NBS CIRCULAR 539
VOLUME 9

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

THE NATIONAL BUREAU OF STANDARDS

Functions and Activities

The functions of the National Bureau of Standards are set forth in the Act of Congress, March 3, 1901, as amended by Congress in Public Law 619, 1950. These include the development and maintenance of the national standards of measurement and the provision of means and methods for making measurements consistent with these standards; the determination of physical constants and properties of materials; the development of methods and instruments for testing materials, devices, and structures; advisory services to government agencies on scientific and technical problems; invention and development of devices to serve special needs of the Government; and the development of standard practices, codes, and specifications. The work includes basic and applied research, development, engineering, instrumentation, testing, evaluation, calibration services, and various consultation and information services. Research projects are also performed for other government agencies when the work relates to and supplements the basic program of the Bureau or when the Bureau's unique competence is required. The scope of activities is suggested by the listing of divisions and sections on the inside of the back cover.

Publications

The results of the Bureau's work take the form of either actual equipment and devices or published papers. These papers appear either in the Bureau's own series of publications or in the journals of professional and scientific societies. The Bureau itself publishes three periodicals available from the Government Printing Office: The Journal of Research, published in four separate sections, presents complete scientific and techincal papers; the Technical News Bulletin presents summary and preliminary reports on work in progress; and Basic Radio Propagation Predictions provides data for determining the best frequencies to use for radio communications throughout the world. There are also five series of nonperiodical publications: Monographs, Applied Mathematics Series, Handbooks, Miscellaneous Publications, and Technical Notes.

Information on the Bureau's publications can be found in NBS Circular 460, Publications of the National Bureau of Standards ($1.25) and its Supplement ($1.50), available from the Superintendent of Documents, Government Printing Office, Washington 25, D. C.

UNITED STATES DEPARTMENT OF COMMERCE · Frederick H. Mueller, *Secretary*
NATIONAL BUREAU OF STANDARDS · A. V. Astin, *Director*

Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, Marlene I. Cook, Thelma Isaacs, and Eloise H. Evans

National Bureau of Standards Circular 539

Volume 9, Issued February 25, 1960

For sale by the Superintendent of Documents, U. S. Government Printing Office, Washington 25, D. C.
Price 40 cents

Contents

Errata

Vol. 5. Page 5, calculated density for ammonium chlorostannate should be 2.398 g/cm^3.

Vol. 6. Page 15, the d-values of the NBS pattern should read 1.4361 instead of 1.4351 and 1.3184 instead of 1.3148.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. 9—Data for 43 Substances

Howard E. Swanson, Marlene I. Cook,[1] Thelma Isaacs,[1] and Eloise H. Evans[1]

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

Included are X-ray data for the following forty-three substances: α-Al_2O_3 (corundum), NH_4N_3, $(NH_4)HCO_3$ (teschemacherite), $(NH_4)_2PtBr_6$, NH_4ReO_4, $(NH_4)_2SO_4$ (mascagnite), $BeAl_2O_4$ (chrysoberyl), $Be_3Al_2(SiO_3)_6$ (beryl), BiOI, $CdBr_2$, $CdCl_2$, $12CaO \cdot 7Al_2O_3$, $Ca_3Fe_2Si_3O_{12}$ (andradite), Cs_2TeBr_6, $CsNO_3$, β-$CrPO_4$, $CoAl_2O_4$, CoO, Co_3O_4, Dy_2O_3, $ErPO_4$, Ho_2O_3, $MgCr_2O_4$ (picrochromite) $MnAl_2O_4$ (galaxite), $MnFe_2O_4$ (jacobsite), Mn_2O_3 (partridgeite), HgO (montroydite), $Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$, $NiAl_2O_4$, Ni_2GeO_4, KBH_4, $K_3Co(NO_2)_6$, K_3ZrF_7, PrOCl, γ-AgI, $AgIO_4$, $NaBH_4$, $SrZrO_4$, S, TeO_2 (tellurite), Tm_2O_3, $TiO_{1.616}$, and ZnI_2.

INTRODUCTION

The National Bureau of Standards in its program[2] for the revision and evaluation of published X-ray data for the X-ray Powder Data File presents data for 43 compounds. This paper is the ninth of a series of "Standard X-ray Diffraction Powder Patterns". These patterns are recommended to replace 41 cards now in the file. The patterns for 12 compounds not represented in the file have been added. These compounds are ammonium bromoplatinate, ammonium perrhenate, cadmium bromide, cesium bromotellurate, dysprosium sesquioxide, erbium phosphate, holmium sesquioxide, neodymium ethylsulfate nonahydrate, nickel germanate, potassium cobaltinitrite, preaseodymium oxychloride, and sodium borohydride.

The experimental procedure and general plan of these reports have not changed from that of the previous volumes of the NBS Circular.[3] However, the basic technique is discussed, in this section, under the same headings that appear in the text of this volume.

ASTM cards. Each section of this Circular contains a table listing the ASTM file card numbers, the three strongest lines, the radiations used, and the literature references for each card. Cards listed in the 1958 index to the Powder Data File [1][4] are included in the table.

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

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

At least two intensity patterns were prepared to check reproducibility of measured values. Samples that gave satisfactory intensity patterns usually had a particle-size average well within the range of 5 to 10 μ, as suggested by Alexander, Klug, and Kummer [2]. A special cell with one open end was used for making intensity measurements. An intensity sample was prepared by clamping a flat piece of glass temporarily over the surface of this holder, and while it was held in a vertical position, the sample was drifted in from the open end. The glass was then carefully removed so that the surface of the sample could be exposed to the X-ray beam. For a few powder samples that did not flow readily or were prone to orient excessively, approximately 50-volume percent of finely ground silica-gel was added

---

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

[2] This project is sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods. This committee is composed of members from the American Society for Testing Materials, the American Crystallographic Association, and the British Institute of Physics. Financial support is also provided by the National Bureau of Standards.

[3] Other volumes were published as follows: Vol. 1 and Vol. 2 June 1953; Vol. 3, June 1954; Vol. 4, March 1955; Vol. 5, October 1955; Vol. 6, September 1956; Vol. 7, September 1957; and Vol. 8, April 1959.

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

as a diluent. The intensity values of each pattern were measured as peak height above background and are expressed as percentages of the strongest line. Additional patterns were obtained for *d*-value measurements. These specimens were prepared by packing into a shallow holder a sample containing approximately 5-weight percent of tungsten powder that served as an internal standard. The lattice constant used for tungsten at 25°C is 3.1648 A, as determined by Jette and Foote [3]. All of the NBS patterns, unless otherwise noted, are made at 25°C, using either filtered copper radiation ($K\alpha_1$), cobalt radiation ($K\alpha_1$), or iron radiation ($K\alpha_1$), having the wavelengths 1.5405 A, 1.7889 A, and 1.9360 A, respectively.

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

Abbreviations used when describing intensities, taken from the literature, without numerical values are: s, strong; m, medium; and w, weak. Other abbreviations used are: B, broad, D, diffuse; db, doublet; and v, very.

Structural data. Although the NBS lattice constants of cubic materials were calculated for each *d*-value, the constant reported is that obtained by averaging the last five lines because of the greater accuracy of measurement in the large-angle region of the pattern. The unit-cell values for each noncubic substance were determined by means of a least-squares calculation made by the IBM 704 from the latter half of the pattern, using those *d*-values for which there was only one possible Miller Index. The number of significant figures reported in the NBS pattern is limited by the quality of each sample and by its structural symmetry.

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

Starting with volume 8 we have adopted a variation in our routine for presenting the space group. In place of both the Schoenflies symbol and the International symbol previously listed, we have dropped the Schoenflies symbol and added the space group number in the International Tables for X-ray Crystallography. It is felt that this number has become useful in locating space group data, while the use of the Schoenflies symbol has diminished.

We have also decided to present orthorhombic cell dimensions only in the "standard" arrangement of a, b, c, as given in the International Tables rather than with a permutation as is occasionally given in the literature.

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

References

[1] Index to the X-ray powder data file, American Society for Testing Materials, Philadelphia, Pa. (1958).

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

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

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

[5] E. Wichers, Report of the Committee on Atomic Weights of the American Chemical Society. J. Am. Chem. Soc. **78**, 3235 (1956).

[6] M. E. Straumanis, Remark concerning the absolute value of Avogadro's number, Phys. Rev. **95**, 566 (1954).

alpha-Aluminum Oxide (corundum), α-Al_2O_3 (trigonal)

ASTM cards

The following pattern is the same pattern shown on ASTM card 5–0712 [1] prepared in 1953 by NBS, but thirteen additional lines have been included. These weak lines were brought out by slower scanning.

NBS sample. The same Mallinckrodt sample was used. It was annealed at 1,400°C for 4 hr in an Al_2O_3 crucible.

Structural data. Bragg [2] in 1922 determined that alpha-aluminum oxide has the corundum-type structure, the space group $R\bar{3}c$ (No. 167) with $6(Al_2O_3)$ per unit hexagonal cell or $2(Al_2O_3)$ per unit rhombohedral cell.

Lattice constants

		a	*c*
		A	*A*
1953	National Bureau of Standards	4.758	12.991 at 26° C

The density of alpha-aluminum oxide calculated from NBS lattice constants is 3.987 g/cm³ at 26° C.

References

[1] NBS (U.S.) Circ. 539 **2**, 20–23 (1953).
[2] W. H. Bragg, The significance of crystal structure, **J.** Chem. Soc. London **121**, 2766–2787 (1922).

hkl hex.	1959 National Bureau of Standards Cu, 1.5405 A at 26° C	
	d	*I*
	A	
012	3.479	74
104	2.552	92
110	2.379	42
006	2.165	<1
113	2.085	100
202	1.964	1
024	1.740	43
116	1.601	81
211	1.546	3
122	1.514	4
018	1.510	7
124	1.404	32
030	1.374	48
125	1.337	1
208	1.276	2
1·0·10	1.239	16
119	1.2343	7
220	1.1898	6
306	1.1600	<1
223	1.1470	4
311	1.1382	1
312	1.1255	5
128	1.1246	2
0·2·10	1.0988	6
0·0·12	1.0831	3
134	1.0781	7
226	1.0426	13
402	1.0175	1
1·2·10	0.9976	11
1·1·12	.9857	<1
404	.9819	2
321	.9431	<1
1·2·11	.9413	<1
318	.9345	3
229	.9178	2
324	.9076	12
0·1·14	.9052	3
410	.8991	6
235	.8884	<1
413	.8804	4
048	.8698	2
1·3·10	.8580	12
3·0·12	.8502	4
2·0·14	.8460	4
146	.8303	22
1·1·15	.8137	4
4·0·10	.8072	11
054	.7988	7
1·0·16	.7970	14
330	.7931	13

Ammonium Azide, NH_4N_3 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
3-0687	2.89 3.12 3.83	Molybdenum	Dow Chemical Co., Midland, Michigan.

Additional published patterns

Source	Radiation
Frevel [1] 1936	Copper K_α

NBS sample. The sample of ammonium azide was prepared in Prof. F. O. Rice's laboratory at the Catholic University of America by E. Miller by neutralizing hydrazoic acid in ether solution with ammonia and crystallizing. The sample was dried over calcium chloride.

The sample is colorless and optically negative. The indices of refraction are $N_\alpha = 1.511$, $N_\beta = 1.606$, $N_\gamma = 1.688$, and $2V = 88°$.

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

Pattern	1	2	3
Dow Chemical Co.	210, 012	202	010
Frevel	202	010	103, 211
National Bureau of Standards	210	012	202

Structural data. Frevel [1] in 1936 determined that ammonium azide has the ammonium hydrofluoride-type structure, the space group Pnma (No. 53), and $4(NH_4N_3)$ per unit cell.

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

hkl	---- Dow Chemical Co. Mo, 0.7107 A		1936 Frevel Cu, 1.5418 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	*I*
200	-----	---	4.48	15	4.48	10
002	-----	---	4.32	18	4.33	11
010	3.84	40	3.81	50	3.811	39
202	3.13	60	3.11	100	3.111	70
210	2.90	100	-----	---	2.899	100
012					2.860	100
301	-----	---	-----	---	2.820	35
103	2.77	40	2.75	35	2.748	42
211						
112	-----	---	-----	---	2.723	6
013	-----	---	-----	---	2.302	5
311	-----	---	2.266	25	2.265	18
400	2.23	20	-----	---	2.232	22
113			2.227	30	2.229	20
004	2.18	10	2.163	15	2.166	9
312	-----	---	2.056	5	2.063	3
402	-----	---	-----	---	1.986	2
204	-----	---	1.947	10	1.950	3
020	1.91	10	1.903	18	1.904	9
021	-----	---	1.860	5	1.860	2
313	-----	---	-----	---	1.822	1
121						
412	-----	---	1.757	8	1.760	7
220	-----	---	-----	---	1.751	7
501						
214	-----	---	1.736	10	1.735	2
122	-----	---	-----	---	1.711	3
105	-----	---	1.702	10	1.702	2
222	-----	---	-----	---	1.623	6
413	-----	---	-----	---	1.602	
511, 314	-----	---	1.589	5	1.591	3
023						
321	-----	---	-----	---	1.579	1
123	-----	---	-----	---	1.565	2
404	-----	---	1.554	5	1.553	2
115						
512	-----	---	-----	---	1.515	1
322	-----	---	-----	---	1.503	2
305	-----	---	-----	---	1.4981	5
223						
414	-----	---	-----	---	1.4399	3
421	-----	---	1.430	10	1.4294	5
024						
513	-----	---	-----	---	1.4116	2
124						
602	-----	---	-----	---	1.4087	4
610	-----	---	1.388	5	1.3866	3
422	-----	---	1.374	5	1.3742	2
206						
611	-----	---	-----	---	1.3700	1
016	-----	---	1.350 [a]	5	1.3501	2

[a] Six additional lines were omitted.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1936	Frevel [1]	8.948	3.808	8.659
1959	National Bureau of Standards	8.936	3.809	8.663 at 25° C

The density of ammonium azide calculated from NBS lattice constants is 1.353 g/cm³ at 25° C.

References

[1] L. K. Frevel, The crystal structure of ammonium azide, NH_4N_3, Z. Krist. **94A**, 197–211 (1936).

