----	2.82	6	-----	-----	-----	-----
102	2.786	4	2.774	s	2.80	100	2.77	100	2.75	100	2.782	s	2.771	100
(a)	-----	-----	-----	-----	-----	-----	-----	-----	2.53	25	-----	-----	-----	-----
(a)	-----	-----	-----	-----	2.29	20	-----	-----	2.25	6	-----	-----	-----	-----
(a)	-----	-----	-----	-----	2.14	20	-----	-----	2.12	6	-----	-----	-----	-----
014	2.055	12	2.056	m	2.05	60	2.04	13	2.04	63	2.053	s	2.050	24
(a)	-----	-----	-----	-----	-----	-----	-----	-----	1.95	13	-----	-----	-----	-----
110	1.892	8	1.877	m	1.89	80	1.88	20	1.871	75	1.884	s	1.879	26
(a)	-----	-----	-----	-----	-----	-----	-----	-----	1.841	6	-----	-----	-----	-----
-----	-----	-----	-----	-----	1.80	60	-----	-----	-----	-----	-----	-----	-----	-----
105	1.785	6	1.765	w	1.78	20	1.77	5	1.76	38	-----	-----	1.768	10
006	1.768		-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	1.757	7
-----	-----	-----	-----	-----	1.71	60	-----	-----	-----	-----	-----	-----	-----	-----
113	1.664	48	1.661	w	-----	-----	1.66	4	1.65	38	-----	-----	1.658	6
(a)	-----	-----	1.594	w	-----	-----	-----	-----	1.59	6	1.602	vw	-----	-----
022	1.566	32	1.551	m	1.56	60	1.56	8	1.53	63	1.559	s	1.556	11
(a)	-----	-----	-----	-----	1.47	20	-----	-----	-----	-----	-----	-----	-----	-----
(a)	-----	-----	-----	-----	1.42	20	-----	-----	1.436	13	-----	-----	-----	-----
204	1.389	20	1.382	m	1.39	60	1.385	4	1.383	25	1.388	m	1.386	6
017	1.370		-----	-----	1.37	40	1.371	1	1.363	13	1.371	w	1.367	4
(a)	-----	-----	-----	-----	-----	-----	-----	-----	1.348	13	-----	-----	-----	-----
025	1.286	28	1.285	m	1.29	70	-----	-----	1.302	6	1.289	m	1.289	5
116	-----	-----	-----	-----	-----	-----	1.284	4	1.286	38	-----	-----	1.284	5
121	1.225	92	1.233	w	-----	-----	-----	-----	-----	-----	-----	-----	1.222	1
108														
212	1.203	24	1.200	m	1.20	70	1.198	5	1.197	50	-----	-----	1.1987	7
(a)	1.185	84	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
009	-----	-----	1.172	vw	-----	-----	-----	-----	-----	-----	1.174	w	1.1722	1
(a)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	1.163	m	-----	-----
124	1.120	36	1.115	m	1.12	50	-----	-----	1.114	25	1.116	m	1.1158	4
207	1.109		-----	-----	1.11	50	1.102	2	1.104	13	-----	-----	1.1062	2
300	1.090	56	1.084	w	1.09	40	1.087	1	1.085	25	1.087	w	1.0857	3
(a)	1.068	60	1.065	w	-----	-----	-----	-----	1.070	13	1.072	m	-----	-----
215	-----	-----	-----	-----	1.06	40	1.064	1	1.063	13	1.064	m	1.0631	3

hkl	1924 Bradley Cu, 1.5405 A		1925 Olshausen Cu, 1.5405 A		---- British Museum Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1942 Harcourt Cu, 1.5405 A		1934 Willott and Evans Cu, 1.5405 A		1953 Swanson and Fuyat 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	
303	1.042	80	1.041	vw	1.04	20	----------	-----	-------	-----	1.034	w	1.0374	2
(a)	1.025	96	-------	-----	-------	-----	----------	-----	-------	-----	-------	-----	----------	-----
119	.998	40	.999	m	-------	-----	----------	-----	.995	25	.997	w	.9948	2
(a)	-----	-----	-------	-----	-------	-----	----------	-----	.966	6	.972	w	----------	-----
127	.955	64	.955	w	-------	-----	----------	-----	.954	13	-------	-----	.9531	2
220	.943	72	.944	w	-------	-----	----------	-----	.940	13	.944	m	.9397	1
1·0·11	.929	44	.925	m	-------	-----	----------	-----	.923	13	.925	w	.9198	3
------	.923		------	-----	-------	-----	----------	-----	-------	-----	.920	vw	----------	-----
------	.910	88	-------	-----	-------	-----	----------	-----	-------	-----	-------	-----	----------	-----
218	-----	-----	.902	w	-------	-----	----------	-----	.899	6	.899	vw	.8995	1
132	.892	52	.895	m	-------	-----	----------	-----	.891	6	.890	w	.8903	2
(a)	-----	-----	.860	m	-------	-----	----------	-----	.864	3	.866	w	----------	-----
------	.855	68	-------	-----	-------	-----	----------	-----	.855	13	.856	w	----------	-----
------	-----	-----	-------	-----	-------	-----	----------	-----	.829	13	-------	-----	----------	-----
------	-----	-----	.834	m	-------	-----	----------	-----	-------	-----	-------	-----	----------	-----

[a] Possible arsenic trioxide lines not superimposed on arsenic lines.

References

[1] A. J. Bradley, The crystal structure of metallic arsenic, Phil. Mag. **47**, 657-671 (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] W. H. Willott and E. J. Evans, An X-ray investigation of the arsenic-tin system of alloys, Phil. Mag. **18**, 114-128 (1934).

[6] H. Stohr, The allotropy of arsenic, Z. anorg. Chem. **242**, 138 (1939).

[7] H. Jung, Centralbl. Min. Geol. (1926) 107-114, as quoted in Z. Krist., Structurbericht **I**, 57 (1913-28).

[8] G. Hagg and A. G. Hybinette, X-ray studies on the systems tin-antimony and tin-arsenic, Phil. Mag. **20**, 913 (1935).

Rhodium, Rh (cubic)

ASTM cards

Card number Old	Card number New	New index lines	Radiation	Source
3188	3333	2.20	Molybdenum, 0.712.	Hall [1] 1921.
	1-1214	1.15		
	1-1214	1.91		
3187	3303	2.20	Molybdenum------	Hanawalt, Rinn, and Frevel [2] 1938.
	1-1205	1.90		
	1-1213	1.15		

Additional published patterns. None.

NBS sample. The rhodium used for the NBS pattern was obtained from the Baker Chemical Company. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of silver; 0.001 to 0.01 percent each of aluminum, iron, iridium, magnesium, manganese, palladium, platinum, and silicon; and 0.0001 to 0.001 percent each of calcium, copper, lead, and ruthenium.

Interplanar spacings and intensity measurements. The Hull 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:

Patterns	1	2	3
Hull------	111	311	200
Hanawalt, Rinn, and Frevel------	111	200	311
Swanson and Fuyat------	111	200	311

Lattice constant. The structure was determined by Hull [1] in 1921. The space group is O_h^5-Fm3m with sodium-chloride-structure type and 4(Rh) per unit cell.

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

Lattice constant in angstroms

1921-----	Hull [1]----------	3.828
1925-----	Barth and Lunde [3]----------	3.803
1928-----	van Arkel [4]----------	3.802
1932-----	Owen and Yates [5]----------	3.8034 at 25°C
1953-----	Swanson and Fuyat----------	3.8031 at 25°C

The density of rhodium calculated from the NBS lattice constant is 12.424 at 25°C.

Rhodium, Rh (cubic)

hkl	1921 Hull Mo, 0.709 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1953 Swanson and Fuyat Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	2.204	100	3.817	2.20	100	3.81	2.1958	100	3.8032
200	1.912	20	3.824	1.90	50	3.80	1.9016	50	3.8032
220	1.353	20	3.827	1.348	30	3.813	1.3446	26	3.8031
311	1.152	30	3.821	1.148	40	3.807	1.1468	33	3.8035
222	1.102	4	3.817	1.101	13	3.814	1.0979	11	3.8032
400	-----	---	-----	.954	4	3.816	.9508	7	3.8032
331	.880	4	3.836	.875	15	3.814	.8724	20	3.8027
420	.855	3	3.824	.854	15	3.819	.8504	14	3.8031
422	.783	2	3.836	.779	8	3.816	------	---	------
511	.737	1	3.830	.734	10	3.814	------	---	------
531	.648	1	3.834	-----	---	-----	------	---	------
Average of the last five lines--------			3.832	-----	---	3.816	------	---	3.8031

References

[1] A. W. Hull, X-ray crystal analysis of thirteen common metals, Phys. Rev. **17**, 571-586 (1921).

[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, Der Einfluss der Lanthaniden Kontraktion auf die Gitterdimensionen der kubischen Platinmetalle, Z. physik. Chem. **117**, 478-490 (1925).

[4] A. E. van Arkel, Eine einfache Methode zur Erhöhung der Genauigkeit bei Debye-Scherrer-Aufnahmen, Z. Krist. **67**, 235-238 (1928).

[5] E. A. Owen and E. L. Yates, Precision measurements of crystal parameters, Phil. Mag. **15**, 472-488 (1933).

Cadmium, Cd (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
3065	3204	2.33	Molybdenum, 0.712.	Hull [1] 1921.
	1-1177	2.79		
	1-1178	1.89		
3043	3203	2.34	Molybdenum------	Hanawalt, Rinn, and Frevel [2] 1938.
	1-1176	2.80		
	1-1175	2.58		

Additional published patterns

Source	Radiation	Wavelength
Roux and Cournot [3] 1928--------	Copper-----	----------
McLennan and Monkman [4] 1929----	Copper-----	----------
Taylor [5] 1932------------------	Copper-----	1.539

NBS sample. The cadmium used for the NBS pattern was prepared by the New Jersey Zinc Co. and is 99.99 percent pure. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent of mercury, 0.0001 to 0.001 percent of silicon, and less than 0.0001 percent each of calcium, copper, iron, magnesium, and lead.

Interplanar spacings and intensity measurements. The d-spacing for the Roux and Cournot and the Taylor patterns were calculated from Bragg angle data. The other three were converted from d-spacings in kX to angstrom units. The Roux and Cournot pattern contains a d-spacing at 2.130 A, which is not possible theoretically. The McLennan and Monkman pattern is incomplete and contains no intensity values.

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

Patterns	1	2	3
Hull----------	101	002	102
Hanawalt, Rinn, and Frevel--	101	002	100
Roux and Cournot----------	101	103	004
Taylor----------	101	112	203
Swanson and Fuyat----------	101	002	100

Lattice constants. The structure was investigated by Hull [1] in 1921. The space group of the hexagonal close packed cell is D^4_{6h}-$P6_3/mmc$ with 2(Cd) per unit cell.

A number of unit cell measurements were converted from kX to angstrom units and were converted from the temperatures indicated in parentheses to 26°C. for comparison with the NBS values. The thermal expansion, according to McLennan and Monkman [4], is 48.2×10^{-6} parallel to the c-axis and 18.5×10^{-6} perpendicular to it.

Lattice constants in angstroms

		a	c
1921-----	Hull [1]----------	2.949	5.572
1929-----	McLennan and Monkman [4]----------	2.971	5.610 at 26°C (18°C)
1931-----	Jenkins and Preston [6]----------	2.9784	5.6155
1932-----	Taylor [5]----------	2.969	5.656
1932-----	Stenzel and Weerts [7]----------	2.9801	5.6191 at 26°C (20°C)
1933-----	Jette and Gebert [8]----------	2.9773	5.6159
1935-----	Jette and Foote [9]----------	2.97918	5.61858 at 26°C (25°C)
1935-----	Kossolapow and Trapesnikow [10]---	2.97910	5.61728 at 26°C
1936-----	Owen and Roberts [11]----------	2.97887	5.61765 at 26°C (18°C)
1941-----	Lu and Chang [12]----------	2.9791	5.6183 at 26°C (21°C)
1947-----	Vegard [13]----------	2.9802	5.6155
1953-----	Swanson and Fuyat----------	2.9793	5.6181 at 26°C

The density of cadmium calculated from the NBS lattice constants is 8.642 at 26°C.

Cadmium, Cd (hexagonal)

hkl	1921 Hull Mo, 0.70926 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.70926 A		1928 Roux and Cournot Cu, 1.5405 A		1929 McLennon and Monkman Cu, 1.5405 A		1932 Taylor Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I	d	I	d	I	d	I
	A		A		A		A		A		A	
002	2.779	33	2.81	40	2.859	vw	--------	-------	--------	-------	2.809	65
100	2.555	17	2.59	30	2.563	w	--------	-------	2.598	vw	2.580	32
101	2.316	100	2.34	100	2.356	vs	--------	-------	2.336	m	2.345	100
-----	--------	-------	--------	-------	2.130	vw	--------	-------	--------	-------	--------	--------
102	1.886	20	1.89	20	1.926	m	1.891	-------	1.900	w	1.901	32
103	1.502	17	1.51	25	1.519	s	1.513	-------	1.520	w	1.516	26
110	1.470	13	1.489	18	--------	-------	1.484	-------	1.489	w	1.490	19
004	1.392	2	1.403	3	1.353	s	--------	-------	--------	-------	1.404	3
112	1.301	17	1.313	27	1.301	w	1.316	-------	1.314	m	1.316	17
200	1.282	0	1.289	2	--------	-------	--------	-------	1.293	w	1.290	2
201	1.245	10	1.255	20	1.216	vw	1.255	-------	--------	-------	1.258	13
104	1.219	2	1.230	2	1.179	vw	1.231	-------	1.231	w	1.234	4
202	1.112	3	1.172	3	1.124	vw	1.171	-------	--------	-------	1.1724	3
203	1.051	3	1.062	5	1.083	vw	1.060	-------	1.062	m	1.0622	5
105	1.020	3	1.022	4	1.033	vw	1.028	-------	1.019	m	1.0303	3
114	1.010	3	--------	-------	1.004	vw	1.020	-------	--------	-------	1.0220	4
210	--------	-------	--------	-------	--------	-------	--------	-------	.9749	w	.9752	2
211	.949	7	.961	10	.951	vw	.958	-------	.9601	m	.9609	9
204	--------	-------	--------	-------	--------	-------	--------	-------	.9517	w	.9501	1
006	--------	-------	--------	-------	--------	-------	--------	-------	--------	-------	.9363	1
212	.910	2	.923	2	--------	-------	.919	-------	.9218	m	.9212	4
106	--------	-------	--------	-------	--------	-------	--------	-------	--------	-------	.8802	2
213	.857	5	.865	4	--------	-------	.864	-------	--------	-------	.8650	10
300	--------	-------	--------	-------	--------	-------	.858	-------	--------	-------	.8600	2
205	.840	2	--------	-------	--------	-------	.846	-------	--------	-------	.8473	1
302	.814	2	.823	2	--------	-------	.821	-------	--------	-------	.8223	5
214	--------	-------	--------	-------	--------	-------	--------	-------	--------	-------	.8010	2

References

[1] A. W. Hull, X-ray crystal analysis of thirteen common metals, Phys. Rev. **17**, 571-588 (1921).

[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. Roux and J. Cournot, Etude cristallographique par rayons X de la structure de dépôts électrolytiques simultanés de deux métaux, Compt. rend. (Paris) **186**, 1733-36 (1928).

[4] J. C. McLennan and R. J. Monkman, On the thermal expansion of zinc and cadmium crystals and on the crystal structure of erbium and niobium, Trans. Roy. Soc. Can. III, **23**, 255-267 (1929).

[5] N. W. Taylor, Solid cadmium amalgams. An X-ray proof of the compound Cd_3Hg, J. Am. Chem. Soc. **54**, 2713-2720 (1932).

[6] C. H. M. Jenkins and G. O. Preston, Some properties of metallic cadmium, J. Inst. Metals **45**, 307-343 (1931).

[7] W. Stenzel and J. Weerts, Präzisionsbestimmung von Gitterkonstanten nichtkubischer Stoffe, Z. Krist. **84**, 20-44 (1932).

[8] E. R. Jette and E. B. Gebert, An X-ray study of the binary alloys of silicon with Ag, Au, Pb, Sn, Zn, Cd, Sb, and Bi, J. Chem. Phys. **1**, 753-755 (1933).

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

[10] G. F. Kossolapow and A. K. Trapesnikow, X-ray investigation of the thermal expansion of Cd, Z. Krist. **91A**, 410-423 (1935).

[11] E. A. Owen and E. W. Roberts, The thermal expansion of the crystal lattices of cadmium, osmium, and ruthenium, Phil. Mag. **22**, 290-304 (1936).

[12] S. S. Lu and Y. L. Chang, The accurate evaluation of lattice spacings from back-reflection powder photographs, Proc. Phys. Soc. (London) **53**, 517-528 (1941).

[13] L. Vegard, Investigation into the structure and properties of solid matter with the help of X-rays, Skrifter Norske Videnskaps-Akad. Oslo I, Mat. Naturv. Kl. 1947, No. 2, 83 p. (1947).

Indium, In (tetragonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2568	2714	2.72	Molybdenum---	Hanawalt, Rinn, and Frevel [1] 1938.
	1-1046	2.29		
	1-1042	1.68		
2599	------	2.70	----------	Hull [2] 1920.
	------	2.29		
	------	1.675		

The Hull pattern was not reproduced in the revised edition of the file or in the 1950 index and is found only in the original card file and index.

Additional published patterns. None.

NBS sample. The indium used for the NBS pattern was obtained from the Fisher Scientific Co. through the NBS Spectrographic Laboratory. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of iron, nickel, silicon, and tin; 0.0001 to 0.001 percent each of aluminum, copper, and calcium; and less than 0.0001 percent of silver.

The intensities were determined from several patterns produced from indium filings and from vaporized indium made by arcing two indium electrodes under water.

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

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

Patterns	1	2	3
Hanawalt, Rinn, and Frevel--------	101	110	112
Hull----------	101	110	112
Swanson and Fuyat----------	101	110	112

Lattice constants. The structure was determined by Hull [2] in 1920. The space group is D_{4h}^{17}-I4/mmm with 2(In) per unit cell. Indium 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. Several *a*-values given in terms of the larger cell produced by a 45° rotation about the *c*-axis were reduced to the true cell size.

Lattice constants in angstroms

		a	*c*
1920	Hull [2]----------	3.25	4.87
1932	Dwyer and Mellor [3]-------	3.251	4.956
1933	Zintl and Neumayr [4]------	3.247	4.946
1933	Shinoda [5]----------	3.246	4.943
1935	Frevel and Ott [6]---------	3.251	4.948
1936	Ageev and Ageeva [7]-------	3.284	5.007
1938	Betteridge [8]----------	3.2514	4.9457
1953	Swanson and Fuyat----------	3.2517	4.9459 at 26°C

The density of indium calculated from the NBS lattice constants is 7.286 at 26°C.

Indium, In (tetragonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1920 Hull Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
101	2.73	100	2.71	100	2.715	100
002	2.46	25	2.42	3	2.471	21
110	2.29	40	2.29	25	2.298	36
112	1.68	30	1.678	10	1.683	24
200	1.62	15	1.620	3	1.625	12
103	1.465	20	1.453	5	1.470	16
211	1.398	30	1.395	10	1.395	23
202	1.358	15	1.351	10	1.358	11
004	--------	------	--------	----	1.2368	3
220	1.146	2	1.152	1	1.1493	5
213	1.090	10	1.082	5	1.0904	12
301	1.057	2	--------	----	1.0587	4
222	1.042	2	--------	----	1.0425	5
310	1.027	2	--------	----	1.0282	8
204	.982	2	--------	----	.9845	1
312	.950	6	--------	----	.9495	3
303	.907	2	--------	----	.9056	2
321	.890	2	--------	----	.8874	4
215	--------	------	--------	----	.8180	3

References

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

[2] A. W. Hull, Arrangement of the atoms in some common metals, Science **52**, 227-229 (1920).

[3] F. D. Dwyer and D. P. Mellor, J. Proc. Roy. Soc. N. S. Wales **66**, 234-239 (1932) as quoted in [7].

[4] E. Zintl and S. Neumayr, Gitterstruktur des Indiums, Z. Elektrochem. **39**, 81-84 (1933).

[5] G. Shinoda, X-ray investigations on the thermal expansion of solids. I., Mem. Coll. Sci. Kyoto Imp. Univ. **16A**, 193-201 (1933).
[6] L. K. Frevel and E. Ott, The X-ray study of indium and the indium-silver system, J. Am. Chem. Soc. **57**, 228 (1935).
[7] N. W. Ageev and V. Ageeva, Solid solutions of indium and lead, J. Inst. Metals **59**, No. 2, 311-316 (1936).
[8] W. Betteridge, The crystal structure of Cd-In alloys rich in In, Proc. Phys. Soc. (London) **50A**, 519 (1938).

Antimony, Sb (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-1273	2002	3.08	Copper----	Dorn and Glockler [1] 1937.
	2-0597	2.31		
	2-0587	2.14		
1940	1911	3.10	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.
	1-0793	2.24		
	1-0802	2.14		
II-1287	2005	3.07	Copper----	Harcourt [3] 1942.
	2-0599	2.23		
	2-0592	2.13		

Additional published patterns. None.

NBS sample. An antimony sample from C.A.F. Kahlbaum was used for the NBS pattern. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent of copper, 0.0001 to 0.001 percent each of bismuth, iron, nickel, lead, silicon, and tin, and less than 0.0001 percent each of silver, aluminum, and calcium.

Interplanar spacings and intensity measurements. The *d*-spacings for the Dorn and Glockler pattern were calculated from Bragg angle data, whereas those for the Hanawalt, Rinn, and Frevel and the Harcourt patterns were converted from kX to angstrom units. Lines at 1.717 A and 1.678 A found in the Dorn and Glockler and the Harcourt patterns, respectively, are possible antimony lines, but they are not in the NBS pattern.

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

Patterns	1	2	3
Dorn and Glockler	102	014	110
Hanawalt, Rinn, and Frevel	102	014	110
Harcourt	102	014	110
Swanson and Fuyat	102	014	212

Lattice constants. The structure was determined by James and Tunstall [4] in 1920. The space group is D_{3d}^5-$R\bar{3}m$ with arsenic-structure-type and 6(Sb) per unit cell.

Several unit-cell measurements have been converted from rhombohedral to hexagonal dimensions and from kX to angstrom units. The Lu and Chang and the Jette and Foote values were converted to 26°C from the temperatures indicated in parentheses, using the coefficient of expansion determined by Erfling [5]. The expansion is 16.18×10^{-6} parallel to the *c*-axis and 8.24×10^{-6} perpendicular to it.

Lattice constants in angstroms

		a	*c*
1933	Jette and Gebert [6]	4.304	11.270
1935	Hägg and Hybinette [7]	4.313	11.263
1935	Jette and Foote [8]	4.3083	11.2743 (25°C)
1937	Dorn and Glockler [1]	4.294	11.263
1941	Lu and Chang [9]	4.307	11.274 (22°C)
1953	Swanson and Fuyat	4.307	11.273 at 26°C

The density of antimony calculated from the NBS lattice constants is 6.697 at 26°C.