Ammonium Bicarbonate, (teschemacherite), $(NH_4)HCO_3$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0868	2.99 5.3 4.02	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of ammonium bicarbonate was obtained from Baker and Adamson Chemical Co., New York. Spectrographic analysis detected no impurities.

The sample is colorless and optically negative. The refractive indices are $N_\alpha = 1.421$, $N_\beta = 1.535$, $N_\gamma = 1.554$. $2V = 24°$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C		*hkl*	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*		*d*	*I*	*d*	*I*
	A		*A*						
110	--------	--------	5.98	4	313	--------	--------	1.8342	2
020	5.3	42	5.34	59	400	--------	--------	1.8137	4
002	--------	--------	4.39	4	060	--------	--------	1.7843	3
012	4.03	27	4.05	45	341	}			
102	--------	--------	3.74	10	323	} --------	--------	1.7564	2
200	3.62	27	3.62	57	411	--------	--------	1.7514	3
022	3.40	7	3.39	12	252	1.69	3	1.6995	4
211	3.20	7	3.195	18	153	}			
122	3.07	10	3.068	30	115	} --------	--------	1.6794	3
131	} 3.00	100	{ 3.005	43	333	--------	--------	1.6502	3
220			{ 2.998	100					
					125	--------	--------	1.6207	5
221	--------	--------	2.841	6	260	--------	--------	1.6019	2
202	2.80	3	2.794	12	431	--------	--------	1.5898	3
212	2.70	7	2.701	18	261	--------	--------	1.5757	<1
113	2.62	7	2.624	21	324	--------	--------	1.5515	2
222	--------	--------	2.476	7	244	--------	--------	1.5345	<1
231	--------	--------	2.443	17	432	--------	--------	1.5165	1
141	} 2.42	10	2.413	8	440	--------	--------	1.5021	1
123					171	--------	--------	1.4752	2
					145	--------	--------	1.4349	3
042	} 2.28	3	2.282	4					
311					511	--------	--------	1.4180	<1
142	--------	--------	2.1781	20	353	}			
240	2.15	20	2.1547	29	315	} --------	--------	1.4044	2
302	--------	--------	2.1152	11	263	}			
104	2.09	3	2.0938	6	414	--------	--------	1.3846	2
024	--------	--------	2.0238	4	362	--------	--------	1.3639	1
151	--------	--------	1.9993	4					
331	}								
124	} --------	--------	1.9505	2					
204	--------	--------	1.8721	2					

Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	131, 220	020	012
National Bureau of Standards	220	02_0	200

Structural data. Mooney [2] in 1932 determined that ammonium bicarbonate has the space group Pccn (No. 56), with $8[(NH_4)HCO_3]$ per unit cell.

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

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1932	Mooney [2]	7.30	10.81	8.78
1959	National Bureau of Standards	7.255	10.709	8.746 at 25° C

The density of ammonium bicarbonate calculated from the NBS lattice constants is 1.545 g/cm³ at 25° C.

References

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

[2] R. C. L. Mooney, Crystal structure of ammonium bicarbonate, Phys. Rev. **39**, 861–862 (1932).

Ammonium Bromoplatinate, $(NH_4)_2PtBr_6$ (cubic)

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C			*hkl*	1959 National Bureau of Standards Co, 1.7889 A at 25° C		
	d	*I*	*a*		*d*	*I*	*a*
	A		*A*				
111	5.99	94	10.38	844	1.0584	8	10.370
200	5.18	100	10.38	933	1.0421	3	10.369
220	3.664	6	10.36	10·0·0	1.0369	3	10.369
311	3.127	48	10.37	10·2·0	1.0166	1	10.367
222	2.994	53	10.37	951	1.0024	5	10.369
400	2.592	90	10.369	10·2·2	0.9977	<1	10.368
331	2.378	14	10.368	953	.9669	4	10.369
420	2.3189	60	10.370	10·4·0	.9627	4	10.369
422	2.1166	3	10.369	10·4·2	.9466	1	10.369
511	1.9954	28	10.368	11·1·1	.9348	<1	10.367
440	1.8329	52	10.368	880	.9164	1	10.368
531	1.7524	25	10.367	11·3·1	.9058	1	10.367
600	1.7281	27	10.369	10·4·4	.9024	3	10.368
620	1.6394	2	10.368	10·6·0	.8890	2	10.367
533	1.5813	6	10.369	11·3·3	.8793	<1	10.367
622	1.5634	9	10.370	10·6·2	.8761	1	10.366
444	1.4966	17	10.369	12·0·0	.8639	2	10.367
711	1.4519	13	10.369	11·5·1	.8551	1	10.367
640	1.4381	11	10.370	12·2·0	.8522	2	10.367
642	1.3858	2	10.370	12·2·2	.8409	1	10.367
731	1.3501	7	10.370	11·5·3	.8327	2	10.367
800	1.2960	5	10.368	12·4·0	.8196	2	10.367
820	1.2573	9	10.368	991	.8120	2	10.367
822	1.2220	1	10.369	12·4·2	.8095	3	10.367
751	1.1973	4	10.369	10·8·2	.7998	1	10.367
662	1.1893	2	10.368	13·1·1	.7927	3	10.366
840	1.1592	12	10.368				
911	1.1382	5	10.369	Average value of last five lines		--------	10.367
842	1.1314	6	10.369				
931	1.0869	3	10.368				

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium bromoplatinate was prepared at NBS from bromoplatinic acid and ammonium bromide. Spectrographic analysis showed no impurities greater than 0.001 percent.

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

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

Pattern	1	2	3
National Bureau of Standards	200	111	400

Structural data. No structural data for ammonium bromoplatinate was found. Due to the similarity of patterns, it is believed to be isostructural with potassium chloroplatinate, with space group Fm3m (No. 225) and $4[(NH_4)_2PtBr_6]$ per unit cell.

Lattice constants

		A
1959	National Bureau of Standards	10.367 at 25° C

The density of ammonium bromoplatinate calculated from NBS lattice constant is 4.235 g/cm³ at 25° C.

Ammonium Perrhenate, NH_4ReO_4 (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium perrhenate was obtained from the Johnson, Matthey and Co., London, England. Their spectrographic analysis detected calcium and magnesium (very faintly visible) as the only impurities.

The sample is colorless and optically positive. The refractive indices are $N_o = 1.646$ and $N_e = 1.679$.

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

Pattern	1	2	3
National Bureau of Standards	112	101	211

Structural data. Beintema [1] in 1937 determined that ammonium perrhenate has calcium tungstate-type structure, the space group $I4_1/a$ (No. 88) and $4(NH_4ReO_4)$ per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1937	Beintema [1]	5.883	12.968
1959	National Bureau of Standards	5.883	12.979 at 25° C

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
	A	
101	5.361	71
112	3.504	100
004	3.245	13
200	2.942	18
202	2.680	2
211	2.581	20
114	2.560	3
105	2.3749	8
213	2.2477	12
204	2.1791	19
220	2.0800	8
222	1.9803	1
301	1.9391	5
116	1.9193	11
215	1.8479	11
312	1.7885	19
107	1.7685	4
224	1.7511	9
321	1.6189	6
305	1.5647	3
323	1.5267	6
217	1.5156	5
400	1.4706	2
411	1.4182	7
316	1.4108	8
109	1.4009	3
325	1.3817	2
332	1.3558	5
307	1.3472	3
404	1.3397	3
420	1.3155	4
228	1.2793	1
219	1.2647	1
415	1.2504	1
1·1·10	1.2390	2

Ammonium Perrhenate, NH_4ReO_4 (tetragonal)

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
327	1.2251	1
424	1.2192	2
501	1.1717	2
336	1.1677	1
309	1.1615	<1
1·0·11	1.1570	<1
512	1.1357	3
503		
417	1.1311	2
408	1.0894	1
514	1.0866	1
329	1.0805	1
2·1·11	1.0767	1
505	1.0714	1
3·1·10	1.0643	1
523	1.0592	<1
440	1.0397	<1
516	1.0183	2
2·0·12	1.0150	2
525	1.0070	<1
532	0.9971	1
507	.9931	<1
444	.9907	1

The density of ammonium perrhenate calculated from the NBS lattice constants is 3.965 g/cm³ at 25° C.

References

[1] J. Beintema, Die Kristallstruktur der Alkaliperiperrhenate und-perjodate, Z. Krist. **97A**, 300–322 (1937).

Ammonium Sulfate (mascagnite), $(NH_4)_2SO_4$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
7–2	4.33 4.39 3.06	Copper	National Bureau of Standards [1] 1956.

Some time ago Dr. deWolff pointed out that the above pattern did not include some additional weak lines that he had measured.

In order to make the above card more complete we have rerun the Johnson Matthey sample used previously. Fine crystals were prepared by adding alcohol to a water solution of the salt. Slow scanning produced the following expanded pattern.

Interplanar spacings and intensity measurements. The original spacings and intensities remain almost unchanged but 28 new lines have been added.

Structural data. Indexing of the powder pattern is based upon the space group Pnma (No. 62) with $4[(NH_4)_2SO_4]$ per unit cell [2]. Unit-cell values were obtained using both old and new spacings for angles higher than 40° (2θ).

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1956	National Bureau of Standards	7.782	5.994	10.64 at 25° C
1959	National Bureau of Standards	7.782	5.993	10.636 at 25° C

The calculated density is 1.769 g/cm³ at 25° C.

References

[1] National Bureau of Standards (U.S.), Circ. 539 **6**, 12 (1956).

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

Ammonium Sulfate (mascagnite), $(NH_4)_2SO_4$ (orthorhombic)

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C		*hkl*	1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*		*d*	*I*
	A				
002	5.31	14	033	1.7400	<1
011	5.22	27	106	1.7275	1
102	4.39	63	133	1.6989	2
111	4.33	100			
200	3.890	35	116	1.6609	<1
			413	1.6401	4
201	3.660	<1	420	1.6324	4
210	3.264	<1	206	1.6130	2
103	3.227	1	421		
202	3.139	30			
211	3.122	22	233	1.5878	<1
			324	1.5788	<1
013	3.055	54	134	1.5647	1
020	2.998	23	422	1.5603	<1
113	2.839	1	026	1.5244	4
212	2.782	3			
121	2.704	5	040	1.4973	5
			126		
004	2.655	13	502	1.4938	5
022	2.611	6	234	1.4782	1
301	2.521	9	017	1.4734	3
122	2.476	2			
213	2.401	3	171	1.4467	<1
			333		
220	2.374	2	405	1.4355	1
311	2.322	17	503	1.4236	3
221	2.317	18	316		
123	2.196	8			
204			226	1.4207	2
			240	1.3985	1
222	2.168	14	712	1.3774	<1
303	2.093	4	432	1.3473	<1
214	2.062	<1	522	1.3369	2
015	2.005	<1			
223	1.973	4	514	1.3109	<1
			406		
400	1.945	4	044	1.3051	1
115	1.942	5	433	1.2973	2
321	1.927	<1	600		
124					
401	1.914	3	144, 601	1.2873	<1
			523		
131	1.904	1	317	1.2806	<1
205	1.867	1	118		
304	1.8557	<1	602	1.2598	<1
402	1.8270	<1			
132	1.8178	<1	515	1.2298	1
			531	1.2200	1
230	1.7762	1	426	1.2008	1
006	1.7729	3			

Beryllium Aluminum Oxide (chrysoberyl), $BeAl_2O_4$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
2-1226	2.08 1.61 3.24	Copper	British Museum.

Additional published patterns

Source	Radiation
Gjessing, Larsson, and Major [2] 1942	Iron
Foster and Royal [3] 1949	Copper
Budnikov, Avetikov, Dudavskij, and Zvjagilskij [4] 1949	Chromium

NBS sample. The sample of chrysoberyl was prepared by E. N. Bunting at NBS by heating beryllium oxide and aluminum oxide at 1,300° C and reheating, after grinding, to 1,400° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of chromium, iron, sodium, and silicon; 0.001 to 0.01 percent each of calcium, magnesium, manganese, and vanadium.

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

Interplanar spacings and intensity measurements. The *d*-values reported by Budnikov, Avetikov, Dudavskij, and Zvjagilskij were converted from kX to angstrom units. The *d*-values reported by Gjessing, Larsson, and Major were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
British Museum	221	222	111
Gjessing, Larsson, and Major	221	222	620
Foster and Royal	221	222	111
Budnikov, Avetikov, Dudavskij, and Zvjagilskij	222	620	040
National Bureau of Standards	221	222	111

Structural data.. Bragg and Brown [1] in 1926 determined that chrysoberyl has the space group Pnma (No. 62) and $4(BeAl_2O_4)$ per unit cell. Their unit-cell measurements have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1926	Bragg and Brown [1]	9.409	5.481	4.429
1959	National Bureau of Standards	9.4041	5.4756	4.4267 at 25° C

The density of chrysoberyl calculated from NBS lattice constants is 3.699 g/cm³ at 25° C.

References

[1] W. L. Bragg and G. B. Brown, The crystal structure of chrysoberyl, Z. Krist. **63**, 122 (1926).

[2] L. Gjessing, T. Larsson, and H. Major, Isomorphous substitutes for aluminum in the compound Al_2BeO_4, Norsk. Geol. Tidsskr. **22**, 92–99 (1942).

[3] W. R. Foster and H. F. Royal, An intermediate compound in the system $BeO \cdot Al_2O_3$-Al_2O_3, J. Am. Ceram. Soc. **32**, 26–34 (1949).