Antimony, Sb (hexagonal)

hkl	1937 Dorn and Glockler Cu, 1.5405A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709A		1942 Harcourt Cu, 1.5405A		1953 Swanson and Fuyat Cu, 1.5405A 25.5°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A	
003	3.71	s	3.72	15	-----	----	3.753	25
011	-----	----	-----	----	-----	----	3.538	4
102	3.092	vs	3.11	100	3.08	100	3.109	100
014	2.251	vs	2.24	63	2.23	33	2.248	70
110	2.142	vs	2.14	63	2.13	33	2.152	56
105	1.926	s	-----	----	1.92	8	1.929	12
006	1.873	s	1.86	15	1.87	8	1.878	35
022	1.763	vs	1.76	44	1.759	17	1.770	26
-----	1.717	w	-----	----	1.678	3	-----	----
204	1.552	vw	1.55	20	1.543	17	1.555	15
017	1.473	s	1.473	13	1.473	8	1.479	13
025	1.433	vw	-----	----	-----	----	1.437	12
116	1.410	s	1.413	20	1.408	17	1.416	63
212	1.362	s	1.363	25	1.358	17	1.368	67
108	1.313	s	1.313	8	-----	----	1.318	30
124	1.257	s	1.261	15	-----	----	1.261	40
009	-----	----	1.246	10	1.254	17	1.252	25
300	1.239	s	-----	----	1.234	17	1.243	30
207	-----	----	1.217	3	1.217	5	1.219	11
215	1.191	s	1.192	3	-----	----	1.1955	12
303	-----	----	-----	----	-----	----	1.1802	5
028	1.123	w	1.122	3	-----	----	1.1243	12
119	1.079	s	-----	----	-----	----	1.0829	32
0·1·10	-----	----	1.077	10	1.077	8	1.0792	16
220	-----	----	-----	----	-----	----	1.0768	12
127	1.056	s	1.049	3	-----	----	1.0609	16
306	1.041	s	1.033	8	1.032	5	1.0369	17
132	1.014	s	-----	----	1.010	3	1.0177	27
218	1.000	vw	-----	----	-----	----	.9966	25
1·0·11	.985	w	-----	----	.987	3	.9882	24

Antimony, Sb (hexagonal)—Con.

hkl	1937 Dorn and Glockler Cu, 1.5405A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709A		1942 Harcourt Cu, 1.5405A		1953 Swanson and Fuyat Cu, 1.5405A 25.5°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
-----	.979	s	-----	----	-----	----	-----	----
314	.967	s	-----	----	-----	----	.9713	15
2·0·10	-----	----	-----	----	.964	5	.9650	8
135	-----	----	-----	----	-----	----	.9402	7
226	.931	s	-----	----	-----	----	.9343	13
402	-----	----	-----	----	-----	----	.9201	8
0·2·11	-----	----	-----	----	-----	----	.8981	10
044	-----	----	-----	----	-----	----	.8853	7
309	-----	----	-----	----	-----	----	.8825	15
1·2·10	-----	----	-----	----	.878	5	.8804	15
317	-----	----	-----	----	-----	----	.8704	7
405	-----	----	-----	----	-----	----	.8612	5
322	-----	----	-----	----	-----	----	.8461	11
0·1·13	-----	----	-----	----	.843	5	.8446	22
138	-----	----	-----	----	-----	----	.8340	5
-----	-----	----	-----	----	-----	----	.8290	16
-----	-----	----	-----	----	-----	----	.8190	8
-----	-----	----	-----	----	-----	----	.8167	22
-----	-----	----	-----	----	-----	----	.8140	13
-----	-----	----	-----	----	-----	----	.8071	7

References

[1] J. E. Dorn and G. Glockler, X-ray study of the structure of copper, lead, cadmium and antimony at high temperatures, J. Phys. Chem. **41**, 499-506 (1937).

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

[4] R. W. James and N. Tunstall, The crystalline structure of antimony, Phil. Mag. **40**, 233-239 (1920).

[5] H. D. Erfling, Studien zur thermischen Ausdehnung fester Stoffe in tiefer Temperatur. II, Ann. Physik. **34**, 136-160 (1939).

[6] E. R. Jette and E. B. Gebert, An X-ray study of the binary alloys of silicon with Ag, Au, Pb, Sn, Zn, Cd, Sb, and Bi, J. Chem. Phys. **1**, 753-755 (1933).

[7] G. Hägg and A. G. Hybinette, X-ray studies on the systems tin-antimony and tin-arsenic, Phil. Mag. **20**, 913-928 (1935).

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

[9] S. S. Lu and Y. L. Chang, The accurate evaluation of lattice spacings from back-reflection powder photographs, Proc. Phys. Soc. (London) **53**, 517-528 (1941).

Iodine, I_2 (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1246	------	3.69 3.09 1.97	Molybdenum----	Hanawalt, Rinn, and Frevel [1] 1938.

This pattern was not reproduced in the revised edition of the file or in the 1950 index and is found only in the original card file and index.

Additional published patterns

Source	Radiation	Wavelength
Harris, Mack, and Blake [2] 1928--	Molybdenum	0.710

NBS sample. The iodine sample used for the NBS pattern was obtained from the Fisher Scientific Co. Chemical analysis at the NBS showed the following impurities: Chlorine and bromine, determined as the chloride, less than 0.005 percent, and total nonvolatiles less than 0.020 percent. The refractive indices are too high to be measured by the usual grain-oil immersion methods.

Interplanar spacings and intensity measurements. The *d*-spacings for both the Hanawalt, Rinn, and Frevel and the Harris, Mack, and Blake patterns were converted from kX to angstrom units. The latter of these contains a very weak line at 1.881 A that does not appear in the NBS pattern or among the permissible calculated lines for iodine.

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

Patterns	1	2	3
Hanawalt, Rinn, and Frevel--------	111	112	132
Harris, Mack, and Blake----------	112	111	020
Swanson and Fuyat----------	112	111	020

Lattice constants. The structure was determined by Harris, Mack, and Blake [2] in 1928. The space group is D_{2h}^{18}-Ccmb (Cmca) with gallium structure type and $4(I_2)$ per unit cell.

Three unit-cell values were converted from kX to angstrom units for comparison with the NBS values. The Straumanis and Sauka values were converted from 25° to 26°C, using their coefficient of expansion [4] of 133.4×10^{-6} parallel to the *a*-axis, 95.0×10^{-6} parallel to the *b*-axis, and 35.1×10^{-6} parallel to the *c*-axis.

Lattice constants in angstroms

		a	*b*	*c*
1927	Ferrari [3]-------	4.770	7.178	9.803
1928	Harris, Mack, and Blake [2].	4.805	7.270	9.800
1943	Straumanis and Sauka [4].	4.79044	7.27007	9.79344 at 26°C
1953	Swanson and Fuyat	4.792	7.271	9.803 at 26°C

The density of iodine calculated from the NBS lattice constants is 4.935 at 26°C.

Iodine, I_2 (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1928 Harris, Mack, and Blake Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
111	3.70	100	3.705	83	3.708	66
020	-------	------	3.623	83	3.635	62
112	3.10	100	3.100	100	3.103	100
113	2.53	8	2.535	17	2.534	14
004	2.44	18	2.458	33	2.456	23
200	-------	------	2.394	vw	2.395	2
201	2.33	15	2.326	27	2.328	20
131	2.11	15	2.108	20	2.112	13
024	2.02	20	2.036	33	2.036	23
220	-------	------	-------	------	2.000	5
132	1.97	30	1.982	------	1.979	28
221	-------	------	1.968	33	1.959	17
203	-------	------	1.933	23	1.933	14
---	-------	------	1.881	vvw	--------	--------
040	1.81	10	1.813	23	1.817	9
133	-------	------	-------	------	1.804	5
115	1.76	10	1.763	20	1.763	13
223	1.71	20	1.709	33	1.707	18
224	-------	------	-------	------	1.551	4
311	-------	------	1.544	23	1.540	7
205	-------	------	-------	------	1.519	4
116	1.51	10	1.516	27	1.515	10
312	-------	------	1.491	vw	1.487	3
044	1.463	8	1.459	20	1.461	6
135	-------	------	-------	------	1.454	3
241	-------	------	1.435	7	1.432	5
313	-------	------	1.407	13	1.408	4
225	1.403	5	-------	------	1.402	2
151	-------	------	1.378	3	1.377	1
152	-------	------	1.339	17	1.338	5
243	-------	------	1.325	w	1.324	7
117	-------	------	1.302	w	1.321	7
136	-------	------	1.202	w	1.305	4

References

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

[2] P. M. Harris, E. Mack, and F. C. Blake, The atomic arrangement in the crystal of orthorhombic iodine, J. Am. Chem. Soc. **50**, 1583-1600 (1928).

[3] A. Ferrari, La struttura cristallina dello iodio, Rend. accad. nazb. Lincei **5**, 582-586 (1927).

[4] M. Straumanis and J. Sauka, Die Gitterkonstanten und Ausdehnungskoeffizienten des Jods, Z. physik. Chem. **B53**, 320-330 (1943).

Hafnium, Hf (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
----	2748 2-0898 2-0885	2.73 1.66 1.42	Zinc-----	Noethling and Tolksdorf [1] 1925.

Additional published patterns

Source	Radiation	Wavelength
Sidhu and McGuire [2] 1952------	Copper------	K_α

NBS sample. The hafnium used for the NBS pattern came from two sources, a cross-sectional slice of an "as deposited" crystal bar supplied by the Atomic Energy Commission and a rolled sheet contributed by the Foote Mineral Co. Both were prepared by the iodide process. The Foote sample was annealed in vacuum for 1 hour at 850°C. Flat surfaces were filed on the AEC sample and then etched with hydrofluoric acid.

The AEC spectrographic analysis of their sample showed the following impurities: 2.0 percent of zirconium, 0.02 percent of iron, 0.001 to 0.01 percent each of silicon, aluminum, titanium, calcium, nickel, and chromium, and less than 0.001 percent each of copper, manganese, magnesium, lead, molybdenum, and tin. Spectrographic analysis of the Foote Mineral Co. sample at the NBS showed the following impurities: 0.1 to 1.0 percent of zirconium, 0.01 to 0.1 percent each of nickel, silicon, and zinc, 0.001 to 0.01 percent each of aluminum, iron, and magnesium, 0.0001 to 0.001 percent of copper, and less than 0.0001 percent of silver.

Interplanar spacings and intensity measurements. The *d*-spacings for the Noethling and Tolksdorf pattern were calculated from Bragg angle data; the *d*-spacings for the Sidhu and McGuire pattern were published in angstrom units. Since the NBS samples were either oriented or large-grained, the rolled sheet and several different surfaces of the chunk were used to obtain all of the *d*-spacings. It was possible to combine these values into one pattern because the reflections in both samples had identical *d*-spacings. The ASTM card for the Noethling and Tolksdorf pattern made with zinc radiation contains a *d*-spacing of 1.50 not found in the original reference, whereas the original reference contains a *d*-spacing of 1.36 not found on the ASTM card. Another Noethling and Tolksdorf pattern made with copper radiation contains an additional *d*-spacing of 1.808 that has not been included in the card-file pattern or in the table in this report because it is not a possible hafnium line. The line at 0.924 angstrom, *hkl* of 300, found in the Sidhu and McGuire pattern is not in the NBS pattern.

The NBS intensity values were the average of four sets of values measured, using filings mixed with silica gel. The three strongest lines for each of the patterns are as follows:

Patterns	1	2	3
Sidhu and McGuire-----	101	100	002
Swanson and Fuyat-----	101	002	100

The strong lines of the Noethling and Tolksdorf pattern do not coincide with the indexed NBS pattern, and they apparently represent quite a different material.

Lattice constants. The structure was determined by Noethling and Tolksdorf [1], who showed its similarity to the zirconium structure. The space group is D^4_{6h}-$P6_3/mmc$ with 2(Hf) per unit cell.

The Noethling and Tolksdorf and the van Arkel lattice constants were converted from kX to angstrom units, whereas the Fast, the Duwez, and the Sidhu and McGuire values were published in angstroms.

Lattice constants in angstroms

		a	*c*
1925	Noethling and Tolksdorf [1]--	3.33	5.47
1927	Van Arkel [3]----------	3.206	5.087
1948	Fast [4]----------	3.187	5.041
1951	Duwez [5]----------	3.1952	5.0569
1952	Sidhu and McGuire [2]-------	3.200	5.061
1953	Swanson and Fuyat----------	3.1967	5.0578 at 26°C

The density of hafnium calculated from the NBS lattice constants is 13.248 at 26°C.

Hafnium, Hf (hexagonal)

hkl	1925 Noethling and Tolksdorf Zn, 1.4351 A		1952 Sidhu and McGuire Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
---	2.84	s	-------	------	--------	--------
100	-------	------	2.77	s	2.768	27
---	2.72	vs	-------	------	--------	--------
002	2.54	w	2.53	s	2.531	34
101	-------	------	2.43	vs	2.428	100
---	2.35	w	-------	------	--------	--------
---	1.99	w	-------	------	--------	--------
102	-------	------	1.868	s	1.866	16
---	1.65	vs	-------	------	--------	--------
110	1.59	w	1.600	s	1.599	14
---	1.53	vw	-------	------	--------	--------
103	-------	------	1.443	s	1.440	16
200	1.41	vs	1.383	w	1.385	2
112	1.36	ms	1.354	s	1.351	16
201	1.31	w	1.337	s	1.336	12
004	1.26	w	1.265	m^+	1.265	4
202	1.23	w	1.216	m	1.214	3
104	-------	------	1.152	m	1.1503	3
203	1.08	ms	1.065	s	1.0697	4
210	-------	------	1.049	w^+	1.0464	1
211	-------	------	1.027	s	1.0247	6
114	.991	w	.993	s	.9917	5
212	-------	------	.968	m	.9671	2
105	.957	ms	.951	s	.9502	5
204	.931	ms	.935	m	.9336	3
---	-------	------	.924	m	--------	--------
213	.907	ms	.890	s	.8891	5
302	-------	------	.868	m	.8668	4
006	-------	------	.844	w	.8428	1
205	-------	------	.817	m	.8168	2
106, 214	.798	s	.807	m	.8060	3

References

[1] W. Noethling and S. Tolksdorf, Die Kristallstruktur des Hafniums, Z. Krist. **62**, 255-259 (1925).

[2] S. S. Sidhu and J. C. McGuire, An X-ray diffraction study of the hafnium-hydrogen system, J. Appl. Phys. **23**, 1257-1261 (1952).

[3] A. E. van Arkel, Das Atomvolum des Zirkoniums und des Hafniums, Z. physik, Chem. **130**, 100-104 (1927).

[4] J. D. Fast, The allotropic transformation of hafnium and a tentative equilibrium diagram of the system zirconium-hafnium, J. Appl. Phys. **23**, 350-351 (1952), as quoted from J. D. Fast, Chem. Weekblad **44**, 621 (1948).

[5] P. Duwez, The allotropic transformation of hafnium, J. Appl. Phys. **22**, 1174-1175 (1951).

Bismuth, Bi (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1710	1659	3.26	Molybdenum	Davey [1] 1925.
	1-0700	2.35		
	1-0699	2.26		
II-1078	1683	3.25	Copper----	Parravano and Caglioti [2] 1930.
	2-0491	1.44	Copper----	Caglioti [3] 1930.
	2-0491	2.35		
1692	1658	3.28	Molybdenum	Hanawalt, Rinn, and Frevel [4] 1938.
	1-0699	2.35		
	1-0688	2.27		
II-1124	1776	3.21	Copper----	Harcourt [5] 1942.
	2-0527	1.44		
	2-0518	2.25		

The Harcourt ASTM card erroneously states that molybdenum radiation was used. The Parravano and Caglioti and the Caglioti patterns are identical except for one line listed 44.47 and 44.42, respectively, and they are combined on one card.

Additional published patterns

Source	Radiation	Wavelength
Solomon and Jones [6] 1931	Copper----------	----------

NBS sample. The bismuth used for the NBS pattern was prepared by the Johnson Matthey & Co. Ltd. Their spectrographic analysis shows less than 0.001 percent each of lead, silicon, copper, iron, aluminum, calcium, magnesium, and sodium.

Interplanar spacings and intensity measurements. The d-spacings of the Davey, the Hanawalt, Rinn, and Frevel, the Harcourt, and the Solomon and Jones patterns were converted from supposed kX to angstrom units. The Parravano and Caglioti pattern, expressed in Bragg angles, was converted directly into angstroms. The Parravano pattern contains four lines with d-spacings 2.982, 2.707, 1.836, and 1.743 not possible in the bismuth structure, as shown by the theoretical pattern.

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

Patterns	1	2	3
Davey----------	102	014	110
Parravano and Caglioti----------	102	212	132
Hanawalt, Rinn, and Frevel-------	102	014	110
Harcourt----------	102	212	110
Solomon and Jones----------	102	014	110
Swanson and Fuyat----------	102	110	014

Lattice constants. The structure was determined by Hassel and Mark [7] in 1924 following several more general investigations. The space group is D^5_{3d}-$R\bar{3}m$ with arsenic-structure type and 6(Bi) per unit cell.

A group of unit-cell determinations were converted from kX to angstrom units for comparison with the NBS values. The Hassel and Mark, the Ehret and Fine, and the Solomon and Jones data also were converted from rhombohedral to hexagonal form. The Hassel and Mark, and the Solomon and Jones values were originally presented in terms of a nonprimitive cell with a-values twice their true length. These have been halved for comparison.

Lattice constants in angstroms

		a	c
1924	Davey [1]----------	4.548	11.853
1924	Hassel and Mark [7]---------	4.55	11.85
1930	Ehret and Fine [8]----------	4.551	11.867
1931	Solomon and Jones [6]-------	4.525	11.799
1935	Jette and Foote [9]---------	4.54643	11.8620
1938	Ievinš, Straumanis, and Karlsons [10]----------	4.54590	11.86225
1953	Swanson and Fuyat----------	4.546	11.860 at 25°C

The coefficient of expansion parallel to the c-axis, as determined by Jacobs and Goetz [11], is approximately 13.8×10^{-6}. The density calculated from the NBS lattice constants is 9.808 at 25°C.

Bismuth, Bi (hexagonal)

hkl	1925 Davey Mo, 0.709 A		1930 Parravano and Caglioti Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1938 Harcourt Cu, 1.5405 A		1931 Solomon and Jones Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	I	d	I	d	I	d	I	d	I	d	I
	A		A		A		A		A		A	
003	3.94	11	---	---	---	---	---	---	---	---	3.95	9
011	3.71	11	---	---	---	---	---	---	---	---	3.74	3
102	3.27	100	3.26	s	3.29	100	3.22	100	3.254	s	3.28	100
---	---	---	2.982	m	---	---	---	---	---	---	---	---
---	---	---	2.707	m	---	---	---	---	---	---	---	---
014	2.35	89	2.346	ms	2.35	50	2.34	33	2.358	m	2.39	40
110	2.26	89	2.258	ms	2.27	50	2.250	67	2.262	m	2.273	41
105	2.02	33	---	---	2.01	7	2.019	17	2.022	w	2.030	8
006	---	---	---	---	---	---	---	---	---	---	1.976	3
113	1.968	45	1.988	w	1.96	13	1.959	17	1.969	m	1.970	10
201	---	---	1.941	w	---	---	---	---	---	---	1.941	1
022	1.866	78	1.886	w	1.86	30	1.854	33	1.866	m	1.868	23
---	---	---	1.836	m	---	---	---	---	---	---	---	---
---	---	---	1.743	mw	---	---	---	---	---	---	---	---
204	1.638	67	1.636	m	1.63	20	1.628	33	1.633	m	1.639	9
017	1.553	33	1.550	ms	1.54	3	1.548	17	1.552	w	1.556	6
025	1.514	22	---	---	---	---	---	---	---	---	1.515	2
116	1.489	67	1.480	ms	1.493	20	1.483	67	1.488	m	1.491	13
212	1.442	78	1.445	s	1.443	27	1.438	100	1.441	m	1.443	16
108	1.386	22	---	---	---	---	1.381	17	1.386	w	1.387	4
124	1.329	45	1.331	ms	1.330	13	1.328	67	1.326	m	1.330	11
009	---	---	---	---	---	---	---	---	---	---	1.319	1
300	1.313	45	1.313	ms	---	---	1.307	33	1.310	m	1.312	6
207	1.286	22	---	---	---	---	1.281	17	1.284	w	1.284	2
215	1.260	11	1.237	mw	---	---	1.257	17	1.259	vw	1.261	2
303	---	---	---	---	---	---	1.243	10	---	---	1.246	1
028	1.184	22	---	---	1.182	3	1.182	17	---	---	1.1843	2
119	1.139	33	---	---	---	---	---	---	---	---	1.1399	4
220	---	---	1.134	mw	1.137	10	1.134	67	1.133	vw	1.1368	4
127	1.118	11	---	---	---	---	1.114	33	---	---	1.1179	2
306	1.093	33	1.094	mw	1.091	7	1.090	67	1.090	vw	1.0932	4
132	1.074	33	1.072	s	1.075	7	1.071	67	1.071	w	1.0738	5
218	1.048	22	---	---	1.047	3	1.049	17	---	---	1.0501	2
1·0·11	---	---	1.043	s	---	---	1.038	17	---	---	1.0399	2
314	1.023	22	1.022	s	1.022	3	1.023	33	---	---	1.0247	3
135	---	---	---	---	---	---	---	---	---	---	.9920	1
226	.986	22	.984	ms	---	---	.984	17	---	---	.9854	3
402	.969	22	.971	ms	---	---	.970	17	---	---	.9709	2
0·2·11	---	---	---	---	---	---	.945	17	---	---	.9455	2
309	.933	22	.927	ms	---	---	.929	17	---	---	.9301	4
1·2·10	---	---	---	---	---	---	---	---	---	---	.9276	2
317	---	---	.919	ms	---	---	.917	17	---	---	.9178	2
1·1·12	---	---	---	---	---	---	---	---	---	---	.9065	2
322	.892	22	---	---	---	---	.893	33	---	---	.8928	2
0·1·13	---	---	.890	ms	---	---	---	---	---	---	.8886	2
138	.878	11	---	---	---	---	.880	10	---	---	.8792	2
2·1·11	---	---	.873	ms	---	---	.874	33	---	---	.8731	2
234	---	---	---	---	---	---	.864	33	---	---	.8640	2
410	.859	11	.860	ms	---	---	.860	33	---	---	.8591	4
047	---	---	---	---	---	---	---	---	---	---	.8511	<1
---	.794	22	---	---	---	---	.829	33	---	---	---	---
---	.752	22	---	---	---	---	.821	17	---	---	---	---

References

[1] W. P. Davey, Precision measurements of the lattice constants of twelve common metals, Phys. Rev. **25**, 753-761 (1925).

[2] N. Parravano and V. Caglioti, Ricerche sul sistema bismuto-selenio, Gazz. chim. ital. **60**, 923-935 (1930).

[3] V. Caglioti, Sulla non esistenza dei sottoioduri di bismuto BiJ_2 e BiJ, Gazz. chim. ital. **60**, 935 (1930).

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

[6] D. Solomon and W. M. Jones, An X-ray investigation of the lead-bismuth and tin-bismuth alloys, Phil. Mag. **11**, 1090-1103 (1931).

[7] O. Hassel and H. Mark, Über die Struktur des Wismuts, Z. Physik. **23**, 269-277 (1924).

[8] W. F. Ehret and R. D. Fine, Crystal structure in the system copper-bismuth, Phil. Mag. **10**, 551-559 (Oct. 1930).

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

[10] A. Ievinš, M. Straumanis, and K. Karlsons, Die Präzisionsbestimmung von Gitterkonstanten nichtkubischer Stoffe (Bi, Mg, Sn) nach der asymmetrischen Methode, Z. physik. Chem. **40B**, 347-356 (1938).

[11] R. B. Jacobs and A. Goetz, The thermal expansion of the bismuth lattice between 25° and 530° Abs., Phys. Rev. **51**, 159-164 (1937).

2.2. Selenides

Zinc Selenide, ZnSe (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-1058	1672	3.28	Molybdenum	General Electric Co., Wembley, England.
	2-0487	2.00		
	2-0479	1.72		
1694	1673	3.28	Molybdenum	New Jersey Zinc Co.
	1-0708	2.00		
	1-0690	1.70		

The radiation given above is that found on the ASTM cards as no published data are available.

Additional published patterns. None.

NBS sample. The zinc selenide used for the NBS pattern is a specially purified sample prepared by the Mallinckrodt Chemical Works. Their spectrographic analysis shows 0.001 to 0.01 percent each of barium, potassium, molybdenum, and sodium, 0.0001 to 0.001 percent each of aluminum, calcium, iron, magnesium, nickel, palladium, and silicon, and less than 0.0001 percent each of silver, bismuth, cadmium, copper, and manganese. Chemical analysis at the NBS showed that the sample contained 44.9 percent zinc as compared to the theoretical amount, 45.3 percent. The refractive index is too high to be measured by grain-oil immersion methods.

Interplanar spacings and intensity measurements. The *d*-spacings for the General Electric and New Jersey Zinc patterns were converted from kX to angstrom units.

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

Pattern	1	2	3
General Electric Company	111	220	311
New Jersey Zinc Company	111	220	311
Swanson and Fuyat	111	220	311

Lattice constant. The structure was investigated by Davey [1] in 1923. The space group is T_d^2-F$\bar{4}$3m with 4(ZnSe) per unit cell.

Several unit cell measurements were converted to angstroms for comparison with the NBS value.

Lattice constant in angstroms

1923	Davey [1]	5.662
1926	Zachariasen [2]	5.672
1953	Swanson and Fuyat	5.667 at 25°C

The density of zinc selenide calculated from the NBS lattice constant is 5.267 at 25°C.