[4] P. P. Budnikov, V. G. Avetikov, E. P. Dudavskij, and A. A. Zvjagilskij, The compound $BeO \cdot 3Al_2O_3$, Doklady Akad. Nauk. SSSR **68**, 313–316 (1949).

hkl	---- British Museum Cu, 1.541 A		1942 Gjessing Larsson and Major Fe, 1.936 A		1949 Foster and Royal Cu, 1.5405 A		1949 Budnikov, Avetikov, Dudavskij and Zvjagilskij Cr, 2.2909 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
200	-------	------	-------	------	-------	------	-------	------	4.71	6
----------	4.47	40	-------	------	-------	------	-------	------	-------	------
101	4.03	60	4.00	12	3.99	30	-------	------	4.01	49
210	3.60	50	3.56	12	-------	------	-------	------	3.570	4
011	-------	------	-------	------	-------	------	-------	------	3.441	4
111	3.24	80	3.24	50	3.22	50	3.29	20	3.232	86
----------	2.85	40	-------	------	-------	------	3.03	10	-------	------
211	-------	------	-------	------	-------	------	2.84	15	2.777	4
020	-------	------	-------	------	-------	------	-------	------	2.737	3
301	2.57	80	2.56	50	2.54	50	2.57	25	2.559	52

Beryllium Aluminum Oxide (chrysoberyl), $BeAl_2O_4$ (orthorhombic)

hkl	---- British Museum Cu, 1.541 A		1942 Gjessing, Larsson and Major Fe, 1.936 A		1949 Foster and Royal Cu, 1.5405 A		1949 Budnikov, Avetikov, Dudavskij and Zvjagilskij Cr, 2.2909 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
220	--------	------	2.37	0	--------	------	--------	------	2.366	7
311	2.33	80	2.31	50	2.31	30	2.30	20	2.317	30
121	2.26	70	2.26	50	2.25	50	2.25	30	2.260	42
002	--------	------	--------	------	--------	------	--------	------	2.212	<1
410	--------	------	--------	------	--------	------	--------	------	2.159	6
102	--------	------	--------	------	--------	------	--------	------	2.155	3
221	2.08	100	2.08	100	2.08	100	2.07	50	2.087	100
401	--------	------	--------	------	--------	------	--------	------	2.078	58
112	1.98	20	2.00	0	--------	------	1.99	<10	2.006	4
411	--------	------	--------	------	--------	------	--------	------	1.941	2
212	1.88	20	--------	------	--------	------	--------	------	1.880	3
321	--------	------	1.87	6	--------	------	1.86	10	1.870	6
302	1.80	60	--------	------	--------	------	1.81	10	1.809	1
501	--------	------	--------	------	--------	------	--------	------	1.732	2
131	--------	------	1.67	25	--------	------	--------	------	1.661	11
511	1.65	40	1.65	12	--------	------	1.64	10	1.651	7
222	1.61	100	1.61	100	1.61	90	1.61	100	1.617	88
402	--------	------	--------	------	--------	------	--------	------	1.613	75
231	--------	------	--------	------	--------	------	--------	------	1.588	1
412	1.56	20	1.55	6	--------	------	1.54	15	1.546	7
610	1.51	50	1.50	25	--------	------	--------	------	1.507	6
331	--------	------	1.489	6	--------	------	1.50	15	1.4858	7
521	1.46	40	1.465	31	1.463	20	1.46	30	1.4629	14
430	--------	------	--------	------	--------	------	--------	------	1.4415	3
113, 203	--------	------	1.410	0	--------	------	1.409	15	1.4086	4
422	--------	------	--------	------	--------	------	--------	------	1.3882	4
040	--------	------	1.371	38	1.370	40	1.374	55	1.3686	21
620	1.36	80	1.362	75	1.361	20	1.354	75	1.3602	27
303	1.34	40	1.336	12	--------	------	--------	------	1.3349	5
313	1.30	70D	1.299	25	--------	------	1.299	35	1.2973	10
123, 701	--------	------	1.287	56	1.286	20	1.289	55	1.2861	13
531	1.26	70	--------	------	--------	------	--------	------	1.2556	4
711, 223	--------	------	1.253	62	1.253	20	1.254	55	1.2519	11
----------	--------	------	--------	------	--------	------	1.218	<10	--------	------
341, 432	1.21	40	1.208	50	--------	------	1.208	45	1.2073	8
----------	--------	------	--------	------	--------	------	1.198	<10	--------	------
630	1.19	40D	--------	------	--------	------	1.188	10	1.1892	3
440	--------	------	--------	------	--------	------	1.183	20	1.1831	3
042, 721	1.16	40	1.164	0	--------	------	1.173	15	1.1643	2
503	--------	------	--------	------	--------	------	--------	------	1.1608	1
441	1.14	50	1.145	19	--------	------	--------	------	1.1429	4
513, 801	--------	------	1.136	6	--------	------	--------	------	1.1361	3
004	1.11	50	1.107	50	--------	------	--------	------	1.1066	5
114, 333 / 204	1.08	60	--------	------	--------	------	--------	------	1.0775	3
523	1.06	60	--------	------	--------	------	--------	------	1.0688	4
151	1.06	20	--------	------	--------	------	--------	------	1.0563	2
632	--------	------	--------	------	--------	------	--------	------	1.0475	2
304, 442	1.04	70	--------	------	--------	------	--------	------	1.0434	10
802	--------	------	--------	------	--------	------	--------	------	1.0383	4
433, 640	--------	------	--------	------	--------	------	--------	------	1.0313	<1

Beryllium Aluminum Oxide (chrysoberyl), $BeAl_2O_4$ (orthorhombic)

hkl	---- British Museum Cu, 1.541 A		1942 Gjessing, Larsson and Major Fe, 1.936 A		1949 Foster and Royal Cu, 1.5405 A		1949 Budnikov, Avetikov, Dudavskij and Zvjagilskij Cr, 2.2909 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
124, 812	1.02	20							1.0200	2
351									1.0067	2
224									1.0023	3
404	1.00	60							1.0011	3
703									0.9933	4
533									.9795	1
822									.9706	<1
252									.9610	<1
343									.9557	3
921									.9533	6
741									.9371	5
10·1·0									.9269	1
551									.9254	2
443									.9230	2
803									.9194	2
813									.9068	1
334, 452									.9057	1
832									.9024	2
650									.8976	1
260									.8958	1
614, 840									.8919	1
161									.8897	2
105									.8814	<1
434, 261									.8780	<1
153									.8757	1
015, 841									.8742	2
10·2·1									.8720	3
115, 552 / 205									.8701	2
10·0·2									.8656	1
044									.8606	7
624									.8584	12
10·1·2									.8551	2
305									.8521	2
353, 244									.8467	2
11·0·1 / 932									.8393	3
262									.8304	7
405									.8284	6
842									.8272	6
10·2·2									.8252	5
923									.8141	4
325									.8101	1
444									.8081	3
561									.8073	3
743									.8040	4
814									.7971	<1
135									.7937	3
515, 752									.7925	2
660, 851									.7886	5
12·0·0									.7836	1

Beryllium Aluminum Silicate (beryl), $Be_3Al_2(SiO_3)_6$ (hexagonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-0079	8.1 3.33 2.92	Copper	British Museum.
2-0080	7.90 3.25 2.87	Copper	Wyandotte Chemical Co., Wyandotte, Mich.
3-0463 3-0464	3.28 2.88 0.81	Copper	Schiebold [1] 1935 (synthetic).
3-0480 3-0481	3.25 2.88 0.81	Copper	Schiebold [1] 1935 (natural).

Card #3-0462 reports *d*-spacings to 1.22; otherwise it has the same data as cards #3-0463 and 3-0464. Therefore, this card is not used in the comparison table.

Additional published patterns

Source	Radiation
Norrish [2] 1947	Copper K_α

NBS sample. The sample of beryl was obtained from Royalston, Mass. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of iron, sodium, and zinc; and 0.001 to 0.01 percent each of magnesium, manganese, strontium, and titanium.

The sample is colorless and optically negative. The refractive indices are $N_o = 1.579$ and $N_e = 1.572$.

Interplanar spacings and intensity measurements. The *d*-values reported by the British Museum and by the Wyandotte Chemical Co. were converted from kX to angstrom units. The three patterns reported by Schiebold were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
British Museum	100	211	110, 002
Wyandotte Chemical Co.	100	112	211
Schiebold (synthetic)	112	211	110, 002
Schiebold (natural)	112	211	110, 002
Norrish	100	112	211
National Bureau of Standards	211	112	100

Structural data. Bragg and West [3] in 1926 determined that beryl has the space group P6/mmc (No. 192) and $2[Be_3Al_2(SiO_3)_6]$ per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1926	Bragg and West [3]	9.23	9.19
1935	Schiebold [1] (synthetic)	9.235	9.203
1935	Schiebold [1] (natural)	9.415	9.226
1935	Schiebold [1] (natural)	9.231	9.188
1947	Norrish [2]	9.188	9.189
1951	Belov and Matveeva [4]	9.206	9.205
1959	National Bureau of Standards	9.215	9.192 at 25° C

The density of beryl calculated from NBS lattice constants is 2.640 g/cm³ at 25° C.

References

[1] E. Schiebold, Verleichende Untersuchungen an naturlichen und synthetischen Smaragdkristallen, Z. Krist. **92,** 435–473 (1935).

[2] K. Norrish, X-ray study of West Australian beryl, J. Roy. Soc. W. Aust. **34,** 1–16 (1947).

[3] W. L. Bragg and J. West, The structure of beryl, $Be_3Al_2Si_6O_{18}$, Proc. Roy. Soc. **111A,** 691–714 (1926).

[4] N. V. Belov and R. G. Matveeva, The determination of parameters of beryl structure by a method of partial projections, Trudy Inst. Krist. Akad. Nauk S. S. S. R. **6,** 69 (1951).

Beryllium Aluminum Silicate (beryl), $Be_3Al_2(SiO_3)_6$ (hexagonal)

hkl	---- British Museum Cu, 1.5418 A		---- Wyandotte Chemical Bo. Cu, 1.5418 A		1935 Schiebold (synthetic) Cu, 1.5418 A		1935 Schiebold (natural) Cu, 1.5418 A		1947 Norrish Cu, 1.5418 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		A	
---	9.4	40	---	---	---	---	---	---	---	---	---	---
100	8.1	100	7.92	100	---	---	---	---	7.93	s	7.98	93
---	5.2	40	---	---	---	---	---	---	---	---	---	---
110, 002	4.7	60	4.61	40	4.64	s	4.60	s	4.60	m	4.60	51
---	4.46	20	---	---	---	---	---	---	---	---	---	---
200, 102	4.08	60	4.01	50	4.04	s	3.99	s	3.96	m	3.99	46
---	3.68	50	---	---	---	---	---	---	---	---	---	---
---	3.33	80	---	---	---	---	---	---	---	---	---	---
112	3.24	20	3.26	100	3.29	vs	3.26	vs	3.25	s	3.254	95
210, 202	3.06	60	3.01	30	3.05	s	3.02	s	3.01	m	3.015	34
211	2.93	80	2.88	100	2.89	vs	2.89	vs	2.86	s–	2.867	100
300	---	---	---	---	2.71	w	---	---	2.65	vvw	2.660	2
212	2.56	50	2.53	40	2.55	s	2.54	s	2.51	m	2.523	30
---	---	---	2.37	10	---	---	---	---	---	---	---	---
220, 302, 004	2.34	40	2.30	10	2.32	ms	2.30	ms	2.289	w	2.293	10
310	2.23	40	---	---	2.22	m	2.21	m	---	---	2.213	6
104	---	---	2.20	20	---	---	---	---	2.203	w	2.208	2
311	2.16	40	2.14	20	2.16	s	2.15	s	2.142	w	2.152	14
222	2.09	20	---	---	2.08	mw	2.06	mw	---	---	2.060	3
114	2.02	60	---	---	---	---	---	---	2.048	vw	2.056	4
312, 204	1.99	20	1.98	40	2.00	s–	1.99	s	1.986	w–m	1.9926	22
---	1.86	20	1.92	20	---	---	---	---	1.922	vvw	---	---
320, 402	1.81	50	---	---	1.85	w	1.84	w	1.821	vw	1.8308	6
321, 313	1.76	60	1.79	30	1.81	ms	1.80	ms	1.784	w	1.7954	17
304	1.72	40	1.73	50	1.75	s	1.74	s	1.733	w–m	1.7397	19
411	---	---	1.71	20	1.72	m	1.71	m	---	---	1.7110	12
322	---	---	---	---	---	---	---	---	1.700	w	1.7007	2
---	1.64	60	1.67	10	---	---	---	---	---	---	---	---
412, 224, 500, 314	1.61, 1.58	50	1.62	30	1.64	s	1.63	s	1.622	w	1.6265	17
			1.59	10	1.60	m	1.61	m	1.589	vw	1.5953	6
323	---	---	1.57	20	1.58	m	1.57	m	---	---	1.5710	9
215	1.55	40	---	---	---	---	---	---	1.561	vw	1.5690	7
330, 006	1.53	60	---	---	1.54	mw	1.53	mw	1.528	vw	1.5349	5
											1.5320	7
413	---	---	1.51	40	1.52	s	1.52	s	1.507	w	1.5138	15
421	1.47	50	---	---	---	---	---	---	---	---	1.4882	1
332, 116	1.44	60	1.45	20	1.46	ms	1.46	ms	1.450	w	1.4566	9
											1.4535	10
510, 422, 324, 206	---	---	1.43	30	1.44	s	1.43	s	1.429	w	1.4324	13
315	1.41	20	1.41	10	1.42	vw	---	---	---	---	1.4148	1
			1.40	10								

Beryllium Aluminum Silicate (beryl), $Be_3Al_2(SiO_6)_3$ (hexagonal)

hkl	---- British Museum Cu, 1.5418 A		---- Wyandotte Chemical Co. Cu, 1.5418 A		1935 Schiebold (synthetic) Cu, 1.5418 A		1935 Schiebold (natural) Cu, 1.5418 A		1947 Norrish Cu, 1.5418 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		A	
512	1.38	50	1.37	20	1.34	s	1.33	s	1.362	w	1.3682	7
216					1.34	w	------	------	------	------	1.3656	6
600	------	----	1.33	20	1.32	vw	1.33	vw	1.328	vvw	1.3306	<1
430												
504	------	----	------	----	1.30	vw	1.30	vw	------	------	1.3117	<1
513												
325	------	----	------	----	1.28	s	1.28	s⁻	------	------	1.2977	<1
520												
602, 334	------	----	1.27	40	1.27	s	1.27	s⁻	1.272	w–m	1.2774	11
415												
521											1.2657	13
432	------	----	1.26	40	1.24	vw	1.23	vw	1.257	w–m	1.2628	9
424												
610	------	----	------	----	1.22	w	1.22	w	------	------	1.2170	2
611												
433									1.200	w–m	1.2062	10
217	------	----	1.20	40	1.21	s	1.21	s⁻			1.2041	9
523	------	----	------	----	1.19	mw	1.18	mw	1.176	vvw	1.1795	1
440, 604												
416	------	----	------	----	1.15	ms	1.15	ms	------	------	1.1511	4
008												
700									1.148	vw	1.1490	4
434	------	----	------	----	1.14	m	1.14	m	1.134	vw	1.1396	3
442												
524	------	----	------	----	1.12	ms	1.12	ms	1.114	vw	1.1173	7
620												
702	------	----	------	----	1.11	mw	1.11	mw	1.104	vvw	1.1066	<1
336	------	----	------	----	1.09	m	1.09	ms	1.083	vvw	1.0848	2
426												
218	------	----	------	----	1.07	ms	1.07	ms	1.073	vvw	1.0752	4
533, 435												
327	------	----	------	----	1.05	s	1.05	s	1.065	vvw	1.0683	5
525												
417	------	----	------	----	1.03	w	1.03	w	1.046	vw	1.0493	6
623	------	----	------	----	------	------	------	------	------	------	1.0485	4
712											1.0405	<1
444	------	----	------	----	1.02	m	1.02	m	1.028	vvw	1.0297	<1
541												
615	------	----	------	----	1.01	w	1.01	w	1.012	vvw	1.0157	3
					[a]		[b]		[c]			

[a] Twenty-nine additional lines are omitted.
[b] Twenty-one additional lines are omitted.
[c] Fourteen additional lines are omitted.