Zinc Selenide, ZnSe (cubic)

hkl	---- General Electric Co. Mo, 0.709 A			---- New Jersey Zinc Co. Mo, 0.709 A			1953 Swanson and Fuyat Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
111	3.288	100	5.695	3.29	100	5.698	3.273	100	5.669
200	2.850	10	5.700	-----	---	-----	2.835	<1	5.670
220	2.008	100	5.679	1.999	80	5.654	2.003	70	5.665
311	1.719	90	5.701	1.704	50	5.652	1.707	44	5.661
222	-----	---	-----	-----	---	-----	1.635	<1	5.664
400	1.417	40	5.668	1.413	8	5.652	1.416	9	5.664
331	1.301	50	5.671	1.298	20	5.658	1.299	13	5.662
420	-----	---	-----	-----	---	-----	1.267	<1	5.666
422	1.156	60	5.663	1.156	30	5.663	1.1561	15	5.664
511	1.091	50	5.669	1.091	10	5.669	1.0901	8	5.664
440	1.002	40	5.668	1.001	2	5.663	1.0018	4	5.667
531	.959	60	5.674	.958	8	5.668	.9577	8	5.666
600	-----	---	-----	-----	---	-----	.9441	<1	5.665
620	-----	---	-----	-----	---	-----	.8958	4	5.666
533	-----	---	-----	-----	---	-----	.8642	2	5.667
622	-----	---	-----	-----	---	-----	.8545	<1	5.668
444	-----	---	-----	-----	---	-----	.8180	2	5.667
Average value of the last five lines			5.669	-----	---	5.664	------	---	5.667

References

[1] W. P. Davey, The crystal structure and densities of Cu_2Se and ZnSe, Phys. Rev. **21**, 380 (1923).

[2] W. H. Zachariasen, Uber die Kristallstrukturen der Selenide von Beryllium, Zink, Cadmium und Quecksilber, Z. physik. Chem. **124**, 436-448 (1926).

2.3. Oxides

Silicon dioxide (alpha-quartz), SiO_2 (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-1034	1597	3.32	Molybdenum, 0.710.	Harrington [1] 1927.
	2-0474	1.82		
	2-0471	1.38		
-------	1535	3.35	No data----	Waldo [2] 1935.
	2-0456	1.81		
	2-0459	1.37		
1612	1472	3.35	Molybdenum	Hanawalt, Rinn and Frevel [3] 1938.
	1-0633	4.25		
	1-0649	1.82		
-------	1471	3.35	Copper-----	Favejee [4] 1939. B
	3-0407	4.26		
	3-0419	1.37		
-------	1534	3.35	Cobalt, 1.786.	Clark [5] 1946.
	3-0427	1.81		
	3-0427	1.54		
II-1007	1533	3.35	Copper-----	British Museum.
	2-0455	1.81		
	2-0458	1.54		
-------	1602	3.32	Iron-------	Allis-Chalmers Mfg. Co.
	3-0454	1.54		
	3-0444	1.81		

The Waldo pattern from the literature is labeled chrysocolla and the ASTM card carries chrysocolla optical data. The pattern contains both quartz and chrysocolla lines, and is not typical of either material. No explanation can be found for reference "B" who is responsible for one line on the Favegee card. The British Museum pattern appears to have been made with copper radiation although molybdenum is listed.

Additional published patterns. None.

NBS sample. The alpha-quartz sample used for the NBS pattern is a natural mineral from Lake Toxaway, Transylvania County, North Carolina. The material was contributed by the Geophysical Laboratory of the Carnegie Institution of Washington. Spectrographic analysis at the NBS showed 0.001 to 0.01 percent of aluminum and 0.0001 to 0.001 percent each of calcium, copper, iron, and magnesium. The NBS sample is uniaxial positive with refractive indices of $\omega = 1.544$ and $\epsilon = 1.553$.

Two additional samples of quartz were considered for use in preparing the NBS pattern. One was a high quality radio grade crystal from Brazil, and the other a synthetic crystal contributed by the Bell Telephone Laboratories. Spectrographic analysis at the NBS indicated that the Brazilian crystal contained a slightly larger percentage of silver, copper, and magnesium than the Lake Toxaway sample while the Bell crystal had a slightly larger percentage of iron and approximately 0.01 percent magnesium.

The synthetic and Lake Toxaway samples showed no appreciable difference in d-spacings. The Brazilian quartz averaged about 0.00006 A smaller than the Lake Toxaway sample for the last seven lines measured.

Interplanar spacings and intensity measurements. All of the patterns were expressed as d-spacings and were converted from kX to angstrom units. The British Museum and Allis-Chalmers patterns were taken from the ASTM cards and the others from the original literature. The Allis-Chalmers pattern contains a number of completely erroneous lines, 30.0, 15.5 and 7.25 and a 1.84 line not allowed by the space group. In addition the pairs of lines at the end of the pattern are presumably $K\alpha_1$ and $K\alpha_2$ doublets of which only the $K\alpha_1$ lines have been included in the comparison table. The 3.73 line added to the Favejee pattern by "B" is not allowed by the space group.

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

Patterns	1	2	3
Harrington----------	101	112	212
Waldo----------	101	112	203,301
Hanawalt, Rinn, and Frevel--	101	100	112
Favejee----------	101	100	203,301
Clark----------	101	112	211
British Museum----------	101	112	211
Allis-Chalmers----------	101	211	112
Swanson and Fuyat----------	101	100	112

Lattice constants. The structure was determined by Bragg and Gibbs [6] in 1925. They found the space group was D_3^4-$P3_121$ or

D_3^6-$P3_221$ according to the rotary sense of the lattice with $3(SiO_2)$ per unit cell. Alpha-quartz is a prototype for other similar structures.

A group of unit cell determinations were converted from kX to angstrom units and Jay's data were converted to 25°C from the temperature indicated in parentheses to compare with the NBS values. The linear thermal expansion according to Sosman [7] for the temperature range 0°C to 100°C is 7.10 to 7.97×10^{-6} parallel to the c-axis and 13.24 to 14.45×10^{-6} perpendicular to it.

Lattice constants in angstroms

		a	c
1925	Bragg and Gibbs [6]	4.90	5.386
1925	Seljakow and Strutinski [8]	4.87	5.37
1927	Harrington [1]	4.913	5.404
1933	Jay [9]	4.9132	5.4045 at 25°C (18°C)
1939	Favejee [4]	4.913	5.404
1947	Novak [10]	4.913	5.404
1950	Keith [11]	4.91304	5.40463 at 25°C
1953	Swanson and Fuyat	4.913	5.405 at 25°C

The density of silicon dioxide calculated from the NBS lattice constants is 2.647 at 25°C.

Silicon dioxide (alpha-quartz), SiO_2 (hexagonal)

hkl	1927 Harrington Mo, 0.709 A		1935 Waldo ----------		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1939 Favegee Cu, 1.5405 A		1946 Clark Co, 1.7902 A		---- British Museum Cu, 1.5405 A		---- Allis-Chalmers Fe, 1.93597 A		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*		*A*		*A*	
---	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	30.0	10	------	-----
---	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	15.5	10	------	-----
---	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	7.25	10	------	-----
100	-----	-----	----	-----	4.26	25	4.27	80	4.26	60	4.30	60	4.22	70	4.26	35
---	-----	-----	----	-----	--------	-----	3.73B	30	-----	-----	-----	-----	------	-----	------	-----
101	3.33	100	3.36	100	3.36	100	3.36	100	3.35	100	3.36	100	3.33	100	3.343	100
110	2.45	30	2.46	40	2.45	15	2.46	60	2.45	40	2.45	60	2.44	40	2.458	12
102	2.28	30	----	-----	2.29	10	2.28	60	2.27	40	2.28	60	2.27	40	2.282	12
111	-----	-----	----	-----	2.23	6	2.24	30	2.23	20	2.22	40	2.22	30	2.237	6
200	2.12	30	----	-----	2.12	9	2.13	50	2.12	40	2.11	60	2.12	40	2.128	9
201	1.979	20	----	-----	1.97	8	1.98	40	1.98	20	1.97	40	1.97	30	1.980	6
---	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	1.84	10	------	-----
112	1.819	80	1.81	80	1.82	25	1.82	70+	1.81	80	1.81	80	1.81	80	1.817	17
003	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	1.801	<1
202	1.668	30	----	-----	1.66	8	1.67	50	1.67	40	-----	-----	1.67	30	1.672	7
103	-----	-----	----	-----	--------	-----	------	-----	1.65	10	1.66	60	1.65	10	1.659	3
210	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	1.60	10	1.608	<1
211	1.543	60	1.54	60	1.54	20	1.54	70	1.54	70	1.540	80	1.54	90	1.541	15
113	1.455	10	----	-----	1.453	2	1.45	20	1.45	10	1.457	40	1.45	20	1.453	3
300	1.418	10	----	-----	--------	-----	1.42	10	1.41	10	1.423	20	1.41	20	1.418	<1
212	1.381	70	----	-----	--------	-----	------	-----	1.38	40	-----	-----	1.38	70	1.382	7
203	}														{1.375	11
301	} ----	-----	1.37	80	1.378	25	1.37	80	1.37	60	1.374	80	1.37	80	{1.372	9
104	1.289	20	(a)	-----	1.302	4	1.29	30	1.28	20	1.288	40	1.28	40	1.288	3
302	1.258	20	----	-----	1.259	3	1.26	40	1.25	20	1.260	40	1.25	60	1.256	4
220	1.230	20	----	-----	1.230	3	1.23	20	1.22	20	1.229	40	1.22	60	1.228	2
213	1.201	20	----	-----	1.202	6	1.20	40	1.20	40	1.204	60	1.20	60	1.1997	5
221	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	1.1973	2
114	1.185	20	----	-----	--------	-----	------	-----	-----	-----	-----	-----	1.18	20	1.1838	4
310	-----	-----	1.18	20	1.182	8	1.18	50	1.18	20	1.182	60	1.18	60	1.1802	4
311	1.156	20	----	-----	1.157	1	1.15	30	1.15	20	1.155	40	1.15	60	1.1530	2
204	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	1.14	20	1.1408	<1
303	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	1.12	10	1.1144	<1
312	1.083	20	----	-----	1.082	4	1.08	40	1.08	40	1.084	60	1.09	10	1.0816	4
400	-----	-----	----	-----	--------	-----	------	-----	1.06	10	1.067	20	1.06	30	1.0636	1

Silicon dioxide (alpha-quartz), SiO_2 (hexagonal)—Con.

hkl	1927 Harrington Mo, 0.709 A		1935 Waldo ----------		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1939 Favegee Cu, 1.5405 A		1946 Clark Co, 1.7902 A		---- British Museum Cu, 1.5405 A		---- Allis-Chalmers Fe, 1.93597 A		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	I	d	I	d	I	d	I	d	I	d	I	d	I	d	I
	A		A		A		A		A		A		A		A	
105	1.046	10	1.05	20	1.050	2	1.05	30	1.04	10	1.051	40	1.05	30	1.0477	2
401	-----	-----	----	-----	--------	-----	------	-----	1.04	10	-----	-----	1.04	30	1.0437	2
214	-----	-----	1.03	20	1.037	1	1.04	30	1.03	10	1.038	40	1.03	30	1.0346	2
223	1.018	10	----	-----	1.017	1	1.02	30	1.01	10	1.017	40	1.01	30	1.0149	2
402 / 115	.993	10	----	-----	--------	-----	.990	40	.987	10	-----	-----	------	-----	.9896	2
313	-----	-----	----	-----	--------	-----	------	-----	.985	10	-----	-----	------	-----	.9872	2
304	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.9781	<1
320	-----	-----	----	-----	--------	-----	------	-----	.974	10	-----	-----	------	-----	.9762	1
321	.963	5	----	-----	--------	-----	------	-----	.958	20	-----	-----	------	-----	.9607	2
410	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.9285	<1
322	.918	5	----	-----	--------	-----	------	-----	.917	10	-----	-----	------	-----	.9182	1
403	-----	-----	----	-----	--------	-----	------	-----	.915	20	-----	-----	------	-----	.9160	3
411	-----	-----	----	-----	--------	-----	------	-----	.912	10	-----	-----	------	-----	.9152	2
224	-----	-----	----	-----	--------	-----	------	-----	.908	10	-----	-----	------	-----	.9090	1
006	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.9008	<1
215	.898	2.5	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8971	2
314	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8889	2
106	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8812	<1
412	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8782	1
305	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8598	<1
116	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8460	<1
501	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8405	<1
404	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8359	<1
206	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8295	3
413	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8254	2
330	.817	2.5	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8189	1
502	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8117	3
225	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8115	3
331	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8096	2
420	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.8041	2
315	-----	-----	----	-----	--------	-----	------	-----	-----	-----	-----	-----	-----	------	.7971	2
421	.793	2.5	----	-----	--------	-----	------	-----	-----	-----	-----	-----	------	-----	.7952	1

[a] Line at 1.32 not included.

References

[1] E. A. Harrington, X-ray diffraction measurements on some of the pure compounds concerned in the study or portland cement, Am. J. Sci. **13**, 467-479 (1927).

[2] A. W. Waldo, Identification of the copper ore minerals by means of X-ray powder diffraction patterns, Am. Mineralogist **20**, 586 (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] J. Ch. L. Favegee, Zur Methodik der röntgenographischen Bodenforschung, Z. Krist. **100**, 430 (1939).

[5] C. B. Clark, X-ray diffraction data for compounds in the system CaO-MgO-SiO_2, J. Am. Ceram. Soc. **29**, 25-30 (1946).

[6] W. H. Bragg and R. E. Gibbs, Structure of α and β quartz, Proc. Roy. Soc. (London) **A109**, 405-427 (1925).

[7] R. B. Sosman, The properties of silica, Reinhold Publishing Corporation, p. 370 (1927).

[8] N. Seljakow, L. Strutinski, and A. Krasnikow, Zur Frage nach der Struktur des Glases, Z. Physik. **33**, 53-62 (1925).

[9] A. H. Jay, The thermal expansion of quartz by X-ray measurements, Proc. Roy. Soc. (London) **A142**, 237 (1933).

[10] J. Novak, Les modifications fibreuses de la silice, Bull. soc. franç. mineral. **70**, 288-299 (1947).

[11] H. D. Keith, Precision lattice-parameter measurements, Proc. Phys. Soc. (London), **63B**, 1034-1036 (1950).

Scandium oxide, Sc_2O_3 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The scandium oxide used for the NBS pattern was obtained from the Fairmount Chemical Co., Inc. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of platinum and silicon; 0.001 to 0.01 percent each of calcium, copper, and magnesium; and 0.0001 to 0.001 percent of barium. The refractive index of the NBS sample is 1.964.

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

Patterns	1	2	3
Swanson and Fuyat-----	222	440	622

Lattice constant. The structure was determined by Zachariasen [1] in 1928. The space group is T^5-$I2_13$ with thallium oxide-structure type and 16 (Sc_2O_3) per unit cell.

The Zachariasen unit cell value has been converted from kX to angstrom units for comparison with the NBS values.

Lattice constant in angstroms

1928-------	Zachariasen [1]----------	9.81
1953-------	Swanson and Fuyat----------	9.845 at 25°C

The density of scandium oxide calculated from the NBS lattice constant is 3.847 at 25°C.

Scandium oxide, Sc_2O_3 (cubic)

hkl	1953 Swanson and Fuyat Cu, 1.5405 A, 25°C		
	d	*I*	*a*
	A		*A*
211	4.021	30	9.849
222	2.841	100	9.842
321	2.631	4	9.844
400	2.461	15	9.844
411	2.321	8	9.847
420	2.202	3	9.848
332	2.099	26	9.845
422	2.009	4	9.842
510	1.9301	20	9.842
521	1.7977	9	9.846
440	1.7406	78	9.846
530	1.6885	5	9.846
600	1.6407	2	9.844
611	1.5968	10	9.843
620	1.5573	4	9.849
541	1.5188	9	9.843
622	1.4839	33	9.843
631	1.4517	12	9.846
444	1.4205	4	9.842
710	1.3924	4	9.846
640	1.3654	3	9.846
721	1.3397	8	9.845
642	1.3158	3	9.847
732	1.2507	3	9.848
800	1.2308	7	9.846
811	1.2120	5	9.846
820	1.1938	4	9.844
653	1.1769	3	9.847
822	1.1603	3	9.845
831	1.1445	4	9.845
662	1.1293	8	9.845
752	1.1147	2	9.845
840	1.1008	3	9.846
Average of the last five lines----------			9.845

References

[1] W. H. Zachariasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO_3, Skrifter utgitt av Det Norske Videnskaps-Akademi i Oslo, I. Mat.-Naturv. Klasse 1928, No. 4, 1928.

Yttrium oxide, Y_2O_3 (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2018	2025	3.05	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
	1-0830	1.87		
	1-0831	1.60		

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [2] 1928	Iron Kα	1.934

NBS sample. The yttrium oxide sample used for the NBS pattern was contributed by the NBS spectrographic laboratory. Their analysis showed the following impurities: 0.01 to 0.1 percent of barium, 0.001 to 0.01 percent each of calcium, erbium, and silicon, and 0.0001 to 0.001 percent each of magnesium, lead, and ytterbium. The NBS sample reacted with the high refractive index liquids, but the index appeared to be above 1.77.

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:

Patterns	1	2	3
Hanawalt, Rinn, and Frevel	222	440	622
Zachariasen	222	440	622
Swanson and Fuyat	222	440	622

Lattice constant. The structure was determined by Zachariasen [3] in 1926. The body-centered cubic cell has thallium oxide-structure type, space group T^5-$I2_13$, and 16 (Y_2O_3) per unit cell.

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

Lattice constant in angstroms

1926	Zachariasen [3]	10.62
1932	Quill [4]	10.61
1953	Swanson and Fuyat	10.604 at 27 °C

The density of yttrium oxide calculated from the NBS lattice constant is 5.031 at 27 °C.

Yttrium oxide, Y_2O_3 (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1928 Zachariasen Fe, 1.93597 A			1953 Swanson and Fuyat Cu, 1.5405 A, 27 °C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
211	4.30	2	10.53	4.33	20	10.61	4.34	16	10.63
----	-----	---	------	[a]3.376	15	-----	------	---	------
222	3.06	100	10.60	3.052	100	10.57	3.060	100	10.600
----	-----	---	-------	[a]2.908	2	-----	------	---	------
400	2.65	16	10.60	2.649	20	10.60	2.652	30	10.608
411	2.51	3	10.65	2.493	5	10.58	2.500	7	10.607
420	2.37	2	10.60	------	---	-----	2.372	1	10.608
332	2.26	3	10.60	2.253	5	10.57	2.261	8	10.605
422	-----	---	-------	------	---	-----	2.165	1	10.606
510	2.07	4	10.55	2.073	20	10.57	2.080	12	10.606
----	-----	---	-------	[a]2.061	20	-----	------	---	------
521	1.93	2	10.57	1.920	5	10.52	1.936	3	10.604
440	1.87	40	10.58	1.864	100	10.54	1.874	46	10.601
530	1.81	2	10.55	------	---	-----	1.818	2	10.601
600	-----	---	-------	1.756	15	10.54	1.769	<1	10.612
611	1.71	2	10.54	1.712	15	10.55	1.720	5	10.603
620	-----	---	-------	------	---	-----	1.677	1	10.606
541	1.64	2	10.63	1.628	10	10.55	1.636	4	10.602
622	1.60	30	10.61	1.589	90	10.54	1.599	31	10.607
631	1.56	2	10.58	1.556	15	10.55	1.563	7	10.601
444	1.52	2	10.53	1.522	15	10.55	1.531	5	10.607
710	-----	---	-------	1.490	5	10.54	1.499	2	10.600
640	-----	---	-------	------	---	-----	1.470	1	10.600
721	-----	---	-------	1.434	15	10.54	1.443	3	10.604
642	-----	---	-------	1.409	8	10.54	1.417	2	10.604
732	1.346	2	10.598	1.339	10	10.54	1.346	2	10.598
800	1.325	2	10.600	1.320	15	10.56	1.325	4	10.600
811	-----	---	-------	1.300	15	10.56	1.305	3	10.602
820	-----	---	-------	1.280	8	10.56	1.287	1	10.613
653	-----	---	-------	1.262	10	10.56	1.267	2	10.600
822	-----	---	-------	1.244	8	10.56	1.249	1	10.598
831	-----	---	-------	1.226	20	10.55	1.233	3	10.607
662	1.217	4	10.610	1.210	50	10.55	1.216	8	10.601
840	1.188	3	[b]10.626	1.1801	30	10.56	1.1854	5	10.603
910	-----	---	-------	1.1658	2	10.56	1.1708	1	10.602
842	-----	---	-------	1.1525	5	10.56	1.1570	1	10.604
921	1.143	2	10.600	1.1387	15	10.56	1.1436	2	10.605
930	1.118	2	10.606	------	---	-----	1.1178	2	10.604
932	-----	---	-------	------	---	-----	1.0939	2	10.606
844	1.083	2	10.611	------	---	-----	1.0821	5	10.602
941	-----	---	-------	------	---	-----	1.0711	2	10.603
10·0·0	-----	---	-------	------	---	-----	1.0606	1	10.606
10·1·1	-----	---	-------	------	---	-----	1.0499	<1	10.603
10·2·0	-----	---	-------	------	---	-----	1.0399	2	10.605
Average of the last five lines			10.605	------	---	10.56	------	---	10.604

[a] K-beta lines.
[b] This value not included in average of last five 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] W. H. Zachariasen, The crystal structure of the sesquioxides and compounds of the type ABO_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. **1928**, No. 4 (1928).

[3] W. H. Zachariasen, The crystal structure of the modification C of the sesquioxides of the rare earth metals and of indium and thallium, Norsk. Geol. Tidsskr. **9**, 310-316 (1926).

[4] L. L. Quill, Die Kristallstruktur des Yttriums, Z. anorg. Chem. **208**, 59-64 (1932).

Molybdenum trioxide, MoO_3 (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1720	1621	3.25	Molybdenum--	Hanawalt, Rinn, and Frevel [1] 1938.
	1-0683	3.80		
	1-0706	3.46		

Additional published patterns. None.

NBS sample. The molybdenum trioxide used for the NBS pattern was obtained from the Merck Chemical Co. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of aluminum, cobalt, manganese, and silicon; 0.001 to 0.01 percent of iron; 0.0001 to 0.001 percent each of copper and magnesium; and less than 0.0001 percent of calcium. The refractive indices are too high to be measured by the usual grain immersion liquids.

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:

Patterns	1	2	3
Hanawalt, Rinn, and Frevel-----	021	110	040
Swanson and Fuyat----------	021	110	040

Lattice constants. The structure was determined by Wooster [2] and Bräkken [3] both in 1931. The space group is D_{2h}^{16}-Pbnm (Pnma) and there are $4(MoO_3)$ per unit cell.

Data for two unit cells were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants in angstroms

		a	*b*	*c*
1931	Wooster [2]----------	3.93	13.97	3.67
1931	Bräkken [3]----------	3.962	13.853	3.701
1953	Swanson and Fuyat------	3.962	13.858	3.697 at 26°C

The density of molybdenum trioxide calculated from the NBS lattice constants is 4.709 at 26°C.

Molybdenum trioxide, MoO_3 (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Cu, 1.5405A		1953 Swanson and Fuyat Cu, 1.5405A, 26°C	
	d	*I*	*d*	*I*
	A		*A*	
020	6.9	24	6.93	34
110	3.81	60	3.81	82
040	3.47	40	3.463	61
120	----------	----------	3.441	44
021	3.26	100	3.260	100
130	3.01	6	3.006	13
101	----------	----------	2.702	19
111	2.67	32	2.655	35
140	----------	----------	2.607	6
041	2.53	8	2.527	12
131	----------	----------	2.332	12
060	2.30	32	2.309	31
150	2.26	6	2.[illegible]	18
141	2.13	6	2.[illegible]	9
160	----------	----------	1.[illegible]	4
200	----------	----------	1.[illegible]	13
061	1.97	24	1.[illegible]	17
002	1.85	24	1.[illegible]	21
230	----------	----------	1.[illegible]	11
170	----------	----------	1.[illegible]	5
161	----------	----------	1.756	5
080	1.73	16	1.733	17
221	1.70	4	1.693	8
112	1.67	12	1.663	13
042	1.63	12	1.631	13
171	1.60	12	1.597	15
180	----------	----------	1.587	6
081	1.57	14	1.569	16
260	1.50	3	1.504	5
251	1.478	8	1.477	10
062	1.443	20	1.443	12
190	----------	----------	1.435	12
270	1.398	6	1.400	5
0·10·0	----------	----------	1.386	5
202	----------	----------	1.352	6

References

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

[2] N. Wooster, The crystal structure of molybdenum trioxide, MoO_3, Z. Krist. **80**, 504-512 (1931).

[3] H. Bräkken, Die Kristallstrukturen der Trioxyde von Chrom, Molybdän und Wolfram, Z. Krist. **78**, 484-488 (1931).

Antimony trioxide (senarmontite), Sb_2O_3 (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1767	1764	3.22	Molybdenum__	Hanawalt, Rinn, and Frevel [1] 1938.
	1-0742	1.96		
	1-0729	1.68		
II-3011	3609	1.96	Iron_____	Mikheev and Dubinina [2] 1938.
	2-1273	3.18		
	2-1283	1.67		British Museum.