Bismuth Oxyiodide, BiOI (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
2-0634	3.02 9.1 2.28	Copper	British Museum.

Additional published patterns. None.

NBS sample. The sample of bismuth oxyiodide was prepared at NBS by reacting Bi_2O_3 with concentrated HI followed by prolonged hydrolysis of the product in boiling water. The X-ray pattern was improved by heating the material in air for 2 hr at 450° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of nickel; and 0.001 to 0.01 percent each of aluminum, cobalt, iron, and silicon.

The color of the sample was dark red-orange. The indices of refraction were too high to be determined by the usual liquid grain immersion method.

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

hkl	British Museum Cu, 1.541 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C		*hkl*	British Museum Mo, 1.541 A		1959 National Bureau of Standards Cu, 1.5405 A at 25°	
	d	*I*	*d*	*I*		*d*	*I*	*d*	*I*
	A		A						
001	9.1	80	9.15	22	312	1.216	20	1.2176	2
002	4.51	60	4.58	7	206	----	----	1.2121	<1
101	----	----	3.661	3	224	1.204	20	1.2017	2
102	3.02	100	3.011	100	117	1.186	10	1.1860	1
110	2.82	60	2.824	53	216	1.161	50	1.1597	1
111	----	----	2.699	3	304	----	----	1.1502	<1
103	2.42	40	2.424	10	008	----	----	1.1436	<1
112	----	----	2.403	7	225	----	----	1.1181	<1
004	2.28	80	2.287	9	314	1.112	60D	1.1058	4
113	----	----	2.072	2	321 108	----	----	1.0993	1
200 104	1.98	60	1.997	24	207	----	----	1.0936	<1
201	----	----	1.985	10	322	1.078	50	1.0768	5
202	1.82	40	1.952	3	305				
005			1.829	3	118 217	1.058	40	1.0601 1.0548	<1 1
114	1.77	60	1.778	15	323	----	----	1.0416	1
212 105	1.66	70	1.664	32	315	1.039	40	1.0393	1
213	----	----	1.541	6	226			1.0363	1
115	1.537	50D	1.5359	3	009	1.019	20	1.0165	<1
006	----	----	1.5246	3	306 400	1.001	20B	1.0028 0.9984	<1 <1
204	1.505	40	1.5045	6					
106	1.427	70	1.4244	4	401 208	----	----	.9925	<1
220	----	----	1.4120	6	109	----	----	.9852	1
214	1.408	50	1.4078	4	316	0.969	40	.9728	1
221	----	----	1.3957	<1	411 218	----	----	.9632	1
222 205	----	----	1.3495	4	119	----	----	.9566	<1
116	1.343	60	1.3422	4	325 412	----	----	.9478	2
007	1.309	20	1.3073	1					
302 215	1.281	40	1.2786	3	330	----	----	.9414	<1
310	1.265	40	1.2634	3					
107	1.242	60	1.2424	2					
303	----	----	1.2200	<1					

Pattern	1	2	3
British Museum	102	001	004
National Bureau of Standards	102	110	212, 105

Structural data. Bannister and Hey [1] in 1935 determined that bismuth oxyiodide has lead fluochloride-type structure, the space group P4/nmm (No. 129), and 2(BiOI) per unit cell.

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

The density of bismuth oxyiodide calculated from NBS lattice constants is 8.006 g/cm³ at 25° C.

Lattice constants

		a	*c*
		A	*A*
1935	Bannister and Hey [1]	4.02	9.16
1941	Sillén [2]	3.992	9.146
1959	National Bureau of Standards	3.994	9.149 at 25° C

References

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

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

Cadmium Bromide, $CdBr_2$ (trigonal)

ASTM cards. None. Card number 3–0088 is a different form.

Additional published patterns

Source	Radiation
Pinsker [1] 1942	Electron diff.

NBS sample. The sample of cadmium bromide was obtained from the City Chemical Corp., New York, as a hydrate. The sample was heated to 550° C to dehydrate and to sharpen the pattern. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of aluminum, iron, and silicon.

The sample was colorless. The indices of refraction were too high to be measured by the oil immersion method.

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

Pattern	1	2	3
Pinsker	110	104	113
National Bureau of Standards	003	110	104

hkl hex.	1942 Pinsker Electron Diffraction		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
003	--------	--------	6.27	100
101	3.42	25	3.40	10
006	--------	--------	3.14	8
104	2.80	70	2.785	19
015	--------	--------	2.546	3
107	--------	--------	2.123	2
009	--------	--------	2.094	7
110	2.00	100	1.993	39
018	1.94	36	1.947	6
113	1.91	70	1.899	15
1·0·10	1.70	14	1.654	3
024	1.62	70	1.621	2
0·0·12	--------	--------	1.570	9
0·1·11	--------	--------	1.5345	1
119	1.44	14	1.4439	4
208	1.40	18	1.3917	5
1·0·13	--------	--------	1.3366	1
0·0·15	1.26	36	1.2561	5
1·1·12	1.24	50	1.2334	10
-------	1.15	18	--------	--------
128	1.14	11	1.1413	3
1·0·16	1.13	11	1.1146	2
1·1·15	--------	--------	1.0625	2
0·1·17	--------	--------	1.0551	1
0·0·18	--------	--------	1.0466	1
0·2·16	--------	--------	0.9734	2
312 / 1·0·19	--------	--------	.9524	2
134 / 1·2·14	--------	--------	.9381	1
3·0·12	--------	--------	.9280	3
315 / 1·1·18	--------	--------	.9265	3
0·1·20	--------	--------	.9087	1
2·1·16	--------	--------	.8741	3

Structural data. Pinsker [1] in 1942 determined that this form of cadmium bromide has the cadmium chloride-type structure, the space group $R\bar{3}m$ (No. 166) and $3(CdBr_2)$ per unit hexagonal cell or $1(CdBr_2)$ per unit rhombohedral cell. Several other forms of cadmium bromide have been reported in the literature by Pinsker [1], Bijvoet and Nieuwenkamp [2], and Hägg, Kiessling, and Linden [3].

Lattice constants

		a	*c*
		A	*A*
1942	Pinsker [1]	4.01	18.88
1943	Hägg, Kiessling, and Linden [3]	3.99	18.78
1959	National Bureau of Standards	3.985	18.841 at 25° C

The density of cadmium bromide calculated from the NBS lattice constants is 5.203 g/cm³ at 25° C.

References

[1] Z. G. Pinsker, Electron di raction of the structure of $CdBr_2$, J. Phys. Chem. USSR **16**, 1–12 (1942).

[2] J. M. Bijvoet and W. Nieuwenkamp, Kürzere Originalmitteilungen und Notizen, Die ⟨⟨Wechselstruktur⟩⟩ von $CdBr_2$, Z. Krist. **86A**, 466–470 (1933).

[3] G. Hägg, R. Kiessling, and E. Linden, The crystal structure of $CdBr_2$ and CdI_2, Arkiv Kemi, Mineral. Geol. No. 4 **16B**, 1 (1943).

Cadmium Chloride, $CdCl_2$ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0169	5.8 2.65 3.28	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of cadmium chloride was obtained from Fisher Scientific Co. Spectrographic analysis shows the following impurities: 0.0001 to 0.001 percent each of aluminum and silicon.

The sample is colorless and optically positive. The indices of refraction are $N_o = 1.681$ and $N_e = 1.719$.

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

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	003	104	101
National Bureau of Standards	003	104	101

Structural data. Pauling [2] in 1929 determined that cadmium chloride has the space group $R\bar{3}m$ (No. 166) and $3(CdCl_2)$ per unit hexagonal cell or $1(CdCl_2)$ per unit rhombohedral cell. Cadmium chloride is used as a structure type and shown to be isomorphous with $MgCl_2$, $ZnCl_2$, $MnCl_2$, and $FeCl_2$ in 1927 [3]. The unit-cell measurements have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	*c*
		A	*A*
1930	Pauling and Hoard [4]	3.86	17.50
1941	Pinsker and Tatarinova [5]	3.85	17.46
1959	National Bureau of Standards	3.844	17.489 at 25° C

The density of cadmium chloride calculated from the NBS lattice constants is 4.080 g/cm³ at 25° C.

Cadmium Chloride, $CdCl_2$ (trigonal)

hkl hex.	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
003	5.8	100	5.85	100
101	3.29	60	3.27	70
102	--------	--------	3.114	11
006	--------	--------	2.925	3
104	2.66	80	2.648	90
015	2.40	25	2.412	28
107	1.99	12	1.998	18
009	--------	--------	1.943	10
110	1.92	40	1.922	31
-------	1.87	4	--------	--------
113	1.83	50	1.826	54
021	1.66	8	1.658	10
202	--------	--------	1.632	3
024	1.56	12	1.556	17
205	1.50	6	1.503	6
0·0·12	} 1.451	4	{ 1.4578	8
0·1·11	}		{ 1.4353	7
027	1.394	2	1.3855	6
119	1.374	4	1.3666	7
208	1.330	6	1.3245	8
211	1.258	6	1.2550	6
1·0·13	--------	--------	1.2473	2
214	1.214	8	1.2092	14
125	1.188	4	1.1846	4
0·0·15	1.166	6	1.1662	9
1·1·12	--------	--------	1.1616	3
2·0·11	--------	--------	1.1500	1
217	1.129	2	1.1239	1
300	1.118	2	1.1097	6
128	1.096	6	1.0905	10
1·0·16	--------	--------	1.0385	6
1·1·15	--------	--------	0.9971	6
1·2·11	--------	--------	.9867	4
309	--------	--------	.9632	7
220	--------	--------	.9612	5
223	--------	--------	.9483	4
131	--------	--------	.9220	4
2·1·13	--------	--------	.9190	4
0·2·16	--------	--------	.9137	3
134	--------	--------	.9036	9
1·0·19	--------	--------	.8871	2
3·0·12	--------	--------	.8829	8
137	--------	--------	.8657	4
318	--------	--------	.8507	7
2·1·16	--------	--------	.8253	8
404	--------	--------	.8176	5
3·0·15	--------	--------	.8036	4
2·2·12	--------	--------	.8024	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] L. Pauling, On the crystal structure of the chlorides of certain bivalent elements, Proc. Nat. Acad. Sci. U.S. **15**, 709–712 (1929).

[3] G. Bruni and A. Ferrari, Z. physik. Chem. **130**, 488–494 (1927).

[4] L. Pauling and J. L. Hoard, The crystal structure of cadmium chloride, Z. Krist. **74**, 546–551 (1930).

[5] Z. G. Pinsker and L. I. Tatarinova, Electronographic investigation of cadmium chloride, Acta Physicochim. U.S.S.R. **14**, 737–744 (1941).

Calcium Aluminate 12:7, $12CaO \cdot 7Al_2O_3$ (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-0912	2.69	Molybdenum	Harrington [1] 1927.
	5.04	Copper	Brownmiller and Bogue [2] 1932.
	2.44		
3-0149	4.85	Copper	Büssem and Eitel [3] 1936.
	2.67		
	2.98		
1-1057	2.68	Molybdenum	Hanawalt, Rinn, and Frevel [4] 1938.
	4.95		
	2.44		

The three ASTM cards above are reported as $5CaO \cdot 3Al_2O_3$; according to Büssem and Eitel [3] and to Thorvaldson and Schneider [5] the formula should be $12CaO \cdot 7Al_2O_3$.

Additional published patterns. None.

NBS sample. The sample of calcium aluminate was prepared by the Portland Cement Association Fellowship at NBS. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of sodium, silicon, and strontium; 0.01 to 0.1 percent each of iron and magnesium; and 0.001 to 0.01 percent each of copper, manganese, and molybdenum.

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

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

Pattern	1	2	3
Harrington	420	422	521
Brownmiller and Bogue	420	400	422
Hanawalt, Rinn, and Frevel	420	211	422
Büssem and Eitel	211	420	422
National Bureau of Standards	420	211	422

Structural data. Büssem and Eitel [3] in 1936, by consideration of the density, came to the conclusion that what was formerly called $5CaO \cdot 3Al_2O_3$ was in fact $12CaO \cdot 7Al_2O_3$. They then found that the space group was $I\bar{4}3d$ (No. 220), with $2(12CaO \cdot 7Al_2O_3)$ per unit cell. $12\ CaO \cdot 7Al_2O_3$ is used as a structure type.

The Büssem and Eitel unit-cell measurement has been converted from kX to angstrom units for comparison with the NBS values. The Harrington value was obtained from the powder pattern rather than his reported value.

Lattice constants

		A
1927	Harrington [1]	11.99
1936	Büssem and Eitel [3]	11.97
1959	National Bureau of Standards	11.982 at 25° C

The density of this compound, using the formula $12CaO \cdot 7Al_2O_3$, calculated from the NBS lattice constant is 2.676 g/cm³ at 25° C.

References

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

[2] L. T. Brownmiller and R. H. Bogue, The system CaO–Na_2O-Al_2O_3, Am. J. Sci. **23**, 501–524 (1932).

[3] W. Büssem and A. Eitel, Die Struktur des Pentacalciumtrialuminats, Z. Krist. **95**, 175–188 (1936).