The orthorhombic antimony trioxide, valentinite, is represented in the ASTM card file by patterns by the British Museum and the Dow Chemical Co.

Additional published patterns

Source	Radiation	Wavelength
Dehlinger [3] 1927____	Copper_____	_____

NBS sample. The antimony trioxide used for the NBS pattern was prepared by the Mallinckrodt Chemical Works. Their spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of lead and silicon; 0.001 to 0.01 percent each of silver, arsenic, calcium, copper, iron, nickel, and tin; 0.0001 to 0.001 percent each of aluminum, gold, barium, bismuth, cadmium, cobalt, sodium, and thallium; and less than 0.0001 percent each of cesium, indium, potassium, lithium, and magnesium.

Interplanar spacings and intensity measurements. The Dehlinger d-spacings were calculated from Bragg angle data and the Hanawalt, Rinn and Frevel and the Boldyrev d-spacings were converted from kX to angstrom units. The British Museum pattern which contains d-spacings at 2.11, 1.159, 1.035 and presumed β-lines at 1.379 and 1.349 not found in the Mikheev and Dubinina pattern, was not published except as the ASTM card with Mikheev and Dubinina and so was not included in the table of d-spacings. The Dehlinger pattern contains two d-spacings at 4.12 and 3.445 angstroms, neither of which are theoretically possible antimony trioxide lines.

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

Patterns	1	2	3
Hanawalt, Rinn, and Frevel__	222	440	622
Mikheev and Dubinina_____	622	222	440
Dehlinger_____	440	622	662
Swanson and Fuyat_____	222	440	400

Lattice constant. The structure was determined by Bozorth [4] in 1923. The space group is O_h^7-Fd3m with $8(Sb_4O_6)$. The structure type is the same as that of cubic arsenic trioxide.

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

Lattice constant in angstroms

1923_____	Bozorth [4]_____	11.16
1927_____	Dehlinger [3]_____	11.16
1938_____	Mikheev and Dubinina [2]_____	11.130
1942_____	Almin and Westgren [5]_____	11.15
1953_____	Swanson and Fuyat_____	11.152 at 26°C

The density of antimony trioxide calculated from the NBS lattice constant is 5.583 at 26°C.

Antimony trioxide (senarmontite), Sb_2O_3 (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1938 Mikheev and Dubinina Fe, 1.93597 A			1927 Dehlinger Cu, 1.5405 A			1953 Swanson and Fuyat 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	6.4	10	11.09	----	----	----	----	----	----	6.44	12	11.15
----	----	----	----	----	----	----	4.12	vw	----	----	----	----
----	----	----	----	----	----	----	3.445	w	----	----	----	----
222	3.23	100	11.18	3.218	8	11.15	3.225	m	11.17	3.218	100	11.147
400	2.79	30	11.14	2.785	5	11.14	2.794	w	11.18	2.788	40	11.152
331	2.57	8	11.18	2.559	3	11.15	2.567	vw	11.19	2.559	11	11.154
422	----	----	----	----	----	----	----	----	----	2.276	2	11.150
511	----	----	----	----	----	----	2.178	w	11.32	2.145	3	11.146
440	1.96	50	11.11	1.966	8	11.12	1.969	s	11.14	1.972	42	11.155
531	----	----	----	----	----	----	----	----	----	1.885	2	11.152
622	1.68	50	11.16	1.676	9	11.12	1.681	s	11.15	1.681	35	11.150
444	1.61	10	11.18	1.604	6	11.11	1.610	m	11.15	1.611	11	11.161
711	1.56	10	11.16	1.558	5	11.13	1.572	w-m	11.23	1.562	7	11.155
----	----	----	----	1.499	1	----	----	----	----	----	----	----
731	1.453	2	11.16	1.449	2	11.13	1.453	w-m	11.16	1.452	3	11.152
800	1.397	6	11.18	----	----	----	1.392	w	11.14	1.394	4	11.152
733	1.358	4	[a]11.12	----	----	----	----	----	----	1.363	4	11.157
662	1.286	15	11.21	1.277	7	11.13	1.280	s	11.16	1.279	12	11.150
840	1.250	10	[a]11.18	1.246	7	11.15	1.248	s	11.16	1.247	8	11.153
911	1.219	1	[a]11.11	1.223	1	11.14	----	----	----	1.224	2	11.151
931	1.186	1	11.32	----	----	----	----	----	----	1.1694	1	11.155
844	1.140	4	[a]11.17	1.136	4	11.13	1.138	m	11.15	1.1384	5	11.154
----	----	----	----	1.121	2	----	----	----	----	----	----	----
951	----	----	----	1.073	7	11.10	----	----	----	1.0783	4	11.154
10·2·2	1.075	8	[a]11.17	----	----	----	----	----	----	1.0732	6	11.153
953	----	----	----	----	----	----	----	----	----	1.0402	1	11.155
11·1·1	----	----	----	----	----	----	----	----	----	1.0056	1	11.153
880	----	----	----	----	----	----	----	----	----	.9856	2	11.151
11·3·1	----	----	----	----	----	----	----	----	----	.9744	3	11.153
11·3·3	----	----	----	----	----	----	----	----	----	.9457	1	11.150
10·6·2	----	----	----	----	----	----	----	----	----	.9425	5	11.152
12·0·0	----	----	----	----	----	----	----	----	----	.9291	3	11.149
11·5·1	----	----	----	----	----	----	----	----	----	.9196	<1	11.150
11·5·3	----	----	----	----	----	----	----	----	----	.8956	<1	11.150
12·4·0	----	----	----	----	----	----	----	----	----	.8817	2	11.153
991	----	----	----	----	----	----	----	----	----	.8734	1	11.151
13·1·1	----	----	----	----	----	----	----	----	----	.8527	3	11.151
10·6·6	----	----	----	----	----	----	----	----	----	.8505	3	11.154
12·4·4	----	----	----	----	----	----	----	----	----	.8406	2	11.152
13·3·1	----	----	----	----	----	----	----	----	----	.8335	3	11.151
13·3·3	----	----	----	----	----	----	----	----	----	.8154	2	11.150
13·5·1	----	----	----	----	----	----	----	----	----	.7986	2	11.152
Average value of last five lines			11.15	----	----	11.13	----	----	11.15	----	----	11.152

[a]Values used for average cell size.

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] V. I. Mikheev and V. N. Dubinina, X-ray powder diagrams of the oxide group, Zap. Len. Gorn. Inst. 1938.

[3] U. Dehlinger, Über die Kristallstruktur der Antimonoxyde, Z. Krist. **66**, 108 (1927).

[4] R. M. Bozorth, The crystal structures of the cubic forms of arsenious and antimonious oxides, J. Am. Chem. Soc. **45**, 1621 (1923).

[5] K. E. Almin and A. Westgren, Lattice parameters of cubic As_4O_6 and Sb_4O_6, Arkiv. Kemi. Mineral. Geol. **15B**, No. 22, (1947).

Lanthanum oxide, La_2O_3 (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-1432	2172 2-0673 2-0688	2.97 3.41 1.96	Molybdenum	General Electric Co. Wembley, England.

The following ASTM card for lanthanum oxide is the pattern for the cubic form at 450°C.

-------	------ 4-0855 4-0856	2.02 1.72 3.30	Copper, 1.5418.	Löhberg [1] 1935.

Additional published patterns

Source	Radiation	Wavelength
Zachariasen [2] 1926	Tungsten	----------

NBS sample. The lanthanum oxide used for the NBS pattern was obtained from the Fairmount Chemical Co. The sample was annealed at 1,200°C for one hour and was mounted in petrolatum to prevent reabsorption of carbon dioxide and water, with which lanthanum oxide readily combines, according to Hüttig and Kantor [3].

Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of calcium, magnesium, and silicon; and 0.0001 to 0.001 percent each of aluminum, copper, iron, and lead.

Interplanar spacings and intensity measurements. The *d*-spacings for the Zachariasen pattern were calculated from Bragg angle data while the General Electric *d*-spacings were converted from kX to angstrom units.

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

Patterns	1	2	3
General Electric Company	101	100	110
Zachariasen	101	112,201	103
Swanson and Fuyat	101	110	102

Lattice constants. The structure was determined by Zachariasen [2] in 1926. The space group is D_3^2-P321 with $1(La_2O_3)$ per unit cell. Lanthanum oxide is a prototype for other similar structures.

Data for two unit cells have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants in angstroms

		a	*c*
1926	Zachariasen [2]	3.94	6.13
1929	Pauling [4]	3.93	5.63
1953	Swanson and Fuyat	3.9373	6.1299 at 26°C

The density of lanthanum oxide calculated from the NBS lattice constants is 6.573 at 26°C.

Lanthanum oxide, La_2O_3 (hexagonal)

hkl	---- General Electric Co., Wembly, Eng. Mo, 0.709A		1926 Zachariasen W, 0.20904A		1953 Swanson and Fuyat Cu, 1.5405A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
100	3.42	60	3.419	40	3.41	34
002	3.07	50	3.076	40	3.063	31
101	2.978	100	2.988	100	2.980	100
102	2.278	50	2.289	50	2.278	58
110	1.964	60	1.975	60	1.968	63
103	1.750	50	1.760	70	1.753	52
200	1.702	10	1.710	10-20	1.705	4
112	1.655	40	1.661	100	1.656	24
201	1.640	30	1.646		1.642	17
004	1.531	10	1.541	10-20	1.532	3
202	1.488	30	1.496	20	1.490	5
104	1.393	10	1.403	30	1.398	2
203	1.307	20	1.315	50	1.309	7
210	1.286	10	1.293	10	1.289	2
211	1.259	30	1.266	70	1.261	12
114	1.206	10	1.214	70	1.209	6
212	---------	--------	1.192	30-40	1.1879	4
105	---------	--------	1.158	50	1.1538	4
204	---------	--------	1.140	40	1.1396	2
300	---------	--------	------	-----	1.1367	4
213	---------	--------	1.094	70	1.0901	7
302	---------	--------	1.070	50	1.0658	4
006	---------	--------	1.026	0-10	1.0220	<1
205	---------	--------	1.000	50	.9952	3
220	---------	--------	------	-----	.9840	3
106	---------	--------	------	-----	.9787	1
310	---------	--------	------	-----	.9459	<1
222	---------	--------	------	-----	.9372	3
311	---------	--------	------	-----	.9345	5
304	---------	--------	------	-----	.9131	2
116	---------	--------	------	-----	.9070	2
215	---------	--------	------	-----	.8883	5
206	---------	--------	------	-----	.8766	1
313	---------	--------	------	-----	.8583	4
107	---------	--------	------	-----	.8480	2
401	---------	--------	------	-----	.8443	1
224	---------	--------	------	-----	.8283	2
314	---------	--------	------	-----	.8050	1
117 216	-------	--------	------	-----	.8007	2

References

[1] K. Löhberg, Über die C-modifikation der Sesquioxyde von Neodym und Lanthan, Z. physik. Chem. **B28**, 402-7 (1935).

[2] W. Zachariasen, Die Kristallstruktur der A-Modifikation 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).

[3] G. F. Hüttig and M. Kantor, Das System Lanthan (III) oxyd/Wasser, Z. anorg. allg. Chem. **202**, 421-428 (1931).

[4] L. Pauling, The crystal structure of the A-modification of the rare earth sesquioxides, Z. Krist. **69**, 415-421 (1929).

Mercury (II) oxide (montroydite), HgO (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-672	1089	3.85	----------	Bird [1] 1932.
	2-0309	2.86		
	2-0305	5.26		
2190	2183	2.96	Molybdenum--	Hanawalt, Rinn, and Frevel [2] 1938.
	1-0882	2.83		
	1-0896	2.40		

Additional published patterns

Source	Radiation	Wavelength
Levi [3] 1924----------	Copper-------	----------
Zachariasen [4] 1927----------	Iron---------	1.934

NBS sample. The red and yellow mercuric oxides used for the NBS pattern were ACS standard samples from the Mallinckrodt Chemical Works. Spectrographic analysis at the NBS showed the following impurities for the yellow form: 0.01 to 0.1 percent each of calcium and magnesium; 0.001 to 0.01 percent each of aluminum, iron, nickel, and silicon; and 0.0001 to 0.001 percent of chromium; and the red form: 0.01 to 0.1 percent each of aluminum, calcium, magnesium, and silicon; and 0.001 to 0.01 percent each of chromium and iron. The refractive indices are too high to be measured by the usual grain-oil immersion methods.

The NBS pattern is that of the yellow oxide as it gave a better pattern than the red form. However, measuring the red pattern as accurately as possible, there were no systematic differences between the two samples and any differences observed were smaller than the experimental error of the apparatus. Therefore, it is believed, at least for powder data, that the two forms are identical and the NBS pattern will serve for both the red and yellow mercuric oxides.

Interplanar spacing and intensity measurements. The *d*-spacings for the Levi and the Zachariasen patterns were calculated from Bragg angle data while *d*-spacings for the Bird and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units.

The controversy concerning the possible existence of two distinct forms of mercuric oxide, the red and the yellow, has been reconciled and the present authors feel both are the same form; the difference in color being due to grain size or some other factor not affecting the structure. The data supports this contention.

The Levi patterns for both the red and yellow oxides are thought to be identical. The Zachariasen *d*-spacings were made on a sample containing sodium chloride which covered four lines of the pattern as indicated in the table. The intensity pattern made without the sodium chloride standard contains these four lines.

Three lines of the Bird pattern, including his first and third strongest lines are due to kleinite, a mercury ammonium chloride of uncertain composition. This contamination is understandable since the pattern was made from a natural mineral sample. Both of the Levi patterns also contain extra lines apparently due to eglestonite, Hg_4Cl_2O.

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

Pattern	1	2	3
Bird----------	------	101	-------
Hanawalt, Rinn, and Frevel--------	011	101	110
Levi, yellow sample----------	112	022	110
Levi, red sample----------	112	022	123
Zachariasen----------	112	130	011
Swanson and Fuyat----------	011	101	110

Lattice constants. The structure was determined by Zachariasen [4] in 1947. The space group is D_{2h}^{13}-Pmnm (Pmmn) with 2(HgO) per unit cell.

The Zachariasen unit cell data were converted to angstrom units for comparison with the NBS values.

Lattice constants in angstroms

		a	*b*	*c*
1927	Zachariasen [4]----------	3.302	3.519	5.513
1953	Swanson and Fuyat-------	3.304	3.519	5.518 at 25°C

The density of mercuric oxide calculated from the NBS lattice constants is 11.211 at 25°C.

Mercury (II) oxide (yellow), HgO (orthorhombic)

hkl	1932 Bird		1938 Hanawalt, Rinn, and Frevel		1924 Levi				1927 Zachariasen		1953 Swanson and Fuyat	
			Mo, 0.709 A		Cu, 1.5405 A				Fe, 1.93597 A		Cu, 1.5405 A, 25°C	
					Yellow HgO		Red HgO					
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		A	
---	[a]5.272	30	---	---	---	---	---	---	---	---	---	---
---	[a]3.856	100	---	---	---	---	---	---	---	---	---	---
---	---	---	---	---	[b]3.10	vw	[b]3.16	vw	---	---	---	---
011	---	---	2.97	100	2.98	w	2.98	w	2.977	70	2.967	100
101	2.870	50	2.84	75	2.83	m	2.86	m	(c)	70	2.834	81
002	---	---	2.76	38	2.73	ms	2.75	w	2.758	50	2.759	58
---	[a]2.622	10	---	---	2.65	m	2.67	ms	---	---	---	---
---	---	---	---	---	[b]2.56	vw	---	---	---	---	---	---
110	2.407	30	2.40	75	2.33	s	2.35	m	2.409	70	2.408	67
---	---	---	---	---	[b]1.95	w	[b]1.97	w	---	---	---	---
112	---	---	1.81	63	1.77	vs	1.79	vs	1.813	100	1.814	49
020	1.766	30	1.75	8	1.73	w	1.74	w	1.761	20	1.759	11
200	---	---	1.64	15	---	---	---	---	1.650	40	1.651	11
013	---	---	---	---	1.63	m	1.64	w	(c)	40	1.630	15
103	---	---	1.60	10	1.60	m	1.61	m	1.608	40	1.607	13
---	---	---	---	---	[b]1.58	m	[b]1.59	mw	---	---	---	---
210	1.500	30	---	---	---	---	1.52	vw	1.495	70	1.495	25
121												
022	---	---	1.489	38	1.47	vs	1.48	s	1.484	40	1.484	12
211	1.444	10	1.443	20	1.42	s	1.43	mw	1.443	60	1.443	18
202	---	---	1.416	8	1.40	m	1.41	w	1.416	40	1.417	11
004	---	---	1.381	5	1.36	w	1.37	mw	1.378	30	1.379	4
212	---	---	---	---	1.30	vw	1.31	vw	---	---	1.315	1
220	---	---	---	---	---	---	---	---	---	---	1.204	5
114	---	---	1.202	13	---	---	---	---	1.197	50	1.1971	10
123	1.182	10	1.189	10	1.19	s	1.19	s	1.186	35	1.1866	9
213	---	---	1.163	5	1.17	ms	1.16	m	1.161	50	1.1605	7
031	1.143	10	1.150	3	1.15	ms	1.15	m	(c)	30	1.1475	4
---	1.134	10	---	---	1.14	w	---	---	---	---	---	---
130	---	---	---	---	---	---	---	---	(c)	80	1.1052	6
222	---	---	1.105	5	1.09	ms	1.11	mw	---	---	1.1039	8
024	---	---	---	---	---	---	---	---	---	---	1.0855	3
301	---	---	1.081	3	1.07	m	1.08	m	---	---	1.0801	3
032												
204	---	---	---	---	---	---	---	---	---	---	1.0589	4
015	---	---	---	---	---	---	---	---	---	---	1.0532	4
310	---	---	1.052	5B	1.05	ms	1.05	ms	---	---	1.0510	4
132	---	---	1.028	3	1.02	m	1.03	mw	---	---	1.0262	5
---	1.015	10	---	---	---	---	---	---	---	---	---	---
033	---	---	---	---	---	---	---	---	---	---	.9890	3
312	---	---	.984	3	.977	ms	.986	m	---	---	.9823	4
303	---	---	---	---	---	---	---	---	---	---	.9450	5
231	---	---	.945	3	.940	ms	.943	mw	---	---	.9425	3
321	---	---	---	---	.917	ms	.921	m	---	---	.9202	4
224	---	---	---	---	[d].903	m	[e].905	mw	---	---	.9072	3

[a]These lines probably kleinite, a mercury ammonium chloride.
[b]These lines probably due to eglestonite, Hg_4Cl_2O.
[c]Lines covered by NaCl-std; the intensity pattern made without standard.
[d]Twelve additional lines omitted.
[e]Seven additional lines omitted.

References

[1] P. H. Bird, A new occurrence and X-ray study of mosesite, Am. Mineralogist **17**, 541-550 (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, Identità cristallografica delle due forme di ossido mercurico, Gazz chim. ital. **54**, 709-712 (1924).

[4] W. Zachariasen, Über die Kristallstruktur des Quecksilberoxyds, Z. physik. Chem. **128**, 421-429 (1927).

2.4. Oxide Hydrates

Alpha-aluminum oxide mono-hydrate (böhmite),[a] α-$Al_2O_3 \cdot H_2O$ (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-3183	3695	1.85	No data	Weiser and Milligan [1] 1932.
	2-1314	2.34		
	2-1316	1.31	Iron	Kovalev [2] 1938.
-------	0277	6.9	Copper	Noll [3] 1936.
	3-0063	6.1		
	3-0065	2.35		
-------	0278	-----	----------	A continuation of the preceding card.
	3-0064			
	3-0066			
1868	1848	3.16	Molybdenum	New Jersey Zinc Company.
	1-0777	1.85		
	1-0774	2.33		
3544	3689	1.85	Molybdenum	Physics Department, Newcastle-on-Tyne, England.
	1-1281	6.20		
	1-1284	3.16		
II-216	0360	6.2	Molybdenum	Imperial Chem. Industries, Billingham, England.
	2-0130	3.17		
	2-0129	2.34		

The Imperial Chemical Co. sample was a mineral specimen while all of the rest were synthetic materials. The seven line Weiser and Milligan pattern combined with the Kovalev pattern on an ASTM card, is called delta-alumina by the authors.

Additional published patterns

Source	Radiation	Wavelength
Schwiersch [4] 1933	----------	----------
Reichertz and Yost [5] 1946	Mo. and Cu.	----------

NBS sample. The alpha-aluminum oxide mono-hydrate used for the NBS pattern was prepared at the Aluminum Co. of America, Aluminum Research Laboratories by digesting alpha-aluminum trihydrate (made by the Bayer process) in steam at 200°C. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of calcium, magnesium, and silicon; 0.001 to 0.01 percent each of iron, manganese, nickel and titanium; and 0.0001 to 0.001 percent each of chromium and copper. The NBS sample was too fine for detailed optical measurements but the average index of the crystal aggregates is 1.64 to 1.65.

Interplanar spacings and intensity measurements. The *d*-spacings for the Weiser and Milligan, the Kovalev, and the Reichertz and Yost patterns were converted from kX to angstrom units while *d*-spacings for the Noll, the New Jersey Zinc, the Physics Department, Newcastle-on-Tyne, the Imperial Chemical Industries, Billingham, England, and the Schwiersch patterns were calculated from Bragg angle data.

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

Patterns	1	2	3
Weiser and Milligan	002	200	041,130
Noll	-------	020	041,130
Kovalev	041,130	002	152
New Jersey Zinc	021	002	041,130
Physics Department, Newcastle	002	020	021
Imperial Chemical Industries	020	021	041,130
Schwiersch	-------	020	021
Reichertz and Yost	020	150,002	021
Swanson and Fuyat	020	021	041,130

Reichertz and Yost measured integrated intensities rather than peak height above background.

Lattice constants. The structure was determined by Reichertz and Yost [5] in 1946. The space group is D_{2h}^{17}-Cmcm with $2(Al_2O_3 \cdot H_2O)$ per unit cell.

Data for two unit cells were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants in angstroms

		a	*b*	*c*
1936	Goldsztaub [6] -------	2.86	11.8	3.79
1946	Reichertz and Yost [5]	2.865	12.26	3.698
1953	Swanson and Fuyat------	2.868	12.227	3.700 at 26°C

The density of böhmite calculated from the NBS lattice constants is 3.070 at 26°C.

[a] The Greek letter designation used is that of the Aluminum Company of America. Böhmite also has been referred to as gamma-alumina monohydrate.