[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] T. Thorvaldson and W. G. Schneider, The composition of "5:3" calcium aluminate, Can. J. Research **19B**, 109–115 (1941).

Calcium Aluminate 12:7, $12CaO \cdot 7Al_2O_3$ (cubic)

hkl	1927 Harrington Mo, 0.7107 A			1932 Brownmiller and Bogue Mo, 0.7107 A			1936 Büssem and Eitel Cu, 1.537 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A	A		A
211	------	------	------	------	------	------	4.84	>100	11.86	4.96	67	12.2	4.89	95	11.98
220	------	------	------	------	------	------	4.23	7	11.96	------	------	------	4.24	4	11.98
310	------	------	------	3.78	m	11.95	3.77	17	11.92	------	------	------	3.79	14	11.98
321	3.21	30	12.0	3.19	m	11.94	3.20	24	11.97	3.20	20	12.0	3.204	25	11.99
400	3.04	40	12.2	2.99	s	11.96	2.98	49	11.91	3.02	23	12.1	2.998	44	11.99
420	2.70	100	12.1	2.68	vs	11.96	2.67	97	11.93	2.69	100	12.0	2.680	100	11.99
332	------	------	------	2.56	m	12.01	2.54	16	11.91	------	------	------	2.556	17	11.99
422	2.45	80	12.0	2.44	s	11.95	2.44	52	11.93	2.44	50	12.0	2.447	52	11.99
510	------	------	------	2.34	m	11.93	2.34	16	11.95	------	------	------	2.350	9	11.98
521	2.19	80	12.00	2.184	s	11.96	2.186	46	11.97	2.19	50	12.0	2.189	40	11.988
530	------	------	------	2.059	w	12.01	2.049	6	11.95	------	------	------	2.054	8	11.979
611	1.949	70	12.01	1.947	s	12.00	1.938	35	11.95	1.94	50	12.0	1.945	28	11.989
----------	------	------	------	1.910	w	------	------	------	------	------	------	------	------	------	--------
541	------	------	------	1.850	w	11.99	1.844	5	11.95	------	------	------	1.850	6	11.982
----------	------	------	------	1.804	vw	------	------	------	------	------	------	------	------	------	--------
631	------	------	------	1.768	w	11.97	1.764	5	11.96	------	------	------	1.767	5	11.982
444	1.728	40	11.97	1.731	m	11.99	1.724	11	11.94	1.73	13	12.0	1.730	11	11.987
710	------	------	------	1.697	w	12.00	1.689	7	11.94	------	------	------	1.695	6	11.983
640	1.663	60	11.99	1.663	s	11.99	1.658	35	11.96	1.66	42	12.0	1.662	27	11.985
721	------	------	------	1.632	m	11.99	1.628	11	11.96	------	------	------	1.630	8	11.982
642	1.603	60	12.00	1.602	s	11.96	1.597	40	11.95	1.59	50	11.9	1.601	31	11.982
----------	------	------	------	1.557	w	------	1.539	9	------	------	------	------	------	------	--------
732	1.523	20	11.99	1.523	m	11.99	------	------	------	1.52	13	12.0	1.522	5	11.982
800	1.501	20	12.01	1.496	w	11.97	1.497	7	11.98	------	------	------	1.498	5	11.985
811	------	------	------	1.475	m	11.98	1.471	9	11.95	1.481	10	12.03	1.475	6	11.981
831	1.397	60	12.02	1.393	s	11.98	1.391	22	11.97	1.398	27	12.03	1.393	16	11.983
752	------	------	------	1.356	vw	11.98	------	------	------	------	------	------	1.356	3	11.976
840	1.345	20	12.03	1.339	w	11.98	------	------	------	1.347	10	12.05	1.340	6	11.983
842	1.313	30	12.03	1.308	m	11.99	------	------	------	1.312	17	12.02	1.307	7	11.982
921	------	------	------	1.293	vw	------	------	------	------	------	------	------	1.292	5	11.982
664	------	------	------	1.277	w	11.98	------	------	------	------	------	------	1.277	4	11.983
930	1.263	20	11.98	1.263	w	11.98	------	------	------	1.264	------	11.99	1.263	4	11.979
932	1.241	10	12.03	1.236	w	11.98	------	------	------	------	------	------	1.236	3	11.982
941	1.212	20	12.00	1.209	w	11.97	------	------	------	1.211	10	11.99	1.210	4	11.980
----------	------	------	------	1.189	vw	------	------	------	------	------	------	------	------	------	--------

Calcium Aluminate 12:7, $CaO \cdot 7Al_2O_3$ (cubic)

hkl	1927 Harrington Mo, 0.7107 A			1932 Brownmiller and Bogue Mo, 0.7107 A			1936 Bussem and Eitel Cu, 1.537 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
10·2·0	1.180	10	12.03	1.173	w	11.96	-----	-----	-----	1.176	10	11.99	1.175	1	11.984
10·3·1	1.144	10	12.00	1.142	vw	11.98	-----	-----	-----	1.143	7	11.99	1.143	2	11.985
10·4·0	1.115	30	12.01	1.112	m	11.98	-----	-----	-----	1.114	13	12.00	1.112	6	11.981
10·4·2	1.091	20	11.95	1.093	w	11.97	-----	-----	-----	1.093	3	11.97	1.094	4	11.980
11·1·0	-----	-----	-----	1.086	w	12.00	-----	-----	-----	-----	-----	-----	1.085	2	11.982
11·2·1	1.066 [a]	20	11.97	1.068 [b]	w	11.99	-----	-----	-----	-----	-----	-----	-----	-----	-----
Average value of last five lines	-----		11.99	-----	-----	11.98	-----	-----	11.97	-----	-----	11.99	-----	-----	11.982

[a] Eleven additional lines were omitted.
[b] Twelve additional lines were omitted.

Calcium Iron Silicate (andradite), $Ca_3Fe_2Si_3O_{12}$ (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
3–0814	2.69 1.61 3.01	Copper	Flint, McMurdie, and Wells [1] 1941.
3–1135	1.61 1.67 1.07	Copper	Menzer [2] 1929.

Additional published patterns. None.

NBS sample. The sample of calcium iron silicate was prepared at NBS by hydrothermal synthesis at 850° C and 20,000 psi using a cold seal bomb. The starting material was a gel made from nitrates of ferric iron and calcium, and ethyl orthosilicate. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, chromium, magnesium, molybdenum, and strontium; 0.0001 to 0.001 percent each of copper, potassium, sodium, nickel, and rubidium.

The sample had a brownish-reddish color. The index of refraction was 1.887.

Interplanar spacings and intensity measurements. The *d*-values reported by Flint, McMurdie, and Wells were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Flint, McMurdie, and Wells	420	642	400
Menzer	642	420	400
National Bureau of Standards	420	400	642

Structural data. Menzer [2] in 1929 determined that andradite was a member of the garnet group, the space group Ia3d (No. 230) and $8(Ca_3Fe_2Si_3O_{12})$ per unit cell.

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

Lattice constants

		A
1929	Menzer [2]	12.044
1935	Zedlitz [3]	12.043
1941	Flint, McMurdie, and Wells [1]	12.04
1959	National Bureau of Standards	12.059 at 25° C

Calcium Iron Silicate (andradite), $Ca_3Fe_2Si_3O_{12}$ (cubic)

hkl	1929 Menzer Cu, 1.5405 A			1941 Flint, McMurdie, and Wells Cu, 1.5405 A			1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
220	4.275	15	12.09	4.25	40	12.0	4.263	13	12.058
400	3.029	59	12.12	3.02	80	12.1	3.015	60	12.060
420	2.709	75	12.11	2.69	100	12.0	2.696	100	12.058
332	2.595	13	12.17	2.57	20	12.0	2.571	13	12.061
422	2.465	50	12.08	2.45	80	12.0	2.462	46	12.063
510	2.379	20	12.13	2.35	40	12.0	2.365	17	12.060
521	2.212	13	12.12	2.20	40	12.0	2.202	17	12.059
611	1.963	28	12.10	1.95	60	12.0	1.9564	24	12.060
620	1.914	17	12.10	1.89	40	12.0	1.9068	10	12.060
-------	1.859	8	----------	----------	------	----------	----------	------	----------
-------	1.790	22	----------	----------	------	----------	----------	------	----------
444	1.739	13	12.05	1.74	20	12.0	1.7406	8	12.059
-------	1.704	8	----------	----------	------	----------	----------	------	----------
640	1.675	50	12.08	1.67	60	12.0	1.6728	25	12.063
721	1.645	10	12.09	----------	------	----------	1.6412	2	12.060
642	1.613	100	12.07	1.61	100	12.0	1.6112	59	12.057
800	1.511	22	12.09	1.51	40	12.1	1.5073	13	12.058
-------	1.458	10	----------	----------	------	----------	----------	------	----------
822	1.425	13	12.10	----------	------	----------	1.4213	3	12.060
840	1.349	45	12.07	1.35	60	12.1	1.3483	13	12.060
842	1.316	45	12.06	1.31	60	12.0	1.3157	18	12.059
664	1.285	45	12.06	----------	------	----------	1.2856	12	12.060
844	1.243	7	12.18	1.25	60	12.1	1.2309	3	12.060
941	1.219	17	12.07	1.21	20	12.0	1.2182	4	12.060
-------	1.183	12	----------	----------	------	----------	----------	------	----------
-------	1.152	5	----------	----------	------	----------	----------	------	----------
-------	1.130	5	----------	----------	------	----------	----------	------	----------
10·4·0	1.119	53	12.06	1.11	60	12.0	1.1195	25	12.057
10·4·2	1.100	53	12.05	----------	------	----------	1.1008	15	12.059
880	1.065	50	12.06	----------	------	----------	1.0659	12	12.059
-------	1.031	7	----------	----------	------	----------	----------	------	----------
12·0·0	1.005	25	12.06	----------	------	----------	1.0049	7	12.059
12·2·0	0.990	25	12.05	----------	------	----------	0.9912	6	12.058
12·2·2	.978	67	12.06	----------	------	----------	.9781	17	12.059
11·6·3	.934	12	12.04	----------	------	----------	.9359	4	12.058
12·6·0	----------	------	----------	----------	------	----------	.8988	7	12.059
12·6·2	----------	------	----------	----------	------	----------	.8889	5	12.058
888	----------	------	----------	----------	------	----------	.8703	4	12.059
14·2·0	----------	------	----------	----------	------	----------	.8527	2	12.060
12·8·0	----------	------	----------	----------	------	----------	.8361	3	12.058
14·4·0	----------	------	----------	----------	------	----------	.8282	6	12.059
14·4·2	----------	------	----------	----------	------	----------	.8205	15	12.059
Average value of last five lines--			12.05	----------	------	12.0	----------	------	12.059

The density of andradite calculated from the NBS lattice constant is 3.849 g/cm³ at 25° C.

References

[1] E. P. Flint, H. F. McMurdie, L. S. Wells, Hydrothermal and X-ray studies of the garnet-hydrogarnet series and the relationship of the series to hydration products of Portland cement, J. Research Nat. Bur. Standards **26,** 13–33 (1941).

[2] G. Menzer, Die kristallstruktur der granate, Z. Krist. Mineral. **69,** 300–396 (1929).

[3] O. Zedlitz, Über titanhaltige kalkeisengranate, II, Zentr. Mineral. Geol., abt. A, 68–78 (1935).

Cesium Bromotellurate, Cs_2TeBr_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium bromotellurate was prepared at the NBS from bromotelluric acid and cesium bromide. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of potassium, sodium, and rubidium; and 0.001 to 0.01 percent each of aluminum, calcium, chromium, iron, magnesium, manganese, molybdenum, silicon, and vanadium.

The color of the sample is deep orange. The index of refraction was not obtained because the sample was too highly colored.

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

Pattern	1	2	3
National Bureau of Standards	222	400	440

Structural data. The structure of cesium bromotellurate has not been published, but it is thought to be isostructural with potassium chloroplatinate because of the similarity of patterns. Ewing and Pauling [1] in 1928 determined the structure of potassium chloroplatinate. The NBS pattern is indexed assuming the space group Fm3m (No. 225) with $4(Cs_2TeBr_6)$ per unit cell.

Lattice constants

		A
1959	National Bureau of Standards	10.919 at 25° C

The density of cesium bromotellurate calculated from the NBS lattice constant is 4.452 g/cm³ at 25°C.

Reference

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

Cesium Bromotellurate, Cs_2TeBr_6 (cubic)

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*
	A		A
111	6.31	27	10.92
200	5.46	4	10.92
220	3.862	37	10.92
311	3.295	17	10.92
222	3.151	100	10.92
400	2.728	86	10.91
331	2.505	6	10.92
420	2.439	4	10.91
422	2.229	16	10.92
511	2.1007	7	10.916
440	1.9301	48	10.918
531	1.8457	6	10.919
620	1.7269	4	10.922
533	1.6656	4	10.922
622	1.6466	24	10.922
444	1.5766	14	10.923
711	1.5294	4	10.922
642	1.4590	6	10.918
731	1.4213	3	10.917
800	1.3649	6	10.919
822	1.2867	2	10.918
662	1.2527	4	10.921
840	1.2209	10	10.920
911	1.1984	2	10.918
664	1.1638	1	10.917
931	1.1449	1	10.922
844	1.1147	5	10.922
933	1.0976	3	10.921
10·2·0	1.0710	2	10.922
951	1.0558	2	10.921
10·2·2	1.0509	3	10.921
953	1.0184	2	10.921
10·4·2	0.9966	3	10.917
11·1·1	.9845	1	10.919
880	.9650	1	10.918
11·3·1	.9540	1	10.919
10·6·0	.9362	1	10.918
10·6·2	.9228	3	10.919
12·0·0	.9098	5	10.918
12·2·2	.8857	2	10.920
12·4·0	.8632	2	10.919
Average value of last five lines			10.919

Cesium Nitrate, $CsNO_3$ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0779	3.15 1.99 1.82	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

X-ray data on ASTM card 4–0575 is for a cubic form of cesium nitrate and was obtained at 170° C.

Additional published patterns. None.

NBS sample. The sample of cesium nitrate was made from solutions of silver nitrate and cesium bromide. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent rubidium; 0.001 to 0.01 percent each of calcium and sodium; and 0.0001 to 0.001 percent each of aluminum, iron, potassium, magnesium, and silicon.

The sample is colorless and optically negative. The indices of refraction are $N_e = 1.554$ and $N_o = 1.560$.

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

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	112	411, 303	330, 114
National Bureau of Standards	112	111	003

Structural data. The most recent work on the structure of cesium nitrate was done by Finbak and Hassel [2] in 1937. They gave the most probable space group as P31m (No. 157) with $9(CsNO_3)$ per unit cell.

Finbak and Hassel [3] report that a cubic phase is stable above 161° C.

Waldbauer and McCann's unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1934	Waldbauer and McCann [4]	10.76	7.70
1959	National Bureau of Standards	10.950	7.716 at 25° C

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
111	4.46	27	4.467	38
112	3.16	100	3.153	100
202	--------	--------	2.996	4
221	2.58	27	2.583	11
003			2.573	38
103	--------	--------	2.483	3
302	--------	--------	2.453	2
222	2.23	23	2.232	21
411	1.99	40	1.999	19
303			1.996	26
330	1.82	33	1.826	18
114			1.820	22
600	1.57	13	1.580	3
224			1.576	6
333	1.49	20	1.4880	6
115			1.4852	10
522	1.41	17	1.4123	6
414			1.4110	9
441	1.34	10	1.3476	1
225			1.3446	5
442	1.28	1	1.2892	2
711	1.24	5	1.2397	4
415			1.2361	5
505	1.19	12	1.1960	5
306			1.1914	4
444	1.11	1	1.1164	2
633	1.08	4	1.0833	6
117			1.0806	4
217				
900	--------	--------	1.0539	2
336	--------	--------	1.0507	2
516	--------	--------	1.0265	1
445	--------	--------	1.0242	1
227	------	--------	1.0220	1

The density of cesium nitrate calculated from the NBS lattice constants is 3.635 g/cm³ at 25° C.

References

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

[2] C. Finbak and O. Hassel, The structure of caesium nitrate, J. Chem. Phys. **5**, 460–461 (1937).

[3] C. Finbak and O. Hassel, Rotation von Anionpolyedern in kubischen Kristallgittern. III. Die Nitrate, Z. physik. Chem. **35**, 25–28 (1937).

[4] L. Waldbauer and D. C. McCann, Caesium nitrate and the perovskite structure, J. Chem. Physics **2**, 615–617 (1934).

beta-Chromium Orthophosphate, β-$CrPO_4$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
*5-0662	2.48 3.51 4.30	Copper	National Bureau of Standards [1] 1951, [2] 1952.

* This ASTM card was reported without indexing.

Additional published patterns. None.

NBS sample. The sample of beta-chromium orthophosphate was prepared at the NBS by heating the unground hexahydrate between 1,000°C and 1,100°C for $\frac{1}{2}$ hr. Longer heating or heating finely ground hexahydrate tends to produce the stable alpha form. Spectrographic analysis showed no impurities greater than 0.001 percent.

The sample has an olive green color. The very fine highly birefringent particles show no extinction positions and have an average index of 1.908.

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

Pattern	1	2	3
National Bureau of Standards	112	111	110

Structural data. Mooney [3] in 1956 determined that beta-chromium orthophosphate has the space group Cmcm (No. 63) and 4($CrPO_4$) per unit cell.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1956	Mooney [3]	5.15	7.77	6.11
1957	Hughes, Lewis and Wilson [4]	5.166	7.750	6.131
1959	National Bureau of Standards	5.165	7.750	6.131 at 25° C

The density of beta-chromium orthophosphate calculated from the NBS lattice constants is 3.971 g/cm³ at 25° C.

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
	A	
110	4.30	74
020	3.874	41
111	3.520	95
021	3.276	51
200	2.582	50
112	2.497	100
130	2.310	54
220	2.148	5
221	2.030	5
202	1.975	37
040	1.938	20
113	1.845	4
023	1.808	6
222	1.760	28
310	1.681	2
042	1.638	20
311	1.621	5
133	1.533	12
241	1.503	5
150	1.4847	4
312	1.4744	16
114, 151	1.4431	7
330	1.4328	10
242	1.3837	37
152	1.3362	6
204	1.3187	6
060, 400	1.2917	10
134	1.2778	14
243	1.2351	1
044, 421	1.2015	8
115	1.1798	3
333	1.1728	1
350	1.1521	2

References

[1] Joint Committee Fellowship Report, Nat. Bur. Standards (U.S.), Oct. 1951.

[2] B. M. Sullivan and H. F. McMurdie, Crystal forms of chromium orthophosphate, J. Research, Nat. Bur Standards **48**, No. 2, 159–162 (1952).

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

[4] J. W. Hughes, I. E. Lewis, and A. J. C. Wilson, Comments on the A.S.T.M. X-ray Powder Data File, Cardiff, Great Britain (1957).

Cobalt Aluminum Oxide, $CoAl_2O_4$ (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-1410	1.43 2.43 1.55	Iron	Natta and Passerini [1] 1929.
3-0896	2.44 2.86 1.43	Molybdenum	Dow Chemical Co.

Additional published patterns

Source	Radiation
Holgersson [2] 1927	Iron

NBS sample. The sample of cobalt aluminate was prepared at NBS by solid state reaction by heating hydroxides of cobalt and aluminum at 1,100° C. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of sodium; 0.01 to 0.1 percent each of calcium, iron, magnesium, manganese, nickel, and silicon; 0.001 to 0.01 percent of copper; and 0.0001 to 0.001 percent of chromium.

The color of the sample was deep blue. The index of refraction could not be determined because the sample was too highly colored.

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

Pattern	1	2	3
Holgersson	511	440	311
Natta and Passerini	440	311	511
Dow Chemical Co.	311	220	440
National Bureau of Standards	311	220	440

Structural data. Holgersson [2] in 1927 determined that cobalt aluminate has the spinel-type structure, the space group Fd3m (No. 227) and $8(CoAl_2O_4)$ per unit cell.

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

Lattice constants

		A
1927	Holgersson [2]	8.09
1929	Natta and Passerini [1]	8.08
1934	Krause and Thiel [3]	8.09
1959	National Bureau of Standards	8.103 at 26° C

hkl	1927 Holgersson Fe, 1.9360 A			1929 Natta and Passerini Fe, 1.9360 A			---- Dow Chemical Co. Mo, 0.7107 A			1959 National Bureau of Standards Cu, 1.5405 A at 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A
220	2.85	m	8.06	2.86	70	8.09	2.87	50	8.117	2.864	66	8.100
311	2.44	s	8.09	2.43	80	8.06	2.44	100	8.092	2.443	100	8.102
400	------	----	------	2.02	60	8.08	2.01	12	8.040	2.026	17	8.104
331	------	----	------	------	----	------	1.86	2	8.108	1.8608	5	8.111
422	------	----	------	1.65	70	8.08	1.65	10	8.083	1.6541	16	8.103
511	1.558	vs	8.10	1.55	80	8.05	1.56	25	8.106	1.5602	34	8.107
440	1.421	vs	8.04	1.428	100	8.09	1.43	50	8.089	1.4324	41	8.103
531	------	----	------	1.365	40	8.07	------	----	------	1.3716	1	8.114
620	------	----	------	1.279	50	8.09	1.27	2	8.032	1.2821	7	8.109
533	------	----	------	1.227	50	8.05	1.23	4	8.066	1.2360	2	8.105
642	------	----	------	1.078	80	8.07	1.08	4	8.082	1.0826	2	8.101
731	1.051	s	8.07	1.051	80	8.07	1.05	8	8.065	1.0551	3	8.104
800	1.012	s	8.10	1.010	80	8.08	------	----	------	1.0131	1	8.105
822	------	----	------	------	----	------	0.955	2	8.103	0.9547	2	8.101
751	------	----	------	------	----	------	.936	2	8.105	.9355	2	8.102
Average value of last five lines			8.08	------	----	8.07	------	----	8.084	------	----	8.103

The density of cobalt aluminate calculated from the NBS lattice constant is 4.416 g/cm³ at 26° C.

References

[1] G. Natta and L. Passerini, Spinelli del cobalto bivalenti; aluminato, cromito, ferrito, e cobaltito cobaltosi, Gazz. chim. ital. **59**, 280–288 (1929).

[2] S. Holgersson, Röntgenographische Untersuchungen der Mineralien der Spinellgruppe und von Synthetisch Dargestellten Substanzen von Spinelltypus, Acta Univ. Lundensis **23**, 5–112 (1927).

[3] O. Krause and W. Thiel, Über keramische Farbkorper II, Ber. deut. keram. Ges. **15**, 111–127 (1934).

Cobalt(II) Oxide, CoO (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–1233	2.12 1.50 2.45	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Bravo [2] 1926	Iron
Natta and Strada [3] 1928	Nickel
Holgersson and Karlsson [4] 1929	Iron

NBS sample. The sample of cobalt oxide was prepared at NBS by heating cobalt hydroxide at hydroxide at 950° C for 12 hr and then at 1,200° C for 1 hr. Spectrographic analysis shows the following impurities: 0.1 to 1.0 percent each of nickel and calcium; 0.01 to 0.1 percent each of silicon and magnesium; and 0.001 to 0.01 each of copper and manganese.

The sample is an opaque black powder.

Interplanar spacings and intensity measurements. The *d*-values reported by Bravo were converted from kX to angstrom units and the *d*-values reported by Natta and Strada and by Holgersson and Karlsson were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Bravo	200	220	311
Natta and Strada	224	420	200
Holgersson and Karlsson	200	220	111
Hanawalt, Rinn, and Frevel	200	220	111
National Bureau of Standards	200	111	220

Cobalt(II) Oxide, CoO (cubic)

hkl	1926 Bravo Fe, 1.937 A			1928 Natta and Strada Ni, 1.6591 A			1929 Holgersson and Karlsson Fe, 1.936 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1959 National Bureau of Standards Co, 1.7889 A at 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A	A		A
111	2.433	m	4.214	2.48	14	4.16	2.496	s	4.263	2.45	67	4.244	2.460	73	4.261
200	2.114	vs	4.218	2.12	39	4.17	2.161	vs	4.255	2.12	100	4.240	2.130	100	4.260
220	1.505	vs	4.246	1.48	34	4.19	1.506	vs	4.256	1.50	100	4.243	1.5062	49	4.260
311	1.287	s	4.257	1.27	9	4.20	1.287	s	4.264	1.283	40	4.255	1.2846	22	4.261
222	1.230	s	4.248	1.21	15	4.20	1.231	s	4.261	1.229	40	4.257	1.2298	15	4.260
----	1.081	w	------	------	------	------	1.067	s	4.263	1.062	10	4.248	1.0651	9	4.260
400	1.065	s	4.260	0.97	9	4.21	------	------	------	0.977	10	4.259	0.9775	13	4.261
331	------	------	------	.94	64	4.20	------	------	------	.953	30	4.262	.9526	28	4.260
420	------	------	------	(a)			------	------	------	(b)					
Average value of last five lines			4.246	------	------	4.20	------	------	4.260	------	------	4.251	------	------	4.260

[a] One additional line was omitted.
[b] Two additional lines were omitted.

Structural data. Cobalt oxide has the sodium chloride-type structure, the space group Fm3m (No. 225), and 4(CoO) per unit cell.

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

Lattice constants

		A
1926	Bravo [2]	4.33
1928	Natta and Strada [3]	4.22
1929	Holgersson and Karlsson [4]	4.262
1929	Ingersoll and Hanawalt [5]	4.25
1929	Passerini and Natta [6]	4.23
1940	Baroni [7]	4.23
1950	Tombs and Rooksby [8]	4.258
1959	National Bureau of Standards	4.260 at 26° C

The density of cobalt oxide calculated from the NBS lattice constant is 6.437 g/cm³ at 26° C.

References

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

[2] F. M. Bravo, Determinacion de la Estructura Cristalina del Oxido de Niquel, del Oxido de Cobalto y del Sulfuro de Plomo, Anal. Espan. Fis y Quim. **24,** 611–646 (1926).

[3] G. Natta and M. Strada, Ossidi ed Ideoossidi del cobalto, Gazz. Chim. Ital. **58,** 419 (1928).

[4] S. Holgersson and A. Karlsson, Roentgenographische Untersuchungen einiger Mischkristallsysteme mit Monoxyden als Komponenten, Z. Anorg. Chem. **182,** 255–271, (1929).

[5] L. R. Ingersoll and J. D. Hanawalt, The gas content, crystal structure and hydrogen absorption of sputtered nickel films, Phys. Rev. **34,** 972–977 (1929).

[6] L. Passarini and G. Natta, Soluzioni Solide Isomorfismo e Simmorfismo tra gli ossidi di metalli bivalenti II, Gazz. Chim. Ital. **59,** 144–154 (1929).

[7] A. Baroni, Sugli Ossidi di Cobalto, Gazz. Chim. Ital. **70,** 483 (1940).

[8] N. C. Tombs and H. P. Rooksby, Structures of monoxide of some transition elements at low temperatures, Nature **165,** 442–443 (1950).

Cobalt(II,III) Oxide, Co_3O_4 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–1152	2.43 1.43 1.56	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of cobalt oxide was prepared at NBS by heating cobalt fluoride to 850° C for 24 hr. Spectrographic analysis shows the following impurities: 0.1 to 1.0 percent each of calcium and nickel; 0.01 to 0.1 percent each of aluminum, iron, magnesium, and silicon; and 0.001 to 0.01 percent each of barium, copper, and manganese.

The sample was a black opaque powder.

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

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	311	440	511
National Bureau of Standards	311	440	220

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1959 National Bureau of Standards Co, 1.7889 A at 24° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	4.68	8	8.11	4.669	22	8.087
220	2.86	20	8.09	2.860	41	8.089
311	2.43	100	8.06	2.438	100	8.085
222	2.34	6	8.11	2.333	11	8.083
400	2.02	13	8.080	2.021	27	8.082
422	1.65	4	8.08	1.6505	11	8.086
511	1.56	25	8.10	1.5559	37	8.085
440	1.43	30	8.09	1.4293	43	8.085
620	-----	---	-----	1.2788	4	8.088
533	1.24	2	8.13	1.2330	11	8.085
622	-----	---	-----	1.2191	6	8.087
444	-----	---	-----	1.1671	3	8.086
711	-----	---	-----	1.1321	2	8.085
642	1.08	1	8.08	1.0803	6	8.084
731	1.06	4	8.14	1.0524	16	8.084
800	1.01	1	8.08	1.0105	7	8.084
822	-----	---	-----	0.9529	4	8.085
751	0.93	2	8.05	.9335	15	8.084
662	-----	---	-----	.9275	5	8.085
	[a]					
Average value of last five lines			8.10	------		8.084

[a] Two additional lines were omitted.