Alpha-aluminum oxide mono-hydrate (böhmite), α-$Al_2O_3 \cdot H_2O$ (orthorhombic)

hkl	1932 Weiser and Milligan		1936 Noll		1938 Kovalev		---- New Jersey Zinc Co.		---- Physics Dept. Newcastle-on-Tyne, England		---- Imperial Chem. Industries, Billingham, England		1933 Schwiersch		1946 Reichertz and Yost		1953 Swanson and Fuyat	
	----------		Cu, 1.5405 A		Fe, 1.93597A		Mo, 0.709A		Mo, 0.709A		Mo, 0.709A		----------		Cu, 1.5405 A and Mo, 0.709A		Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I	d	I	d	I	d	I	d	I	d	I	d	I
	A		A		A		A		A		A		A		A		A	
----	----	----	6.86	100	-----	---	-----	----	-----	---	-----	---	6.91	100	------	-----	-------	----
020	----	----	6.09	100	-----	---	-----	----	6.21	72	6.2	100	6.06	100	6.12	100	6.11	100
----	----	----	3.51	40	-----	---	-----	----	-----	---	-----	---	-----	---	------	-----	-------	----
----	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	3.300	60	------	-----	-------	----
021	3.15	50	3.146	90	3.164	80	3.17	100	3.17	72	3.18	100	3.140	100	3.160	48	3.164	65
----	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	2.938	20	------	-----	-------	----
----	----	----	2.597	50	-----	---	-----	----	-----	---	-----	---	2.605	40	------	-----	-------	----
----	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	2.415	60	------	-----	-------	----
041															2.355			
130	2.36	70	2.340	100	2.349	100	2.33	75	2.350	72	2.34	100	2.331	100	2.341	42	2.346	53
----	----	----	2.037	60	-----	---	-----	----	-----	---	-----	---	2.047	50	------	-----	-------	----
131	----	----	1.977	30	1.979	30	1.980	13	1.979	9	1.985	60	1.988	30	1.977	4	1.980	6
150	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	-----	---	1.859	52	1.860	32
002	1.85	100	1.841	100	1.853	100	1.851	83	1.85	100	1.859	100	1.843	100	1.845		1.850	27
----	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	-----	---	1.785	4	-------	----
022	----	----	1.763	40	1.764	30	1.757	3	1.76	19	1.771	60	1.770	40	1.766		1.770	6
151	----	----	1.657	60	1.667	70	1.659	18	1.659	31	1.663	70	1.657	60	1.660	11	1.662	13
----	1.61	1	1.604	20	-----	---	-----	----	-----	---	-----	---	1.609	30	1.538		-------	----
080	----	----	1.524	50	1.524	60	1.523	1	1.527	9	1.529	60	1.527	50	1.530	-----	1.527	6
132	----	----	1.449	80	1.455	80	1.451	18	1.448	31	1.453	70	1.450	80	1.449		1.453	16
200	1.43	80	1.432	50	-----	---	-----	----	1.431	19	1.433	60	1.438	20	1.429	21	1.434	9
081	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	-----	---	1.413		1.412	1
220	----	----	-------	---	-----	---	1.397	50	1.38	25	-----	---	-----	---	1.392		1.396	2
171	----	----	1.379	60	1.382	50	-----	----	-----	---	1.385	70	1.385	50	1.383	9	1.383	6
062	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	-----	---	1.368		1.369	2
152	1.32	60	-------	---	1.309	100	1.309	26	1.309	50	1.310	80	1.310	80	1.310	18	1.312	15
221	----	----	1.305	80	-----	---	-----	----	-----	---	-----	---	-----	---	1.302		1.303	3
----	----	----	1.285	10	-----	---	-----	----	-----	---	-----	---	-----	---	------	-----	-------	---
----	----	----	1.253	10	-----	---	-----	----	-----	---	-----	---	-----	---	------	-----	-------	----
241	----	----	1.205	20	1.223	20	-----	----	1.224	3	1.222	20	1.224	10	------	-----	1.224	1
023	----	----	-------	---	1.208	20	-----	----	1.204	3	1.207	40	1.211	10	1.206	-----	1.209	2
082	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	-----	---	1.178		1.1782	3
260	----	----	1.175	40	1.177	40	-----	----	1.177	9	1.179	60	1.179	40	1.171	-----	1.1711	<1
----	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	-----	---	1.165		------	----
----	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	-----	---	1.162	-----	------	----
172	----	----	1.157	40	1.158	40	-----	----	1.158	9	1.159	60	1.162	40	1.160		1.1609	3
----	----	----	1.148	60	-----	---	-----	----	-----	---	-----	---	-----	---	------	-----	-------	----
202	1.13	10	1.112	30	1.133	60	1.130	6	1.13	13	1.133	70	1.134	50	1.130	-----	1.1337	5
222	----	----	-------	---	-----	---	-----	----	1.11	6	1.115	60	1.117	20	------	-----	1.1152	2
133	----	----	1.090	5	-----	---	-----	----	-----	---	1.091	30b	-----	---	------	-----	1.0917	<1
280	----	----	1.045	30	-----	---	-----	----	1.043	3	1.047	60	1.046	40	------	-----	1.0459	2
153	----	----	1.021	30	-----	---	-----	----	-----	---	1.029	50	1.027	40	------	-----	1.0281	1
----	----	----	-------	---	-----	---	-----	----	1.023	3	1.019	40	-----	---	------	-----	-------	---
262	----	----	-------	---	-----	---	-----	----	-----	---	.990	20	-----	---	------	-----	.9903	<1
----	----	----	.9795	10	-----	---	-----	----	-----	---	.982	40	.986	10	------	-----	.9818	<1
173	----	----	.9586	10	-----	---	-----	----	-----	---	.951	60	.951	40	------	-----	.9506	2
			.9479	50														
330	----	----	.9304	30	-----	---	-----	----	-----	---	.931	50	.930	30	------	-----	.9310	2
004																		
223	----	----	.9218	50	-----	---	-----	----	-----	---	.925	60	.924	40	------	-----	.9247	2

	1932		1936		1938		----		----		----		1933		1946		1953	
	Weiser and Milligan		Noll		Kovalev		New Jersey Zinc Co.		Physics Dept. Newcastle-on-Tyne, England		Imperial Chem. Industries, Billingham, England		Schwiersch		Reichertz and Yost		Swanson and Fuyat	
hkl	----------		Cu, 1.5405 A		Fe, 1.93597A		Mo, 0.709A		Mo, 0.709A		Mo, 0.709A		----------		Cu, 1.5405 A and Mo, 0.709A		Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*		*A*		*A*		*A*	
----	----	----	-------	---	-----	---	-----	----	-----	---	.915	30	-----	---	------	-----	-------	----
282	----	----	.9091	40	-----	---	-----	----	-----	---	.912	60	.911	40	------	-----	.9105	2
331	----	----	.9013	50	-----	---	-----	----	-----	---	.903	60	.904	40	------	-----	.9023	2
243	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	-----	---	------	-----	.8937	<1
350	----	----	.8896	50	-----	---	-----	----	-----	---	-----	---	.891	40	------	-----	.8907	1
351	----	----	.8662	60	-----	---	-----	----	-----	---	-----	---	.868	50	------	-----	.8660	<1
134	----	----	.8586	50	-----	---	-----	----	-----	---	-----	---	.861	50	------	-----	.8607	1
332	----	----	.8317	60	-----	---	-----	----	-----	---	-----	---	.831	60	------	-----	.8316	2
154	----	----	.8266	60	-----	---	-----	----	-----	---	-----	---	.828	60	------	-----	.8286	3
371	----	----	.8170	30	-----	---	-----	----	-----	---	-----	---	.819	40	------	-----	.8180	1
----	----	----	.8098	20	-----	---	-----	----	-----	---	-----	---	-----	---	------	-----	-------	----
352	----	----	.8016	60	-----	---	-----	----	-----	---	-----	---	.803	60	------	-----	.8026	2
----	----	----	-------	---	-----	---	-----	----	-----	---	-----	---	.792	40	------	-----	-------	----

References

[1] H. B. Weiser and W. O. Milligan, X-ray studies on the hydrous oxides. I. Alumina, J. Phys. Chem. **36**, 3010-3029 (1932).

[2] J. A. Kovalev, Debye-Sherrer diffraction diagrams of some oxide and borate minerals, Materialy TsNIGRI 1938. From A. K. Boldyrev and others, Annales de l'Institut des Mines à Léningrad **11** (2) (1938).

[3] W. Noll, Mineralbildung im System Al_2O_3-SiO_2-H_2O, Neues Jahr. Mineral. **70**, 76 (65-115) (1936).

[4] H. Schwiersch, Thermischer Abbau der natürlichen Hydroxyde des Aluminiums und des dreiwertigen Eisens, Chem. Erde **8**, 252 (1933). From Noll, reference 3.

[5] P. P. Reichertz and W. J. Yost, The crystal structure of synthetic boehmite, J. Chem. Phys. **14**, 495-501 (1946).

[6] S. Goldsztaub, Quelques Observations sur la Boehmite, Bull. soc. franc. mineral. **59**, 348-350 (1936).

Beta-aluminum oxide mono-hydrate (diaspore),[a] β-$Al_2O_3 \cdot H_2O$ (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-2498	3217	2.33	Molybdenum	Hansen and Brownmiller [1] 1928.
	2-1104	2.14		
	2-1106	2.08		
1038	1009	4.00	Molybdenum	Weiser and Milligan [2] 1932.
	1-0446	2.34		
	1-0447	2.13		
II-628	1059	3.99	No data---	British Museum.
	2-0301	2.13	Iron------	Kovalev [3] 1938.
	2-0291	1.64	No data---	Kerr [4] 1932.
			Molybdenum	Weiser and Milligan [2] 1932.
1046	1058	3.99	Molybdenum	Hanawalt, Rinn, and Frevel [5] 1938.
	1-0470	2.31		
	1-0449	1.63		
1056	1057	3.98	Molybdenum	Physics Department, Newcastle-on-Tyne, England.
	1-0469	2.31		
	1-0454	2.13		

The British Museum contributed five lines with d-spacings and intensities of 4.45, 60; 3.60, 20; 2.02, 20; 1.91, 40; 1.76, 20 to the composite pattern, card 2-0291. Because these d-spacings represent only lines not found in any of the other three patterns in the composite, and the complete British Museum pattern apparently was not published, the above data were not presented in the table of d-spacings.

Additional published patterns

Source	Radiation	Wavelength
Rooksby [6] 1929---	----------	----------

NBS sample. The diaspore sample was contributed by the Aluminum Research Laboratories, Aluminum Company of America. It is a mineral from Springfield, Mass. containing 0.18 percent of SiO_2 and 0.64 percent of Fe_2O_3 by chemical analysis at the Aluminum Company. Spectrographic analysis at the NBS showed the following impurities: 0.1 to 1.0 percent each of iron, magnesium, silicon, and titanium, 0.01 to 0.1 percent each of nickel and vanadium, and 0.001 to 0.01 percent each of calcium, chromium, copper, and manganese. The sample is biaxial positive with large 2V, $\alpha = 1.700$ and $\gamma = 1.745$. The β-index was not readily available due to the platy character of the crystal perpendicular to that direction.

Interplanar spacings and intensity measurements. The d-spacings for all the patterns were converted from kX to angstrom units. The pattern from the Physics Department, Newcastle-on-Tyne and the British Museum pattern have not been published except in the ASTM file.

The intensity values for the (010) planes of diaspore are difficult to determine as diaspore commonly grows platy crystals perpendicular to the b-axis. The three strongest lines for each of the patterns are as follows:

Patterns	1	2	3
Hansen and Brownmiller----------	111	121	140
Weiser and Milligan----------	110	111	121
Kerr----------	110	111	121
Kovalev----------	221	121	140
Hanawalt, Rinn, and Frevel----------	110	111	221
Physics Department, Newcastle----------	110	111	121
Rooksby----------	110	111	221
Swanson and Fuyat----------	110	111	121

There are four lines present in some of the patterns that do not appear in the NBS pattern. The lines, d-spacing 4.87 and 4.40 are probably due to the alpha-alumina monohydrate or to one of the trihydrates. The 3.50 line might be due to corundum, and the 2.82 line could be a strong line for either kappa or beta alumina. All the patterns were made

[a] The Greek letter designation used is that of the Aluminum Company of America. Diaspore has also been referred to as alpha-alumina monohydrate.

by using mineral diaspore, as it has never been prepared sufficiently pure or in large enough quantity for an X-ray pattern.

Lattice constants. The structure was determined by Deflandre [7] in 1932. The space group is D_{2h}^{16}-Pbnm (Pnma) with $2(Al_2O_3 \cdot H_2O)$ per unit cell.

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

Lattice constants in angstroms

		a	*b*	*c*
1932	Deflandre [7]	4.41	9.40	2.84
1933	Takane [8]	4.44	9.38	2.81
1935	Ewing [9]	4.41	9.41	2.85
1940	Hoppe [10]	4.43	9.46	2.85
1953	Swanson and Fuyat	4.396	9.426	2.844 at 25°C

The density of diaspore calculated from the NBS lattice constants is 3.380 at 25°C.

Beta-aluminum oxide mono-hydrate (diaspore), β-$Al_2O_3 \cdot H_2O$[a]

hkl	1928 Hanson and Brownmiller, Mo, 0.709 A		1932 Weiser and Milligan, Mo, 0.709 A		1932 Kerr		1937 Kovalev, Fe, 1.93597 A		1938 Hanawalt, Rinn, and Frevel, Mo, 0.709 A		---- Physics Dept. Newcastle, Eng., Mo, 0.709 A		1929 Rooksby		1953 Swanson and Fuyat, Cu, 1.5405 A, 25°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		A		A		A	
---	-------	---	-------	---	4.87	5	-------	---	-------	---	-------	---	-------	---	-------	---
020	-------	---	-------	---	4.68	5	4.699	20	4.71	9	-------	---	4.700	10	4.71	13
---	-------	---	-------	---	-------	---	-------	---	-------	---	4.44	3	-------	---	-------	---
110	-------	---	4.01	100	4.02	100	3.996	60	4.00	100	3.99	100	3.985	100	3.99	100
---	-------	---	-------	---	-------	---	-------	---	-------	---	3.51	6	3.513	20	-------	---
120	-------	---	-------	---	3.28	20	3.256	10	3.21	8	3.22	6	3.222	20	3.214	10
---	-------	---	-------	---	2.83	5	-------	---	-------	---	-------	---	-------	---	-------	---
130	2.58	s	2.58	80	2.59	50	2.559	60	2.56	33	2.57	41	2.563	40	2.558	30
---	-------	---	-------	---	2.52	5	-------	---	-------	---	-------	---	-------	---	-------	---
021	-------	---	-------	---	-------	---	-------	---	-------	---	-------	---	-------	---	2.434	3
101	-------	---	-------	---	-------	---	-------	---	-------	---	2.38	3	-------	---	2.386	5
040	-------	---	-------	---	-------	---	-------	---	2.37	5	-------	---	-------	---	2.356	8
111	2.33	vs	2.34	100	2.328	100	2.318	60	2.31	100	2.31	72	2.317	80	2.317	56
121	2.14	vs	2.13	100	2.148	100	2.134	80	2.12	67	2.13	59	2.128	70	2.131	52
140	2.08	vs	2.08	20	2.088	100	2.076	80	2.06	67	2.07	50	2.076	70	2.077	49
131	-------	---	-------	---	-------	---	-------	---	-------	---	1.898	6	1.896	5	1.901	3
041	1.81	w	1.82	10	1.838	5	-------	---	1.81	7	1.81	6	1.811	10	1.815	8
150	-------	---	-------	---	1.738	5	-------	---	-------	---	-------	---	-------	---	1.733	3
211	1.715	s	1.71	20	-------	---	1.710	40	1.71	20	1.711	19	1.710	30	1.712	15
141	1.675	w	-------	---	-------	---	1.676	20	-------	---	-------	---	-------	---	1.678	3
221	1.634	vs	1.63	100	1.643	100	1.633	100	1.63	83	1.63	59	1.632	80	1.633	43
240	1.604	w	-------	---	-------	---	1.608	30	1.60	5	1.607	6	1.606	20	1.608	12
060	1.574	vw	1.54	10	1.548	5	1.570	20	-------	---	-------	---	-------	---	1.570	4
231	1.525	m	1.50	20	-------	---	1.520	20	1.52	8	1.52	6	1.522	10	1.522	6
160 151	1.483	s	1.47	20	1.498	30	1.480	80	1.480	33	1.481	41	1.480	30	1.480	20
250	-------	---	-------	---	1.438	30	1.429	30	-------	---	-------	---	-------	---	1.431	7
002	1.427	s	-------	---	-------	---	-------	---	1.423	27	1.423	31	1.421	20	1.423	12
320	1.404	m	1.40	80	-------	---	1.403	30	1.403	8	-------	---	1.400	10	1.400	6
061	1.377	s	1.38	10	1.388	30	1.375	60	1.373	20	1.37	31	1.375	30	1.376	16
112	1.338	m	1.34	10	1.353	20	1.340	20	-------	---	-------	---	1.339	10	1.340	5
330	-------	---	1.32	10	-------	---	-------	---	1.333	10	1.333	19	1.328	10	1.329	6
301	1.302	m	-------	---	1.308	20	1.303	30	-------	---	1.299	9	1.303	5	1.304	3
311 170	1.285	m	1.29	10	-------	---	1.286	30	1.293	8	1.286	13	1.287	5	1.289	6
251	-------	---	-------	---	-------	---	-------	---	-------	---	-------	---	-------	---	1.279	1
321	1.250	m	-------	---	1.263	20	1.265	20	1.263	5	1.259	6	-------	---	1.256	4

Beta-aluminum oxide mono-hydrate (diaspore), β-$Al_2O_3 \cdot H_2O$[a]—Con.

hkl	1928 Hanson and Brownmiller Mo, 0.709 A		1932 Weiser and Milligan Mo, 0.709 A		1932 Kerr ----------		1937 Kovalev Fe, 1.93597 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		---- Physics Dept. Newcastle, Eng. Mo, 0.709 A		1929 Rooksby ----------		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	I	d	I	d	I	d	I	d	I	d	I	d	I	d	I
	A		A		A		A		A		A		A		A	
340 132	-------	---	-------	---	-------	---	1.243	20	1.243	7	1.24	13	--------	---	1.243	5
042	-------	---	-------	---	-------	---	1.213	20	1.217	3	--------	---	--------	---	1.218	2
331	1.206	m	-------	---	1.220	20	1.203	40	1.203	5	1.205	9	--------	---	1.204	4
080	-------	---	-------	---	-------	---	1.178	20	--------	---	--------	---	--------	---	1.1783	1
142	1.175	m	-------	---	1.182	20	1.173	40	1.172	9	1.17	13	--------	---	1.1739	7
341	1.142	w	-------	---	1.152	10	1.146	20	1.142	3	1.14	6	--------	---	1.1408	3
400	-------	---	-------	---	1.107	20	--------	---	--------	---	--------	---	--------	---	1.1003	1
410	1.093	m	-------	---	-------	---	1.093	30	1.092	8	--------	---	--------	---	1.0923	3
---	-------	---	-------	---	-------	---	--------	---	--------	---	--------	---	--------	---	--------	---
---	1.068	m	-------	---	1.077	20	--------	---	1.065	7	--------	---	--------	---	--------	---
---	-------	---	-------	---	-------	---	--------	---	--------	---	--------	---	--------	---	--------	---
---	1.041	w	-------	---	1.047	20	--------	---	1.039	4	--------	---	--------	---	--------	---
---	1.004	w	-------	---	1.017	20	--------	---	1.002	3	--------	---	--------	---	--------	---
---	.996	m	-------	---	-------	---	--------	---	--------	---	--------	---	--------	---	--------	---
---	-------	---	-------	---	.982	20	--------	---	--------	---	--------	---	--------	---	--------	---
---	.957	w	-------	---	.962	20	--------	---	--------	---	--------	---	--------	---	--------	---
---	.923	w	-------	---	.932	5	--------	---	--------	---	--------	---	--------	---	--------	---
---	.880	w	-------	---	-------	---	--------	---	--------	---	--------	---	--------	---	--------	---
---	.869	m	-------	---	.877	10	--------	---	--------	---	--------	---	--------	---	--------	---
---	.857	m	-------	---	.863	10	--------	---	--------	---	--------	---	--------	---	--------	---
---	.839	m	-------	---	.841	10	--------	---	--------	---	--------	---	--------	---	--------	---
---	.816	m	-------	---	.820	10	--------	---	--------	---	--------	---	--------	---	--------	---

References

[1] W. C. Hansen and L. T. Brownmiller, Equilibrium studies on alumina and ferric oxide, and on combinations of these with magnesia and calcium oxide, Am. J. Sci. **15**, 225-242 (1928).

[2] H. B. Weiser and W. O. Milligan, X-ray studies on the hydrous oxides I. Alumina, J. Phys. Chem. **36**, 3010 (1932).

[3] J. A. Kovalev, Debye diffraction diagrams of some oxide and borate minerals, Materialy TsNIGRI 1938. From A. K. Boldyrev and others, Annales de l'Institut des Mines à Leningrad **11**, (2)(1938).

[4] P. F. Kerr, The occurence of andalusite and related minerals at White Mountain, California, Econ. Geol. **27**, 614-643 (1932).

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

[6] H. P. Rooksby, An X-ray examination of the effect of heat on aluminum hydroxide, $Al_2O_3 \cdot H_2O$, Trans. Ceram. Soc. (England) **28**, 399-404 (1929).

[7] M. M. Deflandre, Crystal structure of diaspore, Bull. soc. franç. mineral. **55**, 140 (1932).

[8] K. Takané, Crystal structure of diaspore, Proc. Imp. Acad. (Tokyo) **9**, 113, (1933).

[9] F. J. Ewing, The crystal structure of diaspore, J. Chem. Phys. **3**, 203-207 (1935).

[10] W. Hoppe, The crystal structure of α-AlOOH (diaspore) and α-FeOOH (needle iron ore), Z. Krist. **103**, 73-80 (1940).

2.5. Multiple Oxides

Strontium titanate, $SrTiO_3$ (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-4192	3982	1.04	Copper------	Hoffmann [1] 1934.
	2-1457	1.59		
	2-1454	2.76		
2501	2647	2.76	Molybdenum---	New Jersey Zinc Co.
	1-1023	1.94		
	1-1018	1.59		
-------	2667	2.76	No data------	Megaw.
	3-0775	0.80		
	3-0769	1.95		

Additional published patterns. None.

NBS sample. The strontium titanate sample used for the NBS pattern was prepared by the National Lead Co. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of aluminum, barium, calcium, and silicon; and 0.0001 to 0.001 percent each of copper and magnesium. The refractive index of the NBS sample could not be determined because the sample was opaque.

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

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

Patterns	1	2	3
Hoffmann----------	321	211	110
New Jersey Zinc----------	110	200	211
Megaw----------	110	422	200
Swanson and Fuyat----------	110	200	211

Lattice constant. The structure was determined by Goldschmidt [2] in 1927. The space group is O_h^1-Pm3m with perovskite-type structure and $1(SrTiO_3)$ per unit cell.

Hoffmann's lattice constant was converted from kX to angstrom units for comparison with the NBS values.

Lattice constant in angstroms

1935----------	Hoffmann [1]----------	3.907
1953----------	Swanson and Fuyat------	3.9050 at 25°C

The density of strontium titanate calculated from the NBS lattice constant is 5.116 at 25°C.

Strontium titanate, $SrTiO_3$ (cubic)

hkl	1934 Hoffmann Cu, 1.5405 A			---- New Jersey Zinc Mo, 0.709 A			---- Megaw ----------			1953 Swanson and Fuyat 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
100	-------	------	---------	---------	-----	---------	---------	-----	---------	3.90	12	3.90
110	2.76	80	3.90	2.77	100	3.92	2.77	100	3.92	2.759	100	3.902
111	2.25	30	3.897	2.25	10	3.897	2.25	70	3.90	2.253	30	3.902
200	1.951	70	3.902	1.948	30	3.896	1.95	80	3.90	1.952	50	3.904
210	1.744	10	3.900	---------	-----	---------	---------	-----	---------	1.746	3	3.904
211	1.593	90	3.902	1.592	30	3.900	1.60	80	3.92	1.594	40	3.904
220	1.378	80	3.898	1.379	23	3.900	1.38	80	3.90	1.381	25	3.906
300	-------	------	---------	---------	-----	---------	---------	-----	---------	1.302	1	3.906
310	-------	------	---------	1.232	18	3.896	1.23	70	3.89	1.235	15	3.905
311	1.176	50	3.900	1.175	2	3.897	1.18	60	3.91	1.1774	5	3.9050
222	1.127	50	3.904	1.124	3	3.894	1.13	60	3.91	1.1273	8	3.9051
321	1.043	100	3.903	1.043	15	3.903	1.04	80	3.89	1.0437	16	3.9052
400	.976	40	3.904	---------	-----	---------	.978	50	3.91	.9765	3	3.9060
411	.920	60	3.903	---------	-----	---------	.922	70	3.91	.9205	10	3.9053
331	-------	------	---------	---------	-----	---------	---------	-----	---------	.8959	3	3.9051
420	-------	------	---------	---------	-----	---------	.875	80	3.91	.8731	10	3.9046
332	-------	------	---------	---------	-----	---------	.835	70	3.92	.8325	6	3.9048
422	-------	------	---------	---------	-----	---------	.799	100	3.91	.7972	9	3.9054
Average value of last five lines----------			3.903	---------	-----	3.898	---------	-----	3.91	---------	-----	3.9050

References

[1] A. Hoffmann, Untersuchungen über Verbindungen mit Perowkitstruktur, Z. physik. Chem. **28b**, 65 (1935).

[2] V. M. Goldschmidt, Geochem. Verteilungses. der Elemente. Norske Videnskaps-Akad. Oslo, VII (1926) and VIII (1927). From Z. Krist. Strukturbericht **I**, 333 (1913-1928).

Barium titanate, $BaTiO_3$ (tetragonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
----	2570	2.83	Copper	Megaw (pattern unpublished).
	3-0744	1.63		
	3-0725	0.82		
----	2571	-----	----------	A continuation of the preceding card.
	3-0745			
	3-0726			

Additional published patterns. None.

NBS sample. The barium titanate used for the NBS pattern was contributed by the National Lead Co., Titanium Division. The sample was annealed at 1,480°C in a magnesium crucible. After this treatment spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of bismuth and strontium; 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, lead, and silicon; and 0.0001 to 0.001 percent each of manganese and tin. The NBS sample was too finely divided for refractive index measurements.

Interplanar spacings and intensity measurements. The *d*-spacings of the Megaw pattern were assumed to be in angstrom units.

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

Patterns	1	2	3
Megaw	101,110	211	422
Swanson and Fuyat	101,110	111	200

Lattice constants. The structure was determined by Evans [1] in 1951. The space group is C^1_{4v}-P4mm with perovskite-structure type and $1(BaTiO_3)$ per unit cell. The tetragonal cell inverts to the cubic system at approximately 120°C, as reported by Megaw [2] and many others. A number of investigators also report changes below room temperature.

All of the unit cell data have been converted from kX to angstrom units and data for three cells have been converted to 26°C from the temperatures indicated in parentheses.

The mean linear expansion is $3.5 \pm 1.5 \times 10^{-6}$, the change being positive perpendicular to the *c*-axis and negative parallel to it, according to Megaw [2].

Lattice constants in angstroms

		a	*c*
1945	Rooksby [3]	3.9947	4.0277 at 26°C (22°C)
1947	Megaw [2]	3.9947	4.0336 at 26°C (20°C)
1947	de Bretteville [4]	4.00	4.04
1949	Danielson [5]	3.9863	4.0043 at 26°C (25°C)
1953	Swanson and Fuyat	3.994	4.038 at 26°C

The density of barium titanate calculated from the NBS lattice constants is 6.012 at 26°C.

Barium titanate, $BaTiO_3$ (tetragonal)

hkl	---- Megaw Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*
	A		*A*	
001	3.99	20	4.03	12
100			3.99	25
101	2.83	100	2.838	100
110			2.825	
111	2.31	70	2.314	46
002	2.02	70	2.019	12
200	2.00	80	1.997	37
102	1.80	50	1.802	6
201	1.79	60	1.790	8
210			1.786	7
112	1.64	70	1.642	15
211	1.63	100	1.634	35
202	1.42	80	1.419	12
220	1.41	70	1.412	10
212	1.34	50	1.337	5
221			1.332	2
103	1.28	60	1.275	5
301	1.26	70	1.264	7
310			1.263	9
113	1.21	50	1.214	3
311	1.21	60	1.205	5
222	1.16	70	1.1569	7
203	1.12	40	1.1194	<1
302	1.11	40	1.1161	1
320	1.11-	40	1.1082	<1
213	1.07	80	1.0746	7
312	1.07	80	1.0703	12
321	1.07	80	1.0679	12
004	1.01	40	1.0093	1
400	.999	50	.9984	2
104	.978	20	.9784	<1
223	.974	20	.9742	1

Barium titanate, $BaTiO_3$ (tetragonal)—Con.

hkl	---- Megaw Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*
	A		*A*	
322	.971	50	.9710	1
401 } 410	.969	50	.9686	1
114	.950	60	.9506	3
303	.946	60	.9465	1
411 } 330	.942	80	.9419	5
313	.921	60	.9208	2
331	.917	50	.9166	2
204	.900	70	.9008	3
402	.895	70	.8948	5
420	.893	80	.8929	7
214	.878	50	.8787	2
412	.873	50	.8733	1
421	.872	50	.8720	1
323	.855	80	.8552	7
332	.853	80	.8531	6
224	.821	70	.8211	3
422	.817	100	.8167	4
---	.807	10	---	---
---	.804	40	---	---
---	.802	40	---	---
---	.799	40	---	---

Barium titanate, $BaTiO_3$ (tetragonal)—Con.

hkl	---- Megaw Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*
	A		*A*	
---	.791	70	---	---
---	.788	80	---	---
---	.786	80	---	---
---	.784	100	---	---
---	.776	50	---	---

References

[1] H. T. Evans, Jr., The crystal structure of tetragonal barium titanate, Acta Cryst. **4**, 377 (1951).

[2] H. D. Megaw, Temperature changes in the crystal structure of barium titanium oxide, Proc. Roy. Soc. (London) **189A**, 261-283 (1947).

[3] H. P. Rooksby, Compounds of the structural type of calcium titanate, Nature **155**, 484 (1945).

[4] A. P. de Bretteville and S. B. Levin, The lattice constants of a single crystal of barium titanate, Am. Mineralogist **32**, 686 (1947).

[5] G. C. Danielson, Domain orientation in polycrystalline barium titanate, Acta Cryst. **2**, 90-93 (1949).

2.6. Halides

Sodium bromide, NaBr (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
3281	3380	2.10	Molybdenum--	Davey [1] 1923.
	1-1225	2.98		
	1-1230	1.79		
2197	2228	2.96	Molybdenum--	Hanawalt, Rinn, and Frevel [2] 1938.
	1-0900	2.09		
	1-0901	3.44		

Additional published patterns. None.

NBS sample. The sodium bromide used for the NBS pattern was an analytical reagent-grade sample prepared by the Mallinckrodt Chemical Works. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of potassium, 0.001 to 0.01 percent each of aluminum, calcium, iron, and molybdenum, 0.0001 to 0.001 percent each of barium, magnesium, lead, and silicon, and less than 0.0001 percent of copper. The refractive index of the NBS sample is 1.641.

Interplanar spacings and intensity measurements. Both the Davey 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:

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

Lattice constant. The structure, determined by Davey [1] in 1923, is the face-centered, sodium chloride type, O_h^5-Fm3m with 4(NaBr) per unit cell.

A group of unit-cell data was converted from kX to angstrom units for comparison with the NBS values. The coefficient of expansion according to Ievinš, Straumanis, and Karlsons is 42.52×10^{-6}.

Lattice constant in angstroms

1921	Wyckoff [3]	5.96
1923	Davey [1]	5.951
1926	Ott [4]	5.974
1938	Ievinš, Straumanis, and Karlsons [5]	5.97324 at 26°C
1942	Batuecas and Fernandez-Alonso [6]	5.984
1949	Nickels, Fineman, and Wallace [7]	5.9737
1953	Swanson and Fuyat	5.9772 at 26°C

The density of sodium bromide calculated from the NBS lattice constant is 3.200 at 26°C.

Sodium bromide, NaBr (cubic)

hkl	1923 Davey Mo, 0.709 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1953 Swanson and Fuyat Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	3.46	25	5.99	3.45	45	5.98	3.449	64	5.974
200	2.99	80	5.98	2.97	100	5.94	2.988	100	5.976
220	2.10	100	5.94	2.09	63	5.91	2.113	63	5.976
311	1.795	30	5.953	1.79	20	5.94	1.802	21	5.977
222	1.717	30	5.948	1.71	20	5.92	1.725	19	5.976
400	1.486	10	5.944	1.490	10	5.960	1.495	8	5.980
331	1.366	10	5.954	1.365	5	5.950	1.371	7	5.976
420	1.332	30	5.957	1.332	35	5.957	1.337	15	5.979
422	1.215	20	5.952	1.218	10	5.967	1.221	9	5.982
511	----------	--------	----------	1.147	5	5.960	1.1506	4	5.9787
440	1.051	5	5.945	1.055	5	5.968	1.0566	2	5.9770
531	1.007	5	5.957	----------	--------	----------	1.0103	2	5.9770

Sodium bromide, NaBr (cubic)—Con.

hkl	1923 Davey Mo, 0.709 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1953 Swanson and Fuyat Cu, 1.5405 A, 26°C		
	d	I	a	d	I	a	d	I	a
	A		A	A		A	A		A
600	.991	10	5.946	----------	--------	----------	.9963	3	5.9778
620	.940	10	5.945	----------	--------	----------	.9451	2	5.9773
533	----------	--------	----------	----------	--------	----------	.9117	<1	5.9784
622	----------	--------	----------	----------	--------	----------	.9012	2	5.9779
444	----------	--------	----------	----------	--------	----------	.8626	<1	5.9763
711	----------	--------	----------	----------	--------	----------	.8370	1	5.9774
640	----------	--------	----------	----------	--------	----------	.8289	1	5.9773
642	.796	5	5.957	----------	--------	----------	.7987	2	5.9769
Average value of last five lines	----------	----------	5.950	----------	--------	5.960	----------	--------	5.9772

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

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

[5] A. Ievinš, M. Straumanis, and K. Karlsons, Präzisionsbestimmung von Gitterkonstanten hygroskopischer Verbindungen (LiCl, NaBr), Z. physik. Chem. **40B**, 146-150 (1938).

[6] T. Batuecas and J. I. Fernández-Alonso, Pycnometrische Präzisionsmethode für Flüssigkeiten und feste Körper. IV Neubestimmung der Dichte von reinem Kaliumchlorid, Kaliumbromid und Natriumbromid bei 0°C, Z. physik. Chem. **A190**, 272-277 (1942).

[7] J. E. Nickels, M. A. Fineman and W. E. Wallace, X-ray diffraction studies of sodium chloride-sodium bromide solid solutions, J. Phys. & Colloid Chem. **53**, 625-628 (1949).

Cesium bromide, CsBr (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2054	2138	3.03	---------	Davey [1] 1923.
	1-0866	1.75		
	1-0843	2.15		

The following ASTM card for body-centered cesium bromide at 455°C. is also in the file but the ASTM index does not specify that this is a high temperature form.

----	------	3.10	Copper---	Wagner and Lippert [2] 1923.
	4-0608	1.79		
	4-0609	2.19		

Additional published patterns. None.

NBS sample. The cesium bromide sample used for the NBS pattern was prepared at the NBS by R. B. Johannesen from cesium chloride. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of calcium, potassium, and sodium and less than 0.001 percent each of aluminum, barium, copper, iron, magnesium, and silicon. The refractive index of the NBS sample is 1.703.

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

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

Patterns	1	2	3
Davey----------	110	211	200
Swanson and Fuyat----------	110	211	321

Lattice constant. The structure was determined by Wyckoff [3] in 1921. The simple-cubic lattice has space group O_h^1-Pm3m, cesium chloride-structure type, and 1(CsBr) per unit cell.

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

Lattice constant in angstroms

1921-----	Wyckoff [3]----------	4.31
1923-----	Davey [1]----------	4.297
1936-----	Wagner and Lippert [2]-------	4.296
1953-----	Swanson and Fuyat----------	4.2953 at 25°C

The density of cesium bromide calculated from the NBS lattice constant is 4.456 at 25°C.

Cesium bromide, CsBr (cubic)

hkl	1922 Davey Mo, 0.709 A			1953 Swanson and Fuyat Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
100	4.34	1	4.34	4.29	8	4.29
110	3.04	100	4.30	3.039	100	4.298
111	2.42	.75	4.20	2.480	3	4.295
200	2.15	10	4.31	2.148	18	4.296
210	1.929	.75	4.313	1.921	6	4.295
211	1.754	35	4.295	1.754	43	4.296
220	1.523	7	4.308	1.519	18	4.296
300	1.434	.5	4.302	1.432	3	4.296
310	1.359	5	4.297	1.358	16	4.294
311	-------	------	-------	1.295	<1	4.295
222	1.242	1.5	4.304	1.240	6	4.295
320	-------	------	-------	1.1919	1	4.2975
321	1.150	3.5	4.304	1.1482	20	4.2962
400	1.075	.75	4.301	1.0741	1	4.2964
411	1.013	1.5	4.297	1.0125	9	4.2957
331	-------	------	-------	.9856	1	4.2961
420	.959	.75	4.289	.9605	5	4.2955
332	.916	.75	4.296	.9157	3	4.2950
422	.877	.75	4.296	.8768	3	4.2954
500	-------	------	-------	.8590	<1	4.2950
510	.843	1.5	4.297	.8424	9	4.2954
Average of last five lines----------			4.295	--------	-----	4.2953

References

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

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

Cesium dichloroiodide, $CsICl_2$ (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1857	1795	3.16	Molybdenum---	Hanawalt, Rinn, and Frevel [1] 1938.
	1-0758	4.07		
	1-0769	1.71		

Additional published patterns. None.

NBS sample. The cesium dichloroiodide used for the NBS pattern was prepared by R. B. Johannesen at the NBS. The product was purified by recrystallization three times from dilute hydrochloric acid. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of calcium, potassium, and sodium; and less than 0.001 percent each of aluminum, barium, copper, iron, magnesium, and silicon. The refractive indices of the NBS sample are as follows: $\omega = 1.611$ and $\epsilon = 1.645$ with positive optical sign.

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

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

Patterns	1	2	3
Hanawalt, Rinn, and Frevel--------	110	102	124
Swanson and Fuyat------------------	110	102	014

Lattice constants. The structure was determined by Wyckoff [2] in 1920. The space group is D_{3d}^5-$R\bar{3}m$ with $3(CsICl_2)$ per unit cell. Cesium dichloroiodide is representative of the group of similar rhombohedral compounds that possess a distorted cesium chloride-type arrangement.

Wyckoff's lattice constants have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants in angstroms

		a	*c*
1920	Wyckoff [2]------------------	6.331	12.213
1953	Swanson and Fuyat------------	6.328	12.216 at 26°C

The density of cesium dichloroiodide calculated from the NBS lattice constants is 3.888 at 26°C.

Cesium dichloroiodide, $CsICl_2$ (hexagonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*
	A		A	
102	4.08	53	4.081	75
110	3.17	100	3.164	100
014	2.67	40	2.668	50
022	2.51	20	2.499	23
204	2.03	27	2.039	25
212	1.96	20	1.961	15
300	1.82	20	1.827	15
124	1.71	53	1.713	32
220	1.58	13	1.582	9
132	1.475	13	1.475	6
108	----------	----------	1.471	7
314	1.360	20	1.360	10
306				
042	----------	----------	1.337	4
028	1.334	7	1.334	4
231	1.253	8	1.250	5
044				
322	----------	----------	1.231	4
218	1.227	8	1.229	3
410	----------	----------	1.1958	5
0·1·10	1.193	11	1.1923	4
234	1.163	7	1.1624	3
325	1.117	4	1.1169	3
2·0·10				
047	----------	----------	1.0775	2
2·1·10	1.053	7	1.0522	4
421	1.032	5	1.0318	4
242	----------	----------	1.0209	1
333				
424	----------	----------	.9807	1
328	----------	----------	.9705	1
3·1·10	----------	----------	.9522	2
336	----------	----------	.9364	2
520	----------	----------	.8777	1
614	----------	----------	.8060	1
526				

References

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

[2] R. W. G. Wyckoff, The crystal structure of cesium dichloroiodide, J. Am. Chem. Soc. **42**, 1100-1116 (1920).

2.7. Chlorates

Sodium chlorate, $NaClO_3$ (cubic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2227	2296	2.94	Molybdenum---	Hanawalt, Rinn, and Frevel [1] 1938.
	1-0917	3.28		
	1-0908	1.76		

Additional published patterns

Source	Radiation	Wavelength
Kolkmeijer, Bijvoet, and Karssen [2] 1921	Copper---	$K_{\alpha 1}$
Vegard [3] 1922	Copper---	---

NBS sample. The sodium chlorate used for the NBS pattern was procured from the Fisher Scientific Co. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent of calcium; 0.0001 to 0.001 percent each of aluminum, iron, magnesium, and silicon; and less than 0.0001 percent of copper. The refractive index of the NBS sample is 1.515.

Interplanar spacings and intensity measurements. The *d*-spacings for the Kolkmeijer, Bijvoet, and Karssen and the Vegard patterns were calculated from Bragg angle data while 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:

Patterns	1	2	3
Kolkmeijer, Bijvoet, and Karssen-----	210	321	200
Vegard-----	321	210	510
Hanawalt, Rinn, and Frevel-----	210	200	321
Swanson and Fuyat-----	210	200	321

Lattice constant. The structure was determined by Dickinson and Goodhue [4] in 1921. The space group is T^4-$P2_13$ with $4(NaClO_3)$ per unit cell. Sodium chlorate is a prototype for other similar structures.

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

Lattice constant in angstroms

1921	Dickinson and Goodhue [4]-----	6.57
1921	Kolkmeijer, Bijvoet, and Karssen [2]	6.56
1929	Zachariasen [5]-----	6.58
1953	Swanson and Fuyat-----	6.5755 at 25°C

The density of sodium chlorate calculated from the NBS lattice constant is 2.486 at 25°C.

Sodium chlorate, $NaClO_3$ (cubic)

hkl	1921 Kolkmeijer, Bijvoet, and Karssen Cu, 1.5405 A			1922 Vegard Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1953 Swanson and Fuyat Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
110	4.77	w	6.75	4.69	10	6.63	4.66	20	6.59	4.65	23	6.58
111	3.80	w	6.58	3.86	60	6.69	3.80	33	6.58	3.797	35	6.577
200	[a] 3.255	s	6.510	3.292	60	6.584	3.29	67	6.58	3.289	65	6.578
210	2.932	vs	6.556	2.957	70	6.612	2.95	100	6.60	2.941	100	6.576
211	2.673	m	6.547	2.695	50	6.601	2.69	40	6.59	2.685	41	6.577
220	---	---	---	---	---	---	2.32	1	6.56	2.325	2	6.576
221	2.179	m	6.537	2.195	30	6.585	2.18	33	6.54	2.192	26	6.576
310	2.066	vw	6.533	---	---	---	2.07	7	6.55	2.080	6	6.578
311	1.975	w	6.550	1.976	30	6.554	1.98	13	6.57	1.983	11	6.577
222	---	---	---	---	---	---	1.89	1	6.55	1.898	2	6.575

Sodium chlorate, $NaClO_3$ (cubic)—Con.

hkl	1921 Kolkmeijer, Bijvoet, and Karssen Cu, 1.5405 A			1922 Vegard Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A			1953 Swanson and Fuyat 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
320	1.816	vw	6.548	1.828	20	6.591	1.83	7	6.60	1.824	7	6.577
321	1.753	vs	6.559	1.759	100	6.582	1.76	67	6.59	1.757	42	6.574
400	----	----	----	----	----	----	1.64	1	6.56	1.644	2	6.576
410	1.592	w	6.564	1.594	30	6.572	1.59	11	6.56	1.595	10	6.576
411	----	----	----	1.555	10	6.597	1.55	3	6.58	1.550	3	6.576
331	1.505	vw	6.560	1.512	20	6.591	1.51	11	6.58	1.509	7	6.578
420	----	----	----	1.471	10	6.579	1.473	3	6.59	1.470	3	6.574
421	1.435	w	6.576	1.435	30	6.576	1.437	13	6.59	1.435	9	6.576
332	----	----	----	----	----	----	1.407	1	6.60	1.402	2	6.576
422	----	----	----	----	----	----	1.344	1	6.58	1.342	2	6.574
430	----	----	----	----	----	----	1.320	1	6.60	1.315	2	6.575
510	1.287	m	6.562	1.291	70	6.583	1.292	3	6.59	1.2895	14	6.5752
511	----	----	----	1.263	30	6.563	1.267	5	6.58	1.2657	5	6.5768
520	----	----	----	1.224	30	6.591	1.224	5	6.59	1.2208	4	6.5742
521	----	----	----	1.200	20	6.573	1.202	5	6.58	1.2004	5	6.5749
522	----	----	----	1.142	10	6.560	1.147	3	6.59	1.1445	2	6.5747
530	----	----	----	----	----	----	1.132	1	6.60	1.1276	2	6.5750
531	----	----	----	1.110	10	6.567	1.116	3	6.60	1.1114	2	6.5751
600	----	----	----	----	----	----	1.096	1	6.58	1.0958	1	6.5748
610	----	----	----	----	----	----	----	----	----	1.0810	1	6.5755
611	----	----	----	1.068	10	6.584	1.070	3	6.60	1.0666	2	6.5750
620	----	----	----	1.043	10	6.597	1.044	1	6.60	1.0397	2	6.5756
621	----	----	----	1.027	70	6.576	1.030	8	6.60	1.0269	8	6.5754
541	----	----	----	----	----	----	----	----	----	1.0146	4	6.5754
533	----	----	----	----	----	----	----	----	----	1.0027	4	6.5751
630	----	----	----	----	----	----	----	----	----	.9803	2	6.5761
631	----	----	----	----	----	----	----	----	----	.9697	1	6.5768
632	----	----	----	----	----	----	----	----	----	.9393	1	6.5751
710	----	----	----	----	----	----	----	----	----	.9299	3	6.5754
711	----	----	----	----	----	----	----	----	----	.9207	1	6.5751
720	----	----	----	----	----	----	----	----	----	.9033	3	6.5761
721	----	----	----	----	----	----	----	----	----	.8949	2	6.5761
Average of the last five lines			6.564	----	----	6.577	----	----	6.60	----	----	6.5755

[a] *d*-spacing 3.553, vw was omitted as it cannot be indexed.

References

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

[2] N. H. Kolkmeijer, J. M. Bijvoet, and A. Karssen, Investigation by means of X-rays of the crystal structure of sodium chlorate and sodium bromate, Koninkl. Akad. Wetenschap. Amsterdam **23**, 644-653 (1921).

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

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

[5] W. H. Zachariasen, The crystal structure of sodium chlorate, Z. Krist. **71**, 517-529 (1929).

2.8. Carbonates

Calcium carbonate (aragonite), $CaCO_3$ (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
----	3106	2.46	Rhodium----------	Bragg [1] 1924.
	3-0894	1.23		
	3-0893	1.86		
----	1506	3.35	Copper, 1.53923--	Olshausen [2] 1925.
	3-0417	2.70		
	3-0425	2.36		
----	2357	2.92	Copper----------	Norton [3] 1937.
	3-0680	1.86		
	3-0670	1.85		
----	3604	1.97	Iron----------	Allis-Chalmers.
	3-1062	3.39		
	3-1067	3.26		
----	1531	3.39	Copper----------	British Museum.
	3-0426	1.99		
	3-0405	2.72		
1560	1456	3.40	Molybdenum------	Hanawalt, Rinn, and Frevel.
	1-0628	1.98		
	1-0628	2.70		

The Bragg pattern is a single crystal pattern which accounts for the duplicate d-spacings and the absence of intensities in certain cases. The Norton card is mislabeled calcite.

Additional published patterns. None.

NBS sample. The aragonite used for the NBS pattern was prepared by H. E. Kissinger of the NBS. Solutions of potassium carbonate and calcium chloride were heated to boiling and poured quickly together into a third beaker. The resulting mixture was digested until precipitation was complete and then filtered. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent each of silicon and strontium; 0.001 to 0.01 percent each of aluminum, barium, copper, iron, magnesium, nickel, and lead; and 0.0001 to 0.001 percent each of silver, manganese, and tin. The NBS sample is optically negative with the following refractive indices: $\alpha = 1.529$, $\beta = 1.680$, γ was not obtainable due to the acicular crystal form.

Interplanar spacings and intensity measurements. The Bragg, Olshausen, and Norton data were converted from Bragg angles to d-spacings in angstroms. The Allis-Chalmers, British Museum, and Hanawalt, Rinn, and Frevel d-spacings were converted from kX to angstrom units. In the Bragg pattern the reflections of zero intensity listed on the ASTM card have been dropped and only one of the two possible intensities given for certain d-spacings is included in the table of patterns. The 3.06 d-spacing of the Hanawalt, Rinn, and Frevel pattern is the strong line for calcite.

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

Patterns	1	2	3
Olshausen----------	111	------	112
Norton----------	002	041	132,230
Allis-Chalmers----------	221	111	021
British Museum----------	111	221	121
Hanawalt, Rinn, and Frevel--------	111	221	-------
Swanson and Fuyat----------	111	221	021

The Bragg intensity values for the three strongest lines were not included in this table as they represent single crystal data.

Lattice constants. The structure, determined by Bragg [1] in 1924, is the orthorhombic pseudo-hexagonal potassium nitrate-type structure with space group D_{2h}^{16}-Pbnm (Pnma) and 4($CaCO_3$, aragonite) per unit cell.

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

Lattice constants in angstroms

		a	b	c
1924	Bragg [1]----------	4.95	7.96	5.73
1925	Olshausen [2]----------	4.965	7.977	5.748
1953	Swanson and Fuyat-------	4.959	7.968	5.741 at 26°C

The density of aragonite calculated from the NBS lattice constants is 2.930 at 26°C.