Structural data. Cobalt oxide is a member of the spinel group, the space group being Fd3m (No. 227) with $8(Co_3O_4)$ per unit cell [5].

Lattice constants

1928	Hendricks and Albrecht	8.06
1928	Natta and Strada	8.08
1929	Holgersson and Karlsson	8.124
1934	Kraus and Thiel [2]	8.07
1946	Gulbransen and Hickman	8.11
1959	National Bureau of Standards	8.084 at 24° C

The density of cobalt oxide calculated from the NBS lattice constants is 6.054 g/cm³ at 24° C.

References

[1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. **10**, 451–512 (1938).

[2] O. Kraus and W. Thiel, Über Keramische Farbkörper, Ber. Deut. Keram. Ges. **15**, 101 (1934).

[3] E. A. Gulbransen and J. W. Hickman, An electron diffraction study of oxide films formed on iron, cobalt, nickel, chromium, and copper at high temperatures. Metals Technol. **13**, A. I. M. M. E. Tech. Pub. 2068 (1946).

[4] S. Holgersson and A. Karlsson, Über einige neue Kobaltite vom Spinelltypus. Z. Anorg. Chem. **183**, 384–394 (1929).

[5] S. B. Hendricks and W. H. Albrecht, X-ray and chemical investigations of various oxides of iron and cobalt, Ber. deut. Keram. Ges. **61B**, 2153–61 (1928).

[6] G. Natta, M. Strada, Spinelli del cobalto trivalenti: cobaltito cobaltoso e cobaltito di zinco, Rend. Accad. Naz. Lincei **7**, 1024–1030 (1928).

Dysprosium(III) Oxide, Dy_2O_3 (cubic)

ASTM cards. None.

Additional published patterns

Source	Radiation
Zachariasen [1] 1928	Iron

NBS sample. The sample of dysprosium sesquioxide was prepared by the Lindsay Chemical Co., West Chicago, Ill. Their analysis showed the following impurities: a total of less than 0.1 percent of holmium and yttrium oxides and traces of other rare earths. The sample was annealed at 1,100° C for a period of 16 hr.

The sample was colorless. The index of refraction was not determined because the sample was too fine-grained.

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

Pattern	1	2	3
Zachariasen	222	440	622
National Bureau of Standards	222	440	400

Structural data. Pauling and Shappell [9] in 1930 determined that dysprosium sesquioxide has the thallium oxide type structure (rare earth type C), the space group Ia3(No. 206) and $16(Dy_2O_3)$ per unit cell.

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

hkl	1928 Zachariasen Fe, 1.9360 A			1959 National Bureau of Standards Co, 1.7889 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
211	4.37	15	10.69	4.35	15	10.656
222	3.067	100	10.62	3.079	100	10.665
321	2.845	3	10.65	2.850	2	10.664
400	2.655	30	10.62	2.666	42	10.663
411	2.496	8	10.59	2.514	8	10.667
420	------	---	------	2.3856	2	10.669
332	2.260	5	10.60	2.2733	6	10.663
422	------	---	------	2.1765	1	10.663
431	2.077	15	10.59	2.0911	11	10.663
521	1.931	5	10.58	1.9479	3	10.669
440	1.872	100	10.59	1.8848	44	10.662
433	1.818	5	10.60	1.8288	3	10.664
600	1.760	18	10.56	1.7779	<1	10.667
611	1.718	15	10.59	1.7298	6	10.663
620	1.675	<2	10.59	1.6865	1	10.666
541	1.635	10	10.60	1.6458	5	10.666
622	1.596	100	10.58	1.6079	34	10.666
631	1.561	15	10.59	1.5726	7	10.666
444	1.529	20	10.59	1.5395	8	10.666
543	1.497	10	10.59	1.5087	3	10.668
640	1.468	5	10.58	1.4793	1	10.667
721	1.440	15	10.58	1.4517	4	10.668
642	1.415	10	10.59	1.4255	2	10.667
732	1.345	10	10.59	1.3548	3	10.668
800	1.324	20	10.59	1.3334	5	10.667
811	1.304	25	10.59	1.3131	4	10.667
820	1.285	10	10.60	1.2935	2	10.666
653	1.267	15	10.60	1.2748	3	10.666
822	1.250	10	10.60	1.2570	2	10.666
831	1.233	25	10.61	1.2399	5	10.666
662	1.226	60	10.68	1.2234	10	10.665
840	1.1862	40	10.610	1.1926	8	10.667
833	1.1713	8	10.607	1.1779	1	10.666
842	1.1581	8	10.614	1.1638	2	10.666
921	1.1453	20	10.621	1.1501	3	10.666

Dysprosium(III) Oxide, Dy_2O_3 (cubic)

hkl	1928 Zachariasen Fe, 1.9360 A			1958 National Bureau of Standards Co, 1.7889 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
851	1.1187	20	10.613	1.1243	3	10.666
932	------	---	------	1.1001	3	10.666
844	------	---	------	1.0886	7	10.666
941	------	---	------	1.0774	3	10.666
10·0·0	------	---	------	1.0666	2	10.666
10·1·1	------	---	------	1.0562	1	10.667
10·2·0	------	---	------	1.0458	4	10.665
943	------	---	------	1.0361	1	10.667
10·2·2	------	---	------	1.0264	10	10.667
10·3·1	------	---	------	1.0170	4	10.666
871	------	---	------	0.9989	5	10.665
10·4·0	------	---	------	.9903	4	10.666
10·3·3	------	---	------	.9818	3	10.665
10·4·2	------	---	------	.9736	4	10.665
954	------	---	------	.9656	3	10.665
11·2·1	------	---	------	.9501	4	10.665
880	------	---	------	.9427	2	10.665
10·4·4	------	---	------	.9283	2	10.665
11·3·2	------	---	------	.9214	4	10.665
10·6·0	------	---	------	.9145	2	10.665
11·4·1	------	---	------	.9079	3	10.665
Average value of last five lines		---	10.613	------	---	10.665

Lattice constants

		a
		A
1925	Goldschmidt, Barth, and Lunde [3]	10.65
1928	Zachariasen [1]	10.65
1939	Bommer [4]	10.650
1954	Templeton and Dauben [5]	10.667
1959	National Bureau of Standards	10.665 at 25° C

The density of dysprosium sesquioxide calculated from the NBS lattice constant is 8.167 g/cm³ at 25° C.

References

[1] W. Zachariasen, The crystal structure of the sesquoixides and compounds of the type ABO_3, Skrifter Norske Videnskaps-Akad., Oslo I. Mat.-Naturv. Kl. 1928, No. 4 (1928).

[2] L. Pauling and M. D. Shappell, The crystal structure of Bixbyite and the C-modification of the sesquioxides, Z. Krist. **75**, 128–142 (1930).

[3] V. M. Goldschmidt, T. Barth, and G. Lunde, Isomorphie und Polymorphie der Sesquioxide, die Lanthaniden-Kontraktion und ihre Konsequenzen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. No. **7**, 1–59 (1925).

[4] H. Bommer, Die Gitterkonstanten der C-Formen der Oxyde der seltenen Erdmetalle, Z. anorg. u. allgem. Chem. **241**, 273–280 (1939).

[5] D. H. Templeton and C. H. Dauben, Lattice parameters of some rare earth compounds and a set of crystal radii, J. Am. Chem. Soc. **76**, 5237–5239 (1954).

Erbium Phosphate, $ErPO_4$ (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of erbium phosphate was prepared hydrothermally at 400° C from erbium oxide and dilute phosphoric acid. Spectrographic analysis showed no impurities greater than 0.01 percent.

The sample has a pink color. The indices of refraction were not determined because of the small particle size.

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

Pattern	1	2	3
National Bureau of Standards	200	112	101

Structural data. The structure of erbium phosphate has not been published. It is thought to have a zirconium silicate-type structure because of similarity of patterns. The NBS pattern was indexed assuming the space group to be $I4_1/amd$ (No. 141) with $4(ErPO_4)$ per unit cell.

Lattice constants

		a	*c*
		A	*A*
1959	National Bureau of Standards	6.863	6.007 at 25° C

The density of erbium phosphate calculated from the NBS lattice constants is 6.155 g/cm³ at 25° C.

Erbium Phosphate, $ErPO_4$ (tetragonal)

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C		*hkl*	1959 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*		*d*	*I*
	A			*A*	
101	4.52	56	325	1.0161	2
200	3.432	100	631	1.0081	2
211	2.733	23	613	0.9833	5
112	2.554	67	116	.9808	<1
220	2.426	19	415	.9743	1
202	2.261	11	701	.9678	1
301	2.1382	25	640	.9520	3
103	1.9224	14	543	.9451	3
321	1.8144	19	444	.9441	<1
312	1.7596	44	721	.9313	1
400	1.7157	13	712	.9238	6
213	1.6771	9	604	.9095	6
411	1.6039	5	316		
420	1.5347	10	505	.9041	1
303	1.5063	2	624	.8797	5
004	1.5023	4	525	.8745	2
332	1.4244	12	732	.8631	5
323	1.3792	10	800	.8579	2
204	1.3759	<1	723	.8529	2
431	1.3379	6	107	.8514	1
413	1.2802	10	811	.8429	<1
224	1.2769	<1	426	.8380	1
521	1.2465	1	820	.8324	1
512	1.2283	9	217	.8267	1
440	1.2120	2	802	.8225	1
105	1.1832	2	660	.8089	1
600	1.1438	5	644	.8040	8
503	1.1321	<1	307	.8033	<1
404	1.1301	6	516		
215	1.1189	4	545	.8000	1
611	1.1089	2	831	.7962	<1
532	1.0957	8	813	.7833	<1
620	1.0851	4	327	.7823	<1
424	1.0732	9			
541	1.0550	1			

Holmium(III) Oxide, Ho_2O_3 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of holmium sesquioxide was prepared by the Lindsay Chemical Co., West Chicago, Ill. Their analysis showed the following impurities: a total of less than 0.1 percent of erbium and dysprosium oxides and traces of other rare earths. The sample was annealed at 1,100° C for a period of 16 hr.

The sample was colorless. The index of refraction was not determined because the sample was too fine-grained.

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

Pattern	1	2	3
National Bureau of Standards	222	440	400

Structural data. Pauling and Shappell [3] in 1930 determined that holmium sesquioxide has the thalliumoxide type structure (rare earth type C), the space group Ia3(No. 206) and 16(Ho_2O_3) per unit cell.

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

Holmium(III) Oxide, Ho_2O_3 (cubic)

hkl	1959 National Bureau of Standards Co, 1.7889 A at 25° C			hkl	1959 National Brueau of Standards Co, 1.7889 A at 25° C		
	d	I	a		d	I	a
	A		A		A		A
211	4.334	14	10.616	662	1.2171	8	10.610
222	3.061	100	10.604	840	1.1861	7	10.609
321	2.835	2	10.608	833	1.1715	1	10.608
400	2.651	41	10.606	842	1.1576	1	10.610
411	2.500	7	10.606	921	1.1440	3	10.609
420	2.3723	1	10.609				
332	2.2613	5	10.606	851	1.1182	2	10.608
422	2.1652	1	10.607	932	1.0942	3	10.609
431	2.0796	10	10.604	844	1.0827	6	10.608
521	1.9361	3	10.604	941	1.0715	2	10.607
				10·0·0	1.0608	2	10.608
440	1.8754	42	10.609				
433	1.8195	3	10.609	10·1·1	1.0504	1	10.608
600	1.7670	<1	10.602	10·2·0	1.0400	4	10.606
611	1.7204	6	10.605	943	1.0302	1	10.607
620	1.6767	1	10.604	10·2·2	1.0206	7	10.606
541	1.6366	5	10.606	10·3·1	1.0112	4	10.606
622	1.5989	30	10.606				
631	1.5637	7	10.606	871	0.9934	3	10.606
444	1.5311	7	10.608	10·4·0	.9848	4	10.607
543	1.4997	2	10.604	10·3·3	.9764	2	10.607
				10·4·2	.9682	4	10.606
640	1.4706	1	10.605	954	.9603	3	10.607
721	1.4434	3	10.607				
642	1.4170	2	10.604	11·2·1	.94491	4	10.6066
732	1.3468	3	10.605	880	.93744	2	10.6059
800	1.3259	4	10.607	10·4·4	.92317	2	10.6064
				11·3·2	.91625	4	10.6064
811	1.3056	4	10.607	10·6·0	.90949	2	10.6064
820	1.2863	2	10.607				
653	1.2680	3	10.609	Average value of last five lines---		--------	10.6063
822	1.2503	1	10.609				
831	1.2333	4	10.609				

Lattice constants

		A
1925	Goldschmidt, Barth, and Lunde [2]---	10.60
1927	Zachariasen [1]----------	10.60
1954	Templeton and Dauben [4]----------	10.607
1959	National Bureau of Standards--------	10.606 at 25° C

The density of holmium sesquioxide calculated from the NBS lattice constant is 8.413 g/cm³ at 25° C.

References

[1] W. 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 (1927).

[2] V. M. Goldschmidt, T. Barth, and G. Lunde, Isomorphie und Polymorphie der Sesquioxide, die Lanthaniden-Kontraktion und ihre Konsequenzen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. No. **7**, 1–59 (1925).

[3] L. Pauling and M. D. Shappell, The crystal structure of Bixbyite and the C-modification of the sesquioxides, Z. Krist. **75**, 128–142 (1930).

[4] D. H. Templeton and C. H. Dauben, Lattice parameters of some rare earth compounds and a set of crystal radii, J. Am. Chem. Soc. **76**, 5237–5239 (1954).

Magnesium Chromite (picrochromite) $MgCr_2O_4$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
2-1228	2.08 1.60 1.47	Chromium	Holgersson [1] 1930.