Calcium carbonate (aragonite) $CaCO_3$ (orthorhombic)

hkl	1924 Bragg Rh, 0.61326 A		1925 Olshausen Cu, 1.5405 A		1937 Norton Cu, 1.5405 A		---- Allis-Chalmers Fe, 1.93597 A		---- British Museum Cu, 1.5405 A		---- Hanawalt, Rinn, and Frevel Mo, 0.70926 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26℃	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*		*A*	
110	-------	----	4.287	m	-------	----	-------	----	-------	----	-------	------	4.21	2
---	-------	----	3.745	w	-------	----	-------	----	-------	----	-------	------	-------	------
111	-------	----	3.348	s	-------	----	3.40	80	3.40	100	3.41	100	3.396	100
021	-------	----	-------	----	3.23	6	3.27	60	-------	----	3.30	48	3.273	52
---	-------	----	-------	----	-------	----	-------	----	-------	----	3.06	2	-------	------
002	2.855	34	-------	----	2.92	100	-------	----	3.02	30	2.89	2	2.871	4
121	-------	----	-------	----	-------	----	2.73	10	2.73	80	-------	------	2.730	9
---	-------	----	2.693	s	-------	----	2.70	20	-------	----	2.71	64	2.700	46
---	-------	----	-------	----	-------	----	2.58	10	-------	----	-------	------	-------	------
200	2.471	100	2.457	m	-------	----	2.49	20	2.51	65	2.50	48	2.481	33
---	-------	----	-------	----	2.39	25	2.39	10	-------	----	-------	------	2.409	14
112	-------	----	2.358	s	-------	----	2.37	20	2.36	80	2.36	48B	2.372	38
130	2.328	60	-------	----	-------	----	2.32	40	-------	----	-------	------	2.341	31
022	2.316	61	-------	----	-------	----	-------	----	-------	----	-------	------	2.328	6
040	-------	----	2.192	w	2.20	38	-------	----	2.19	65	2.19	11	2.188	11
220	2.094	63	2.076	w	-------	----	2.10	20	2.09	65	2.10	24	2.106	23
221	1.980	26	1.982	s	-------	----	1.97	100	1.99	100	1.98	100	1.977	65
041	-------	----	1.881	m	1.86	63	1.88	60	1.88	65	1.88	64	1.882	32
202	1.866	68	-------	----	-------	----	-------	----	-------	----	-------	------	1.877	25
132 230	------	----	1.801	w	1.83	63	1.81	40	1.83	65	1.82	32	1.814	23
141	-------	----	-------	----	-------	----	-------	----	-------	----	-------	------	1.759	4
113	-------	----	-------	----	-------	----	-------	----	1.74	80	1.74	40	1.742	25
231	-------	----	1.728	s	-------	----	1.73	40	-------	----	-------	------	1.728	15
---	-------	----	-------	----	-------	----	1.72	40	-------	----	-------	------	-------	------
222	-------	----	-------	----	-------	----	-------	----	-------	----	-------	------	1.698	3
---	-------	----	1.631	vw	-------	----	-------	----	-------	----	1.63	2	-------	------
311	-------	----	1.551	w	1.59	6	1.55	10	1.56	30	1.56	6	1.557	4
232	-------	----	-------	----	-------	----	-------	----	-------	----	1.53	2	1.535	2
241	-------	----	-------	----	1.49	13	1.49	10	-------	----	1.50	6	1.499	4
321	-------	----	1.474	w	-------	----	-------	----	-------	----	1.473	8	1.475	3
151	-------	----	-------	----	1.44	13	1.46	10	-------	----	-------	------	1.466	5
---	1.428	7	-------	----	-------	----	-------	----	-------	----	-------	------	-------	------
312	-------	----	-------	----	-------	----	-------	----	-------	----	1.413	8	1.411	5
330	-------	----	1.404	w	-------	----	-------	----	1.39	30	-------	------	1.404	3
242 331	1.363	21	1.354	m	-------	----	1.36	20	1.37	30	1.365	6	1.365	3
114	-------	----	-------	----	-------	----	-------	----	-------	----	-------	------	1.358	3
060	1.320	19	-------	----	-------	----	-------	----	-------	----	-------	------	1.328	2
332	-------	----	-------	----	-------	----	1.26	10	-------	----	1.266	6	1.261	6
400	1.236	70	1.238	m	-------	----	-------	----	1.25	30	1.243	13	1.240	7
134 410	------	----	-------	----	-------	----	1.23	20	-------	----	1.212	6	1.224	5
243 062	------	----	1.204	vw	-------	----	-------	----	-------	----	-------	------	1.205	6
153	-------	----	-------	----	-------	----	-------	----	-------	----	1.192	2	1.1892	5
162 260	1.164	42	1.163	w	1.17	13	1.17	20	-------	----	1.175	8	1.1712	6
421	1.158	4	-------	----	-------	----	1.15	20	-------	----	-------	------	1.1599	3
---	-------	----	-------	----	-------	----	-------	----	-------	----	1.132	5	-------	------
---	-------	----	-------	----	-------	----	-------	----	-------	----	1.112	2	-------	------
e360	1.047	40	1.034	m	-------	----	1.03	20	-------	----	-------	------	-------	------
225	-------	----	1.007	m	-------	----	-------	----	-------	----	-------	------	-------	------

Calcium carbonate (aragonite) $CaCO_3$ (orthorhombic)—Con.

hkl	1924 Bragg Rh, 0.61326 A		1925 Olshausen Cu, 1.5405 A		1937 Norton Cu, 1.5405 A		---- Allis-Chalmers Fe, 1.93597 A		---- British Museum Cu, 1.5405 A		---- Hanawalt, Rinn, and Frevel Mo, 0.70926 A		1953 Swanson and Fuyat 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*	
450	.990	9	.975	vd	----------	----	----------	----	----------	----	----------	------	----------	------
173	.952	18	.957	w	----------	----	----------	----	----------	----	----------	------	----------	------
---	.933	2	.936	m	----------	----	----------	----	----------	----	----------	------	----------	------
---	.926	6	----------	----	----------	----	----------	----	----------	----	----------	------	----------	------
325	.913	2	.914	m	----------	----	----------	----	----------	----	----------	------	----------	------
381	(b)	----	.896	m	----------	----	----------	----	----------	----	----------	------	----------	------

[a] This and succeeding indices are taken from Olshausen's data.
[b] Twelve additional lines are omitted.

References

[1] W. L. Bragg, The structure of aragonite, Proc. Roy. Soc. (London), **105A**, 16-39 (1924).

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

[3] F. H. Norton, Accelerated weathering of feldspars, Am. Mineralogist **22**, 1-14 (1937).

Strontium carbonate (strontianite), $SrCO_3$ (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1394	1309	3.53	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
	1-0562	2.45		
	1-0556	2.05		
II-893	1377	3.49	Copper----	British Museum.
	2-0405	2.42		
	2-0397	2.03		
II-893a	1378	-----	----------	A continuation of the preceding card.
	2-0406			
	2-0398			

The British Museum pattern was made using a natural mineral specimen from Strontian, Argyll, Scotland.

Additional published patterns

Source	Radiation	Wavelength
J. J. Lander [2] 1949--------	Copper-------	1.5418

NBS sample. The strontium carbonate used for the NBS pattern was specially purified material contributed by the Mallinckrodt Chemical Works. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of barium; 0.001 to 0.01 percent each of calcium and lithium; 0.0001 to 0.001 percent each of aluminum, potassium, manganese and sodium; and less than 0.0001 percent each of copper, iron, magnesium, and silicon. The refractive indices of the NBS sample are: $\alpha = 1.517$, $\beta = 1.663$ and $\gamma = 1.667$ with negative optical sign.

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

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

Patterns	1	2	3
Hanawalt, Rinn, and Frevel--------	111	130	221
British Museum----------	111	130	221
Lander----------	111	021	221
Swanson and Fuyat----------	111	021	221

Four d-spacings of the British Museum pattern, 6.71, 6.09, 4.83, and 3.11 cannot be indexed and are probably due to mineral contamination.

Lattice constants. The structure was determined by Wilson [3] in 1928. The space group is D_{2h}^{16}-Pmcn (Pnma) with potassium nitrate-structure type and $4(SrCO_3)$ per unit cell. A rhombohedral form of $SrCO_3$ stable above 912°C is also known, according to J. J. Lander [2].

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

Lattice constants in angstroms

		a	b	c
1928	Wilson [2]----------	5.128	8.421	6.094
1953	Swanson and Fuyat-------	5.107	8.414	6.029 at 26°C

The density of strontium carbonate calculated from the NBS lattice constants is 3.785 at 26°C.

(See table on next page)

References

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

[2] J. J. Lander, Polymorphism in the alkaline earth carbonates, J. Chem. Phys. **17**, 892-901 (1949).

[3] T. A. Wilson, The lattice constants and the space groups of $BaCO_3$ and $SrCO_3$, Phys. Rev. **31**, 305 (1928).

Strontium carbonate, $SrCO_3$ (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		---- British Museum Cu, 1.5405 A		1949 Lander Cu, 1.5418 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
-----	------	---	6.71	40	------	---	------	---
-----	------	---	6.09	40	------	---	------	---
-----	------	---	4.83	20	------	---	------	---
110	------	---	4.24	20	4.32	3	4.367	14
020	------	---	3.87	60	4.18	3	4.207	6
-----	------	---	------	---	[a] 3.90	3	------	---
111	3.54	100	3.50	100	3.50	100	3.535	100
021	------	---	3.38	60	3.42	50	3.450	70
-----	------	---	3.11	20	------	---	------	---
002	------	---	2.98	40	2.98	20	3.014	22
121	------	---	2.82	60	------	---	2.859	5
012	------	---	2.71	60	2.81	20	2.838	20
102	------	---	------	---	2.58	10	2.596	12
200	2.57	8	2.55	40	2.54	20	2.554	23
112	------	---	------	---	2.46	30	2.481	34
130	2.45	40	2.42	80	2.44	30	2.458	40
022	------	---	------	---	------	---	2.4511	33
211	------	---	2.25	40	2.25	5	2.2646	5
220	2.18	8	2.16	40	2.17	15	2.1831	16
040	------	---	2.09	20	2.090	5	2.1035	7
221	2.05	40	2.03	80	2.040	50	2.0526	50
041	1.98	8	1.975	60	1.973	30	1.9860	26
202	------	---	1.936	60	1.936	30	1.9489	21
132	1.90	16	1.881	70	1.893	40	1.9053	35
141	------	---	------	---	------	---	1.8514	3
113	------	---	------	---	1.816	30	1.8253	31

Strontium carbonate, $SrCO_3$ (orthorhombic)—Con.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		---- British Museum Cu, 1.5405 A		1949 Lander Cu, 1.5418 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
023	1.81	32	1.802	70	1.804	10	1.8134	16
231	------	---	------	---	------	---	1.8023	4
222	------	---	1.756	20	1.758	5	1.7685	7
042	------	---	1.704	20	1.716	3	1.7253	5
310	------	---	1.654	20	1.660	5	1.6684	3
240	------	---	------	---	1.617	5	1.6236	4
311	------	---	1.603	60	1.602	20	1.6080	13
150	------	---	------	---	------	---	1.5981	3
241	------	---	1.556	60	1.562	20	1.5676	13
151	------	---	1.531	60	1.537	20	1.5447	11
004	------	---	------	---	1.500	3	1.5072	3
223	------	---	1.471	40	1.473	8	1.4782	6
312	------	---	------	---	------	---	1.4596	4
330	------	---	1.443	50	------	---	1.4551	9
242	------	---	------	---	------	---	1.4293	6
114	------	---	1.413	60	1.420	10	1.4246	7
152	------	---	1.392	20	------	---	1.4120	5
060	------	---	1.354	20	------	---	1.4024	4
332	------	---	1.305	70	------	---	1.3103	10
204	------	---	------	---	------	---	1.2977	4
313	------	---	1.278	60	------	---	1.2840	13
400	------	---	(b)	---	------	---	1.2766	4

[a] Probably beta line for 111.
[b] Twelve additional lines have been omitted.

2.9. Nitrates

Potassium nitrate (niter), KNO_3 (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
1188	1132	3.77	Molybdenum__	Hanawalt, Rinn, and Frevel [1] 1938.
	1-0497	3.03		
	1-0493	2.66		

The two additional patterns, one by Barth and the other by Finbak and Hassel, were made at 115°C and represent high temperature forms.

II-2104	2910	2.60	Copper_____	Barth [2] 1939.
	2-0982	1.81		
	2-0991	2.15		
_____	1650	3.25	Copper_____	Finbak and Hassel [3] 1937.
	3-0474	2.73		
	3-0482	2.08		

Additional published patterns

Source	Radiation	Wavelength
Edwards [4] 1931__	Molybdenum_____	_____

NBS sample. The potassium nitrate used for the NBS pattern was obtained from the Mallinckrodt Chemical Works. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent sodium; 0.001 to 0.01 percent each of aluminum, calcium, and iron; 0.0001 to 0.001 percent each of barium, magnesium, lead and silicon; and less than 0.0001 percent of copper. The refractive indices of the NBS sample are as follows: α is too low for the usual liquids (1.335), $\beta = 1.505$, and $\gamma = 1.509$.

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

The Edwards pattern contains no powder intensity data, although Edwards did extensive single crystal work on potassium nitrate.

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

Patterns	1	2	3
Hanawalt, Rinn, and Frevel_____	111	012	130
Swanson and Fuyat_____	111	021	012

The literature reference for Edwards' pattern lists some indices which are not in complete agreement with those assigned to the corresponding d-spacings of the NBS pattern.

Lattice constants. The structure was determined by Zachariasen [5] in 1928. The space group is D_{2h}^{16}-Pmcn (Pnma) with $4(KNO_3)$ per unit cell. Orthorhombic potassium nitrate is a prototype for other similar structures. This form designated KNO_3II is reported to change at 127.7°C to KNO_3I, a rhombohedral form, and on cooling below 125°C to another rhombohedral form, KNO_3III, all according to Kracek, Barth, and Ksanda [6]. The two patterns in the card file made at 115°C by Barth [2] and by Finbak and Hassel [3] do not agree with either of the high temperature forms described by Kracek, Barth, and Ksanda.

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

Lattice constants in angstroms

		a	b	c
1928	Zachariasen [5]_____	5.41	9.16	6.42
1931	Edwards [4]_____	5.44	9.19	6.46
1953	Swanson and Fuyat_____	5.414	9.164	6.431 at 26°C

The density of potassium nitrate calculated from the NBS lattice constants is 2.104 at 26°C.

Potassium nitrate, KNO_3 (orthorhombic)

hkl	1931 Edwards Mo, 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I
	A		A		A	
110	4.70	------	4.67	12	4.66	23
020	------	------	-------	-------	4.58	11
111	3.78	------	3.78	100	3.78	100
021	------	------	-------	-------	3.73	56
002	------	------	-------	-------	3.215	5
121	------	------	-------	-------	3.070	15
012	3.04	------	3.04	36	3.033	55
102	2.78	------	2.78	8	2.763	28
200	------	------	-------	-------	2.707	17
130	------	------	2.67	28	2.662	41
112	2.654	------	-------	-------	2.647	55
022	------	------	-------	-------	2.632	20
211	2.419	------	-------	-------	2.409	7
122	------	------	-------	-------	2.367	4
220	2.339	------	-------	-------	2.332	9
040	------	------	-------	-------	2.292	5
221	2.199	------	2.19	24	2.192	41
041	------	------	-------	-------	2.159	20
202	------	------	-------	-------	2.071	13
132	2.063	------	2.06	8	2.050	18
113	1.941	------	1.96	12	1.947	24
023	------	------	-------	-------	1.942	6
222	------	------	-------	-------	1.888	3
042	------	------	-------	-------	1.866	2
142	------	------	-------	-------	1.763	6
240	------	------	1.76	4	1.750	2
150	------	------	-------	-------	1.733	1
311	------	------	-------	-------	1.707	4
241	1.685	------	-------	-------	1.688	6
151	------	------	-------	-------	1.677	4
321	1.626	------	-------	-------	1.624	3
014	------	------	-------	-------	1.585	3
312	1.557	------	-------	-------	1.552	2
242	------	------	1.54	4	1.536	2
114, 024	1.519	------	-------	-------	1.519	6

Potassium nitrate, KNO_3 (orthorhombic)—Con.

hkl	1931 Edwards Mo, 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I
	A		A		A	
124	------	------	-------	-------	1.461	1
332	------	------	-------	-------	1.399	5
204	------	------	-------	-------	1.381	5
134	------	------	-------	-------	1.376	2
214, 313	------	------	1.368	4	1.365	4
243, 400	------	------	-------	-------	1.354	8
153	------	------	-------	-------	1.350	8
260	------	------	-------	-------	1.330	4

References

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

[2] F. T. W. Barth, Die Kristallstruktur der Druckmodifikation des Saltpeters, Z. physik. Chem. **B43**, 448-450 (1939).

[3] C. Finbak and O. Hassel, Kristallchemie der Nitrate einwertiger Kationen II, Z. physik. Chem. **B37**, 75-80 (1937))

[4] D. A. Edwards, A determination of the complete crystal structure of potassium nitrate, Z. Krist. **80**, 154-163 (1931).

[5] W. H. Zachariasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO_3, Skrifter Norske Videnskaps-Akad. Oslo, I. Mat. Naturv. Kl. **10**, 14 (1928).

[6] F. C. Kracek, F. T. W. Barth, and C. J. Ksanda, Molecular rotation in the solid state and the polymorphic relation of the univalent nitrates, Phys. Rev. **40**, 1034 (1932).

2.10. Sulfates and Sulfites

Sodium sulfite, Na_2SO_3 (hexagonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
----	1138	3.77	Molybdenum-----	Zachariasen and Buckley [1] 1931.
	3-0311	2.72		
	3-0305	2.58		
2565	2695	2.72	Molybdenum-----	Hanawalt, Rinn, and Frevel [2] 1938.
	1-1040	2.57		
	1-1039	1.87		

The Zachariasen pattern found in the ASTM file is a combination of single-crystal *d*-spacings and powder-intensity data.

Additional published patterns. None.

NBS sample. The sodium sulfite used to make the NBS pattern was an analytical reagent grade sample prepared by the Mallinckrodt Chemical Works. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of calcium; 0.001 to 0.01 percent each of aluminum, iron, molybdenum, and strontium; 0.0001 to 0.001 percent each of barium, magnesium, lead, and silicon; and less than 0.0001 percent of copper. The sample used for the NBS pattern is optically negative with the following refractive indices: $\omega = 1.568$ and $\epsilon = 1.517$.

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

The *d*-spacings of the Zachariasen and Buckley single-crystal pattern of nil intensity have been omitted from the table, but many points, which combined would make a single powder diffraction line or which would be invisible, still remain.

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

Patterns	1	2	3
Zachariasen and Buckley----------	101	110	102
Hanawalt, Rinn, and Frevel--------	110	102	202
Swanson and Fuyat----------	102	110	101

Lattice constants. The structure was determined by Zachariasen and Buckley [1] in 1931. The space group is C_{3i}^1-$P\bar{3}$ with $2(Na_2SO_3)$ per unit cell.

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

Lattice constants in angstroms

		a	*c*
1931	Zachariasen and Buckley [1]----	5.452	6.145
1953	Swanson and Fuyat----------	5.459	6.160 at 25°C

The density of sodium sulfite calculated from the NBS lattice constants is 2.633 at 25°C.

Sodium sulfite, Na_2SO_3 (hexagonal)

hkl	1931 Zachariasen and Buckley Mo, 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
100	4.72	vw	4.72	3	4.73	5
101	3.741	vs	3.73	67	3.75	60
002	3.072	m	3.08	27	3.078	55
110	2.724	vs	2.73	100	2.728	78
102	2.574	vs	2.58	100	2.580	100
111	2.489	m	2.49	20	2.495	11
200	2.361	w	2.35	11	2.364	4
201	2.204	m	2.20	20	2.207	9
003	2.048	vw	------	-------	--------	--------
112	2.038		2.02	3	2.043	2
103	1.879	s-vs	------	-------	1.883	<1
202	1.870		1.87	100	1.876	34
210	1.783	mw	1.78	11	1.788	3
211	1.713	vvw	1.71	1	1.714	1
113	1.637	w	1.63	3	1.641	2
300	1.573	ms	1.57	40	1.576	12
203	1.546	s	------	-------	--------	--------
212	1.543		1.54	53	1.546	16
004	1.536		------	-------	1.540	1
104	1.461	m	1.463	17	1.465	15
220	1.362	ms	1.363	27	1.365	6
114	1.338	vvvw	-------	-------	1.342	1
310	1.309	vw	-------	-------	1.311	<1
204	1.287	m	1.285	13	1.291	8
311	1.280				1.283	2
303	1.248	vvw	1.248	1	1.250	1
222	1.246					
132	1.204	ms	1.203	20	1.207	11
214	1.164	m	1.163	20	1.1668	13
401	1.159				-------	--------

Sodium sulfite, Na_2SO_3 (hexagonal)—Con.

hkl	1931 Zachariasen and Buckley Mo, 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
313	1.103		------	-------	--------	--------
402	1.102	m	1.102	8	1.1033	4
304	1.099		------	-------	1.0926	1
321	1.067	vvw	-------	-------	1.0683	2
410	1.030		1.032	8	1.0315	4
006	1.024		------	-------	--------	--------
403	1.022		------	-------	--------	--------
322	1.021	ms	1.023	13	1.0232	4
224	1.019		------	-------	--------	--------
411	1.016		------	-------	--------	--------
215	-----	-------	-------	-------	1.0145	< 1
314	-----	-------	.998	5	.9983	2
116	-----	-------	.962	7	.9605	3
404	-----	-------	-------	-------	.9374	< 1
330						
331	-----	-------	-------	-------	.9038	< 1
306	-----	-------	-------	-------	.8600	2
422	-----	-------	-------	-------	.8580	3
226	-----	-------	-------	-------	.8206	2
512	-----	-------	-------	-------	.8186	2
504	-----	-------	-------	-------	.8058	1

References

[1] W. H. Zachariasen and H. E. Buckley, The crystal lattice of anhydrous sodium sulfite, Na_2SO_3, Phys. Rev. **37**, 1295 (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).

Potassium sulfate (arcanite), K_2SO_4 (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2298	2417	2.89	Molybdenum, 0.712.	Goeder [1] 1928.
	1-0954	3.01		
	1-0939	2.08		
2308	2418	2.88	Molybdenum--	Hanawalt, Rinn, and Frevel [2] 1938.
	1-0955	3.00		
	1-0944	2.08		
11-1343	2077	3.02	Copper, Kα, 1.539.	Goubeau, Kolb, and Krall [3] 1938.
	2-0628	2.91		
	2-0626	2.10		
-------	2078	3.01	----------	Bredig [4] 1942.
	3-0599	2.90		
	3-0608	2.23		
-------	2420	2.88	Copper, Kα--	O'Daniel and Tscheischwili [5] 1942.
	3-0695	2.99		
	3-0695	2.07		

Additional published patterns. None.

NBS sample. The potassium sulfate used for the NBS pattern was contributed by the Mallinckrodt Chemical Works. Spectrographic analysis at the NBS showed the following impurities: 0.01 to 0.1 percent of sodium; 0.001 to 0.01 percent of calcium; 0.0001 to 0.001 percent each of aluminum, magnesium, and silicon; and less than 0.0001 percent each of silver, barium, copper, and iron. The refractive indices of the NBS sample are as follows: $\alpha = 1.493$, $\beta = 1.495$, and $\gamma = 1.498$, with 2V of 70° and positive optical sign.

Interplanar spacings and intensity measurements. The *d*-spacings for the Goeder, the Goubeau, Kolb, and Krall, and the O'Daniel and Tscheischwili patterns were calculated from Bragg angle data, whereas those for the Hanawalt, Rinn, and Frevel and the Bredig patterns were converted from kX to angstrom units.

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

Patterns	1	2	3
Goeder	130	022-112	042
Hanawalt, Rinn, and Frevel	130	022-112	042
Goubeau, Kolb, and Krall	022-112	130	042
Bredig	022-112	130	113-212
O'Daniel and Tscheischwili	130	022-112	032
Swanson and Fuyat	130	022-112	200

Lattice constants. The structure was determined by Ehrenberg and Hermann [6] in 1929. The space group is D_{2h}^{16}-Pmcn (Pnma) with $4(K_2SO_4)$ per unit cell. Potassium sulfate is a prototype for other similar structures.

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

Lattice constants in angstroms

		a	*b*	*c*
1916	Ogg and Hopwood [7]	5.743	10.028	7.439
1927	Koch-Holm and Schönfeldt [8]	5.29	10.27	7.52
1928	Gossner [9]	5.86	10.08	7.34
1928	Goeder [1]	5.783	10.084	7.533
1938	Goubeau, Kolb, and Krall [3]	5.83	10.05	7.43
1942	Bredig [4]	5.77	10.07	7.48
1953	Swanson and Fuyat	5.772	10.072	7.483 at 25°C

The density of potassium sulfate calculated from the NBS lattice constants is 2.660 at 25°C.

(See table on next page)

Potassium sulfate, K_2SO_4 (orthorhombic)

hkl	1928 Goeder Mo, 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1938 Goubeau, Kolb, and Krall Cu, 1.5405 A		1942 Bredig ----------		1942 O'Daniel and Tscheischwili Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*	
020	--------	--------	5.0	2	--------	--------	-------	-----	--------	--------	5.03	8
021	4.19	30	4.20	24	--------	--------	4.19	m	4.12	w	4.176	28
111	--------	--------	--------	--------	4.23	w	-------	-----	--------	--------	4.160	23
002	3.76	25	3.74	8	3.86	vw	3.76	vw	3.68	w	3.743	18
012	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	3.508	6
121	--------	--------	3.39	5	3.351	vw	-------	-----	3.371	vw	3.384	13
102	--------	--------	--------	--------	--------	--------	-------	-----	3.095	vvw	3.140	9
031	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	3.062	8
022 / 112	3.00	90	3.01	80	3.028	s	3.02	vs	2.983	ms	3.001	77
130	2.883	100	2.88	100	2.921	s	2.91	vs	2.871	s	2.903	100
200	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	2.886	53
122	2.676	5	2.67	2	--------	--------	-------	-----	2.682	vvw	2.665	7
211	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	2.602	2
040	2.513	30	2.51	12	2.522	m	2.520	m	--------	--------	2.518	13
032	--------	--------	--------	--------	--------	--------	-------	-----	2.491	ms	2.499	15
013	2.424	40	2.41	20	2.455	m	2.426	m	2.413	m	2.422	25
041	--------	--------	--------	--------	--------	--------	2.389	w	--------	--------	2.386	13
221	--------	--------	--------	--------	--------	--------	-------	-----	2.370	w	2.374	17
113 / 212	2.223	40	--------	--------	2.254	m	2.230	s	2.273	vvw	2.230	19
141	--------	--------	2.21	24	--------	--------	-------	-----	2.201	m	2.206	14
231	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	2.101	6
042	2.081	50	2.08	40	2.104	s	2.087	s	2.072	ms	2.089	25
222	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	2.082	25
033	2.022	5	2.00	5	2.015	w	-------	-----	1.994	w	2.002	7
142	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	1.964	4
051	1.950	5	1.94	4	1.956	w	-------	-----	1.933	vw	1.945	7
232	--------	--------	1.88	10	--------	--------	-------	-----	--------	--------	1.889	12
004	--------	--------	--------	--------	1.873	m	-------	-----	1.874	mw	1.870	8
213	1.835	30	1.85	4	--------	--------	-------	-----	1.841	w	1.855	6
052	1.765	15	1.76	3	--------	--------	-------	-----	1.771	vw	1.774	5
114	--------	--------	--------	--------	--------	--------	-------	-----	1.743	vw	1.752	4
302	--------	--------	--------	--------	1.715	m	-------	-----	--------	--------	1.711	5
143	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	1.694	9
124	1.681	30	1.68	10	--------	--------	-------	-----	1.679	mw	1.679	5
330	--------	--------	--------	--------	1.669	w	-------	-----	1.662	mw	1.669	8
034	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	1.634	4
331	--------	--------	--------	--------	--------	--------	-------	-----	1.627	vw	1.629	3
251	1.619	20	1.62	4	--------	--------	-------	-----	1.613	vw	1.613	4
134	--------	--------	1.57	6	1.590	m	-------	-----	1.567	m	1.5715	7
214	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	1.5508	1
062	1.528	25	--------	--------	--------	--------	-------	-----	--------	--------	1.5312	1
252	1.508	5	--------	--------	--------	--------	-------	-----	--------	--------	1.5105	1
341	1.493	5	--------	--------	1.494	vw	-------	-----	--------	--------	1.4977	2
015	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	1.4807	2
260	--------	--------	--------	--------	--------	--------	-------	-----	--------	--------	1.4513	5
400	1.441	30	1.442	10	--------	--------	-------	-----	--------	--------	1.4427	8
025 / 115	--------	--------	--------	--------	1.435	m	-------	-----	--------	--------	1.4332	9
234	--------	--------	1.421	3	--------	--------	-------	-----	--------	--------	1.4219	10

Potassium sulfate, K_2SO_4 (orthorhombic)—Con.

hkl	1928 Goeder Mo, 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1938 Goubeau, Kolb, and Krall Cu, 1.5405 A		1942 Bredig		1942 O'Daniel and Tscheischwili Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	I	d	I	d	I	d	I	d	I	d	I
	A		A		A		A	A	A		A	
071	--------	--------	--------	--------	1.411	w	-------	-----	--------	--------	1.4129	12
170	1.398	5	1.394	3	--------	--------	-------	-----	--------	--------	1.3966	4
054	--------	--------	--------	--------	1.371	m	-------	-----	--------	--------	1.3707	2
163	--------	--------	1.352	6	--------	--------	-------	-----	--------	--------	1.3534	7
----	[a]	--------	[b]	--------	[c]	--------	-------	-----	--------	--------	--------	--------

[a] Thirteen additional lines omitted.
[b] Twelve additional lines omitted.
[c] Twenty-five additional lines omitted.

References

[1] F. P. Goeder, The crystal structure of potassium sulfate, Proc. Nat. Acad. Sci. U. S. **14**, 766-771 (1928).

[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. Goubeau, H. Kolb, and H. G. Krall, Das System Kaliumsulfat-Kaliumsulfid, Z. anorg. Chem. **236**, 45-56 (1938).

[4] M. A. Bredig, Isomorphism and allotropy in compounds of the type A_2XO_4, J. Phys. Chem. **46**, 750-764 (1942).

[5] H. O'Daniel and L. Tscheischwili, Zur Struktur von K_2BeF_4, Sr_2SiO_4 und Ba_2SiO_4, Z. Krist. **104**, 348-357 (1942).

[6] W. Ehrenberg and C. Hermann, Die Raumgruppe von Kaliumsulfat, Z. Krist. **70**, 163-170 (1929).

[7] A. Ogg and F. Hopwood, A critical test of the crystallographic law of valency volumes, a note on the crystalline structure of the alkali sulphates, Phil. Mag. **32**, 518-525 (1916).

[8] E. Koch-Holm and N. Schönfeldt, Raumgitteranalyse von Kaliumsulfat and Kaliumselenat, Wiss. Veröffentl. Siemens-Konzern **6**, 177-187 (1927).

[9] B. Gossner, Über die Kristallstruktur von Glaserite und Kaliumsulfat, Neues Jahrb. Mineral. B.-Bd. **57A**, 89-116 (1928).

Barium sulfate (barite), $BaSO_4$ (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
3277	3377	2.10	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
	1-1224	3.44		
	1-1229	3.10		
II-2765	3378	2.11	Copper	British Museum.
	2-1183	3.42		
	2-1199	3.08		

Additional published patterns. None.

NBS sample. The material used for the NBS pattern was prepared by the Mallinckrodt Chemical Works. Their spectrographic analysis shows 0.001 to 0.01 percent of iron, 0.0001 to 0.001 percent each of aluminum and strontium and less than 0.0001 percent each of calcium, copper and magnesium. The NBS sample is too finely divided for determination of the refractive indices.

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

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

Patterns	1	2	3
Hanawalt, Rinn, and Frevel	113,312	210	211
British Museum	113,312	210	211
Swanson and Fuyat	210	211	113

Lattice constants. The structure was determined by Rinne, Hentschel, and Schiebold [2] in 1924. The space group is D_{2h}^{16}-Pnma with $4(BaSO_4)$ per unit cell.

A group of unit cell values were converted to angstroms for comparison with the NBS values. The Allison value for the *a*-direction was multiplied by two.

Lattice constants in angstroms

		a	*b*	*c*
1924	Allison [3]	8.916	5.459	7.18
1924	Rinne, Hentschel, and Schiebold [2]	8.90	5.46	7.16
1925	Pauling and Emmett [4]	8.864	5.441	7.11
1925	James and Wood [5]	8.87	5.44	7.14
1925	Wyckoff and Merwin [6]	8.916	5.459	7.18
1926	Basche and Mark [7]	8.87	5.46	7.15
1946	Walton and Walden [8]	8.8701	5.4534	7.1507
1953	Swanson and Fuyat	8.878	5.450	7.152 at 26°C

The density of barium sulfate calculated from the NBS lattice constants is 4.480 at 26°C.

Barium sulfate (barite), $BaSO_4$ (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		---- British Museum Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
200	-------	-------	------	------	4.44	17
011	4.36	20	4.28	40	4.34	36
111	3.90	25	3.83	40	3.90	57
201	-------	-------	------	------	3.77	12
002	3.58	10	3.56	40	3.576	31
210	3.45	63	3.43	80	3.442	100
102	3.32	35	3.31	60	3.317	67
211	3.11	63	3.09	80	3.101	97
112	2.84	40	2.85	50	2.834	53
301	2.73	45	2.73	50	2.734	16
020					2.726	47
212	2.47	15	2.47	20	2.481	14
311	-------	-------	------	------	2.444	2
220	2.31	10	2.33	60	2.322	15
103	-------	-------	------	------	2.303	6
302	-------	-------	2.28	20	2.281	7
221	2.20	15	2.21	40	2.209	27
113	2.10	100	2.11	100	2.120	80
312					2.104	76
410	2.04	10	2.06	40	2.056	23
222	-------	-------	------	------	1.947	<1
321	1.92	5	1.93	20	1.930	7
303	1.85	15	1.86	50	1.857	16
004	-------	-------	------	------	1.787	3
031	-------	-------	------	------	1.760	9
313	1.74	8	1.75	40	1.754	9
131	-------	-------	------	------	1.726	5
501	-------	-------	------	------	1.723	6

Barium sulfate (barite), $BaSO_4$ (orthorhombic)—Con.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		---- British Museum Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I
	A		A		A	
230	-------	-------	1.68	50	1.681	7
421	1.67	15	------	------	1.673	14
114	-------	-------	------	------	1.669	10
231	1.63	8	1.64	40	1.636	8
132	-------	-------	1.594	40	1.593	8
502	1.58	10	------	------	1.590	7
323	-------	-------	1.537	60	1.534	18
512	1.52	25	------	------	1.526	11
024	-------	-------	------	------	1.495	3
124	1.468	7	1.483	40	1.474	10
521	-------	-------	------	------	1.457	3
610 133	------	-------	1.429	60	1.426	8
503	1.423	20	------	------	1.424	16
332	-------	-------	------	------	1.421	13
430	-------	-------	1.406	50	1.406	7
611	-------	-------	------	------	1.401	10
015	-------	-------	1.384	40	1.384	6
431 513	------	-------	------	------	1.378	5
040	-------	-------	1.360	40	1.363	6
414	-------	-------	------	------	1.349	5
215	-------	-------	1.324	40	1.321	6
240 620	------	-------	1.308	40	1.300	5
523 134	------	-------	1.268	60	1.262	13
142 504	1.258	18	------	------	1.260	10
---	-------	-------	1.222	50	--------	--------
---	1.192	8	1.202	50	--------	--------
---	1.095	13	------	------	--------	--------
---	1.028	5	------	------	--------	--------

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. Rinne, H. Hentschel, and E. Schiebold, Zum Feinbau von Anhydrit und Schwerspat, Z. Krist. **61**, 164-176 (1924).

[3] S. K. Allison, The reflection of X-rays by barite, Am. J. Sci. **8**, 261-276 (1924).

[4] L. Pauling and P. H. Emmett, The crystal structure of barite, J. Am. Chem. Soc. **47**, 1026-1030 (1925).

[5] R. W. James and W. A. Wood, The crystal structure of baryte, celestine and anglesite, Proc. Roy. Soc. (London) **A109**, 598-620 (1925).

[6] R. W. G. Wyckoff and H. E. Merwin, The space group of barite ($BaSO_4$), Am. J. Sci. **9**, 286-295 (1925).

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

[8] G. Walton and G. H. Walden, Jr., The nature of the variable hydration of precipitated barium sulfate, J. Am. Chem. Soc. **68**, 1750-1753 (1946).

Lead sulfate (anglesite), $PbSO_4$ (orthorhombic)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
2117	2119	3.00	Molybdenum_____	Hanawalt, Rinn, and Frevel [1] 1938.
	1-0862	2.06		
	1-0867	4.26		
----	3457	2.07	Copper_____	British Museum.
	3-1006	3.00		
	3-1019	4.22		
----	3458	-----	----------	A continuation of the preceding card.
	3-1007			
	3-1020			

Additional published patterns. None.

NBS sample. The lead sulfate sample used for the NBS pattern was prepared by the National Lead Co. Spectrographic analysis at the NBS showed 0.001 to 0.01 percent each of bismuth, iron, and silicon, 0.0001 to 0.001 percent each of silver, aluminum, copper, and magnesium and less than 0.0001 percent of calcium. The refractive indices are too high to be determined by grain-oil immersion methods.

Interplanar spacings and intensity measurements. The Hanawalt and British Museum *d*-spacings were converted from kX to angstrom units. The *d*-spacing 4.69 of the British Museum pattern is not possible according to the space group.

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

Patterns	1	2	3
Hanawalt, Rinn, and Frevel_____	211	122,113	011
British Museum_____	122,113	211	011
Swanson and Fuyat_____	211	011	210

Lattice constants. The structure was determined by James and Wood [2] in 1925. The space group is D_{2h}^{16}-Pnma with 4($PbSO_4$) per unit cell.

Data for two unit cells were converted to angstrom units for comparison with the NBS values.

Lattice constants in angstroms

		a	*b*	*c*
1925	James and Wood [2]_____	8.27	5.39	6.94
1926	Basche and Mark [3]_____	8.48	5.39	6.96
1953	Swanson and Fuyat_____	8.480	5.398	6.958 at 25°C

The density of lead sulfate calculated from the NBS lattice constants is 6.323 at 25°C.

Lead sulfate (anglesite), $PbSO_4$ (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		---- British Museum Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
101	-------	-------	------	------	5.381	3
---	-------	-------	4.69	25	--------	--------
011	4.27	80	4.23	75	4.26	87
111	3.81	28	3.79	25	3.813	57
201	3.62	8	------	------	3.622	23
002	3.48	8	------	------	3.479	33
210	3.34	60	3.35	75	3.333	86
102	3.22	40	3.21	50	3.220	71
211	3.01	100	3.01	85	3.001	100
112	2.76	32	2.77	25	2.773	35
020	2.69	32	2.70	50	2.699	46
301	-------	-------	------	------	2.618	8
212	2.40	12	2.41	50	2.406	17
311	-------	-------	------	------	2.355	<1
220	2.27	12	2.29	50d	2.276	20
103	-------	-------	------	------	2.235	5
302	-------	-------	------	------	2.193	7
221	2.16	16	2.16	50	2.164	26
022	-------	-------	------	------	2.133	5
122, 113	2.06	100	2.07	100	2.067	76
312	-------	-------	------	------	2.031	34
401	2.02	40	2.01	75	2.028	48
410	1.97	20	1.98	50	1.973	21
222	1.90	4	------	------	1.905	3
321	1.87	4	1.88	25	1.879	6
303	1.78	12	1.79	50	1.793	15
031, 004	1.73	6	1.75	25	1.741	8
412	-------	-------	------	------	1.716	3
322	1.70	12	1.70	50	1.703	16
230	-------	-------	------	------	1.656	7
501	1.65	4	1.65	25	1.648	3
421	-------	-------	1.62	50	1.621	19
231	1.61	20	------	------	1.611	10
132	1.57	4	------	------	1.571	6
214	-------	-------	------	------	1.542	2
502	-------	-------	------	------	1.525	1

Lead sulfate (anglesite), $PbSO_4$ (orthorhombic)—Con.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		---- British Museum Cu, 1.5405 A		1953 Swanson and Fuyat Cu, 1.5405 A, 25°C	
	d	I	d	I	d	I
	A		A		A	
323	1.493	16	1.49	50	1.493	15
512	-------	-------	1.47	25	1.467	7
124	-------	-------	------	------	1.441	8
314	-------	-------	1.43	25	1.429	4
521	-------	-------	------	------	1.406	3
133	-------	-------	1.40	25	1.402	7
332	-------	-------	------	------	1.391	4
601	-------	-------	------	------	1.385	2
105 503	-------	-------	1.37	50	1.371	6
610	-------	-------	------	------	1.368	7
233	-------	-------	1.35	50	1.348	4
611	-------	-------	------	------	1.341	5
---	-------	-------	(a)	------	--------	--------

[a] This pattern contains thirteen additional 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] R. W. James and W. A. Wood, The crystal structure of barytes, celestine and anglesite, Proc. Roy. Soc. (London) **109A**, 598-620 (1925).

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

2.11. Phosphates

Potassium dihydrogen phosphate, KH_2PO_4 (tetragonal)

ASTM cards

Card number		New index lines	Radiation	Source
Old	New			
II-2022	2812 2-0932 2-0948	2.65 1.96 3.76	Molybdenum, 0.7076.	Hendricks [1] 1927.
2669	2813 1-1062 1-1072	-----	----------	This card is the same source and pattern as the card above.
1229	1135 1-0499 1-0505	3.72 2.90 1.95	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.

The second set of Hendricks cards as listed above gives the same pattern but with the lattice constants in their proper order (on the original card c was larger than a).

Additional published patterns

Source	Radiation	Wavelength
West [3] 1930-----	Rhodium----------	----------

NBS sample. The monobasic potassium phosphate used for the NBS pattern was reagent grade material prepared by the Mallinckrodt Chemical Works. Spectrographic analysis at the NBS showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium and iron; 0.0001 to 0.001 percent each of barium, magnesium, lead, silicon, and strontium; and less than 0.0001 percent of copper. The NBS sample is uniaxial negative with $\omega = 1.511$ and $\epsilon = 1.468$.

Interplanar spacings and intensity measurements. The Hanawalt, Rinn, and Frevel Bragg angle data were converted into d-spacings in angstroms. The Hendricks d-spacings were converted from kX to angstrom units.

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

Patterns	1	2	3
Hendricks----------	220	231,132	200
Hanawalt, Rinn, and Frevel-------	200	112	231,132
Swanson and Fuyat----------	200	112	132

Lattice constants. The structure was determined by West [3] in 1930. The space group is D_{2d}^{12}-$I\bar{4}2d$ with $4(KH_2PO_4)$ per unit cell.

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

Lattice constants in angstroms

		a	c
1930	West [3]----------	7.45	6.98
1947	Ubbelohde and Woodward [4]-----	7.452	6.959 at 20°C
1953	Swanson and Fuyat----------	7.448	6.977 at 26°C

The density of potassium dihydrogen phosphate calculated from the NBS lattice constants is 2.335 at 26°C.

Potassium dihydrogen phosphate, KH_2PO_4 (tetragonal)

hkl	1927 Hendricks Mo. 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I
	A		A		A	
101	5.142	5	5.1	10	5.10	22
200	3.763	80	3.73	100	3.726	100
121	------	------	3.01	8	3.008	12
112	------	------	2.91	100	2.910	75
220	2.650	100B	2.64	16	2.636	23
202	------	------	2.54	6	2.547	10
130	2.358	10	2.34	12	2.356	5
301					2.341	10
103	2.212	10	2.22	3	2.220	5
231	1.966	90B	1.95	40	1.982	9
132					1.953	37
213	------	------	1.90	2	1.907	4
400	------	------	-------	-------	1.863	2
141	------	------	-------	-------	1.750	1
303	------	------	-------	-------	1.698	<1
240	1.672	15	1.66	6	1.667	8

Potassium dihydrogen phosphate, KH_2PO_4 (tetragonal)—Con.

hkl	1927 Hendricks Mo, 0.709 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Fuyat Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I
	A		A		A	
204	1.576	40	1.57	8	1.580	7
332					1.569	7
233	------	------	-------	-------	1.545	<1
242	------	------	-------	-------	1.504	<1
224	1.456	1[illegible]	1.453	4	1.454	5
152	1.351	20	1.348	6	1.348	8
440	1.316	>1	1.321	2	1.318	3
404	1.273	15	1.273	4	1.273	7
600	------	------	-------	-------	1.242	1
244	1.205	30	1.202	6	1.205	5
352	------	------	-------	-------	1.1998	2
260	1.179	------	1.177	2	1.1785	2
602	------	------	-------	-------	1.1702	1
116	1.136	------	-------	-------	1.1348	1
361	------	------	1.010	2	1.0966	<1
136	1.043	------	-------	-------	1.0424	2
460	------	------	-------	-------	1.0333	<1
552	1.009	------	-------	-------	1.0087	3
264	------	------	-------	-------	.9763	<1
732	------	------	-------	-------	.9422	<1

References

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

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

[3] J. West, A quantitative X-ray analysis of the structure of potassium dihydrogen phosphate, Z. Krist. **74**, 306-332 (1930).

[4] A. R. Ubbelohde and I. Woodward, Structure and thermal properties associated with some hydrogen bonds in crystals, Proc. Roy. Soc. (London) **A188**, 358-371 (1947).

2.12. Bromoösmates

Ammonium bromoösmate, $(NH_4)_2OsBr_6$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The ammonium bromoösmate used for the NBS sample was prepared by R. B. Johannesen at the NBS. Spectrographic analysis at the Bureau showed the following impurities: 0.01 to 0.1 percent of silicon, 0.001 to 0.01 percent of magnesium, and 0.0001 to 0.001 percent each of copper and iron. The refractive indices of the NBS sample could not be determined as the sample was opaque.

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

Patterns	1	2	3
Swanson and Fuyat	200	111	400

Lattice constants. No X-ray data appears to have been published for ammonium bromoösmate. From related compounds such as ammonium chloroplatinate the material was found to be face-centered cubic with a lattice constant of approximately 10 angstroms. The structure is cubic face-centered with $4[(NH_4)_2OsBr_6]$ per unit cell and probably space group O_h^5-Fm3m.

Lattice constant in angstroms

1953	Swanson and Fuyat	10.398 at 25°C

The density of ammonium bromoösmate calculated from the NBS lattice constant is 4.169 at 25°C.

Ammonium bromoösmate, $(NH_4)_2OsBr_6$ (cubic)

hkl	1953 Swanson and Fuyat Cu, 1.5405 A, 25°C		
	d	*I*	*a*
	A		*A*
111	6.0	97	10.4
200	5.20	100	10.40
220	3.68	5	10.41
311	3.135	40	10.398
222	3.002	55	10.399
400	2.600	83	10,400
331	2.385	12	10.396
420	2.325	51	10.398
422	2.121	<1	10.391
511	2.001	20	10.398
440	1.838	49	10.397
531	1.756	20	10.389
600	1.733	23	10.398
533	1.585	5	10.394
622	1.567	8	10.394
444	1.501	12	10.399
711	1.456	10	10.398
640	1.443	8	10.406
642	1.389	<1	10.394
731	1.353	5	10.393
800	1.300	4	10.400
733	1.270	1	10.395
820	1.261	8	10.398
751	1.201	3	10.401
662	1.1927	3	10.398
840	1.1628	8	10.400
911	1.1414	3	10.399
842	1.1343	4	10.396
931	1.0900	3	10.398
844	1.0611	5	10.397
933	1.0455	<1	10.403
10·0·0	1.0397	<1	10.397
951	1.0048	2	10.394
Average of last five lines			10.398

References. None.

3. CUMULATIVE INDEX TO VOLUMES I, II, AND III

☆ U. S. GOVERNMENT PRINTING OFFICE : 1954 O - 298034

PERIODICALS OF THE NATIONAL BUREAU OF STANDARDS

The National Bureau of Standards is engaged in fundamental and applied research in physics, chemistry, mathematics, and engineering. Projects are conducted in thirteen fields: electricity, optics and metrology, heat and power, atomic and radiation physics, chemistry, mechanics, organic and fibrous materials, metallurgy, mineral products, building technology, applied mathematics, electronics, and radio propagation. The Bureau has custody of the national standards of measurement and conducts research leading to the improvement of scientific and engineering standards and of techniques and methods of measurement. Testing methods and instruments are developed; physical constants and properties of materials are determined; and technical processes are investigated.

JOURNAL OF RESEARCH

The Journal presents research papers by authorities in the specialized fields of physics, mathematics, chemistry, and engineering. Complete details of the work are presented, including laboratory data, experimental procedures, and theoretical and mathematical analyses. Annual subscription: domestic, $5.50; foreign, $6.75.

TECHNICAL NEWS BULLETIN

Summaries of current research at the National Bureau of Standards are published each month in the Technical News Bulletin. The articles are brief, with emphasis on the results of research, chosen on the basis of their scientific or technologic importance. Lists of all Bureau publications during the preceding month are given, including Research Papers, Handbooks, Applied Mathematics Series, Building Materials and Structures Reports, Miscellaneous Publications, and Circulars. Each issue contains 12 or more two-column pages; illustrated. Annual subscription: domestic, $1.00; foreign, $1.35.

BASIC RADIO PROPAGATION PREDICTIONS

The Predictions provide the information necessary for calculating the best frequencies for communication between any two points in the world at any time during the given month. The data are important to all users of long-range radio communications and navigation, including broadcasting, airline, steamship, and wireless services, as well as to investigators of radio propagation and ionosphere. Each issue, covering a period of one month, is released three months in advance and contains 16 large pages, including pertinent charts, drawings, and tables. Annual subscription: domestic, $1.00; foreign, $1.25.

Order all publications from the Superintendent of Documents
U. S. Government Printing Office, Washington 25, D. C.


DEPARTMENT OF COMMERCE
UNITED STATES OF AMERICA