Additional published patterns

Source	Radiation
Passerini and Bruni [2] 1929	Iron
Andrews [6] 1951	Cobalt

NBS sample. The sample of magnesium chromite was prepared at the NBS by fusion of MgO and Cr_2O_3 in a carbon arc with subsequent heating to remove carbides. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of sodium and silicon; 0.01 to 0.1 percent of aluminum, calcium, and iron; and 0.001 to 0.01 percent of copper, nickel, strontium, and titanium.

The color of the sample was dark brownish-green. The index of refraction was too high to be measured by the usual oil immersion method.

Interplanar spacings and intensity measurements. Several patterns were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Passerini and Bruni	440	400	444
Holgersson	400	511	440
Andrews	440	840	311
National Bureau of Standards	311	111	400

hkl	1929 Passerini and Bruni Fe, 1.9373 A			1930 Holgersson Cr, 2.2909 A			1951 Andrews Co, 1.790 A			1959 National Bureau of Standards Cu, 1.5405 A at 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A
111	------	----	------	------	----	------	4.81	vvw	8.331	4.813	65	8.335
220	2.863	2	8.10	2.942	20	8.321	2.946	vw	8.333	2.945	13	8.331
311	2.449	17	8.12	2.514	80	8.338	2.512	ms	8.331	2.512	100	8.331
222	2.343	1	8.12	------	----	------	2.406	vw	8.335	2.406	12	8.335
400	2.040	42	8.16	2.083	100	8.332	2.083	ms	8.332	2.083	56	8.332
331	------	----	------	------	----	------	1.912	vvw	8.334	1.912	5	8.334
422	1.676	3	8.21	------	----	------	1.701	vw	8.333	1.701	2	8.333
511	1.589	11	8.26	1.603	100	8.329	1.604	m	8.334	1.603	39	8.332
440	1.463	100	8.28	1.474	100	8.338	1.4731	s	8.333	1.4731	53	8.333
531	1.404	4	8.31	------	----	------	1.4085	vw	8.333	1.4089	13	8.335
620	1.315	2	8.32	1.319	20	8.342	1.3177	vvw	8.334	1.3176	1	8.333
533	1.270	9	8.33	1.273	100	8.348	1.2709	mw	8.334	1.2711	13	8.335
622	1.254	2	8.32	------	----	------	1.2563	mw	8.333	1.2563	9	8.333
444	1.200	33	8.31	------	----	------	1.2028	mw	8.333	1.2028	9	8.333
711	------	----	------	------	----	------	1.1668	w	8.333	1.1666	8	8.331
642	------	----	------	------	----	------	1.1135	vw	8.333	1.0136	2	8.333
731	------	----	------	------	----	------	1.0849	ms	8.333	1.0850	10	8.334
800	------	----	------	------	----	------	1.0417	mw	8.334	1.0417	4	8.334
822	------	----	------	------	----	------	0.9821	vvw	8.333	0.9821	<1	8.333
751	------	----	------	------	----	------	.9622	ms	8.333	.9623	6	8.334
662	------	----	------	------	----	------	.9559	mw	8.333	.9559	1	8.333
840	------	----	------	------	----	------	.9317	s	8.333	.9317	6	8.333
911	------	----	------	------	----	------	.9147	m	8.333	.9146	4	8.332
931	------	----	------	------	----	------	------	----	------	.8736	5	8.333
844	------	----	------	------	----	------	------	----	------	.8505	9	8.333
933	------	----	------	------	----	------	------	----	------	.8375	2	8.333
951	------	----	------	------	----	------	------	----	------	.8056	8	8.333
10·2·2	------	----	------	------	----	------	------	----	------	.8019	3	8.334
Average value of last five lines			8.32	------	----	8.338	------	----	8.333	------	----	8.333

Structural data. Passerini and Bruni [2] in 1929 showed that magnesium chromite has the spinel-type structure, the space group Fd3m (No. 227) and 8($MgCr_2O_4$) per unit cell.

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

Lattice constants

		A
1929	Passerini and Bruni [2]	8.31
1930	Holgersson [1]	8.34
1946	Lovell, Rigby, and Green [3]	8.33
1946	Rait [4]	8.325
1946	Verwey, Haayman, and Heilman [5]	8.33
1951	Andrews [6]	8.323
1959	National Bureau of Standards	8.333 at 26° C

The density of magnesium chromite calculated from the NBS lattice constant is 4.414 g/cm³ at 26° C.

References

[1] S. Holgersson, Röntgenographische Untersuchungen einiger synthetisch dargestellten Chromspinelle, Z. anorg. Chem. **192**, 123–128 (1930).

[2] L. Passerini and S. Bruni, Ricerche Sugli Spinelli, Rend. Accad. Naz. Lincei **9**, 338–343 (1929).

[3] G. H. B. Lovell, G. R. Rigby, and A. T. Green, An investigation of chrome ores, Iron and Steel Inst. Spec. Report **32**, 153–170 (1946).

[4] J. R. Rait, An X-ray investigation into the constitution of chrome ores, Iron and Steel Spec. Report **32**, 175–209 (1946).

[5] E. J. W. Verwey, P. W. Haayman, and E. L. Heilman, On the crystalline structure of ferrites and analogous metal oxides, Philips Tech. Rev. **9**, 185–190 (1946).

[6] K. W. Andrews, An X-ray study of spinels in relation to chrome magnesite refractories, Trans. Brit. Ceram. Soc. **50**, 47–74 (1951).

Manganese Aluminate (galaxite), $MnAl_2O_4$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–1302	1.40 2.50 2.39	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Holgersson [2] 1927	Iron
Clark, Ally, and Badger [3] 1931	Molybdenum

NBS sample. The sample of manganese aluminate was made at NBS by heating $MnCO_3$ and $Al(OH)_3$ to 1,300° C for 24 hr. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of cobalt and sodium; 0.01 to 0.1 percent silicon; and 0.001 to 0.01 percent each of chromium, copper, iron, and magnesium.

The color of the sample was brown. The index of refraction could not be determined because the sample was too dark.

Interplanar spacings and intensity measurements. The *d*-values reported by Clark, Ally, and Badger [3] were modified to correspond to a wavelength change of K_{α_1} 0.712 to K_{α_1} 0.7093 A. The *d*-values reported by Holgersson [2] and Hanawalt, Rinn, and Frevel [1] were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	---	311	222
Holgersson	311	400	511
Clark, Ally, and Badger	311	220	511
National Bureau of Standards	311	220	440

Structural data. Bragg [4] in 1915 determined the structure of the spinel group. Manganese aluminate has the spinel-type structure, the space group Fd3m (No. 227), and 8($MnAl_2O_4$) per unit cell.

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

Lattice constants

		A
1927	Holgersson [2]	8.28
1931	Clark, Ally, and Badger [3]	8.24
1931	Krause and Thiel [5]	8.29
1959	National Bureau of Standards	8.258 at 25° C

The density of manganese aluminate calculated from the NBS lattice constant is 4.077 g/cm³ at 25° C.

References

[1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. **10**, 451–512 (1938).

[2] S. Holgersson, X-ray examination of the minerals of the spinel group and of synthesized substances of the spinel type, Lunds Univ. Årsskr. **23**, No. 9, 1–112 (1927).

[3] G. L. Clark, A. Ally, and A. E. Badger, The lattice dimensions of spinels, Am. J. Sci. **22**, 539–546 (1931).

[4] W. H. Bragg, The structure of the spinel group of crystals, Nature **95**, 561 (1915).

[5] O. Krause and W. Thiel, The structure of some ceramic coloring materials containing aluminum oxide, Z. Anorg. Chem. **203**, 120–128 (1931).

Manganese Aluminate (galaxite), $MnAl_2O_4$ (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1927 Holgersson Fe, 1.9373 A			1931 Clark, Ally, and Badger Mo, 0.7093 A			1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A
220	2.93	17	8.29	2.921	w	8.26	2.91	70	8.231	2.921	58	8.262
311	2.50	50	8.29	2.499	vs	8.29	2.48	100	8.225	2.494	100	8.265
222	2.39	50	8.28	------	----	------	2.38	5	8.245	2.383	10	8.254
400	------	----	------	2.073	vs	8.29	2.057	20	8.228	2.065	21	8.260
422	------	----	------	------	----	------	1.678	20	8.220	1.6862	19	8.260
511	------	----	------	1.588	vs	8.25	1.590	70	8.262	1.5896	41	8.262
440	------	----	------	1.461	vs	8.262	1.460	70	8.259	1.4600	44	8.259
----------	1.401	100	------	------	----	------	------	----	------	------	----	------
620	------	----	------	------	----	------	1.300	5	8.222	1.3060	7	8.260
533	------	----	------	1.261	vw	8.272	1.259	10	8.256	1.2596	11	8.262
642	------	----	------	------	----	------	1.101	10	8.239	1.1037	9	8.262
731	------	----	------	1.075	s	8.256	1.075	20	8.257	1.0749	22	8.257
800	------	----	------	------	----	------	1.032	10	8.256	1.0322	12	8.256
822	------	----	------	------	----	------	0.970	20	8.231	0.9732	7	8.258
751	------	----	------	------	----	------	.951	20	8.236	.9534	19	8.257
931	------	----	------	------	----	------	.866	10	8.261	.8656	16	8.257
844	------	----	------	------	----	------	.842	10	8.250	.8429	27	8.259
10·2·0	------	----	------	------	----	------	.809	5	8.250	.8097	11	8.257
951	------	----	------	------	----	------	.798	10	8.255	.7983	17	8.258
Average value of last five lines			8.29	------	----	8.266	------	----	8.250	------	----	8.258

Manganese Ferrite (jacobsite), $MnFe_2O_4$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
8-15	2.56 2.12 1.64	Iron	McAndrew [1] 1952.

Additional published patterns

Source	Radiation
Holgersson [2] 1927	Iron
Passerini [3] 1930	Iron

NBS sample. The sample of jacobsite was prepared at NBS by solid state reaction at approximately 1,100° C between Fe_2O_3 and $MnCO_3$ using KCl as a flux. The KCl was washed out after the reaction was completed. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of titanium and zinc; 0.01 to 0.1 percent each of aluminum and silicon; and 0.001 to 0.01 percent each of chromium, copper, calcium, magnesium, molybdenum, and nickel.

The sample was a blackish opaque powder.

Interplanar spacings and intensity measurements. The pattern reported by Passerini was converted from kX to angstrom units. The *d*-values for the Holgersson pattern were calculated from Bragg angle data. The indices for the three strongest lines for each pattern are as follows:

Pattern	1	2	3
McAndrew	311	400	511
Holgersson	311	400	731
Passerini	440	800	311
National Bureau of Standards	311	440	220

Structural data. Bragg [4] in 1915 described the structure of the spinel group. Jacobsite has the spinel-type structure, the space group Fd3m (No. 227), and $8(MnFe_2O_4)$ per unit cell.

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

Manganese Ferrite (jacobsite), $MnFe_2O_4$ (cubic)

hkl	1952 McAndrew Fe, 1.9373 A			1927 Holgersson Fe, 1.9373 A			1930 Passerini Fe, 1.9373 A			1959 National Bureau of Standards Fe, 1.93597 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	4.94	40	8.56	------	----	------	------	----	------	4.906	21	8.497
220	3.01	40	8.51	3.03	w	8.57	2.97	9	8.41	3.005	37	8.500
311	2.56	100	8.49	2.59	vs	8.59	2.54	30	8.43	2.563	100	8.501
222	2.45	3	8.49	------	----	------	------	----	------	2.450	11	8.487
400	2.12	60	8.48	2.16	vs	8.64	2.11	24	8.44	2.124	26	8.495
422	1.739	10	8.56	------	----	------	1.73	10	8.46	1.7342	20	8.496
511	1.636	60	8.50	1.66	s	8.63	1.631	18	8.48	1.6355	34	8.498
440	1.501	60	8.49	1.46	vw	8.64	1.500	100	8.48	1.5031	42	8.503
531	1.435	5	8.49	------	----	------	1.437	3	8.50	1.4376	2	8.505
620	1.339	3	8.47	------	----	------	1.346	8	8.51	1.3441	3	8.501
533	1.296	20	8.50	1.309	w	8.58	1.300	14	8.52	1.2962	21	8.500
622	1.278	5	8.48	------	----	------	1.284	5	8.52	1.2810	14	8.497
444	1.225	10	8.49	1.233	vw	8.54	1.230	18	8.52	1.2276	8	8.505
711	1.191	3	8.50	------	----	------	1.194	1	8.53	1.1898	10	8.497
642	1.134	5	8.49	1.148	w	8.59	1.139	13	8.52	1.1355	7	8.501
731	1.108	40	8.51	1.114	vs	8.56	1.112	24	8.54	1.1063	28	8.498
800	1.062	20	8.50	1.071	s	8.57	1.067	35	8.54	1.0623	12	8.498
751	0.982	40D	8.50	------	----	------	------	----	------	0.9815	21	8.500
Average value of last five lines----			8.50	------	----	8.57	------	----	8.53	------	----	8.499

Lattice constants

		A
1927	Holgersson [2]----------	8.572
1930	Passerini [3]----------	8.532
1934	Krause and Thiel [5]----------	8.597
1952	McAndrew [1]----------	8.505
1959	National Bureau of Standards--------	8.499 at 25° C

The density of jacobsite, calculated from the NBS lattice constant, is 4.989 g/cm³ at 25° C.

References

[1] J. McAndrew, The cell edge of jacobsite, Am. Min. **37,** 453–460 (1952).
[2] S. Holgersson, Röntgenographische Untersuchungen der Spinelle, Acta Univ. Lundensis **23,** 22–112 (1927).
[3] L. Passerini, Ricerche sugli spinelli, Gazz. chimi. itali. **60,** 389–399 (1930).
[4] W. H. Bragg, The structure of magnetite and the spinels, Nature **95,** 561 (1915).
[5] O. Krause and W. Thiel, Ueber keramische Farbkörper, Ber. deut. keram. Ges. **15,** 101–110 (1934).

Manganese(III) Oxide (partridgeite), Mn_2O_3 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
2-0896	2.72 1.66 1.42	Iron	Zachariasen [1] 1928.

Additional published patterns

Source	Radiation
Drucker and Hüttner [2] 1928----------	Iron
Wretblad [3] 1930----------	Chromium
Morozov and Kuznecov [4] 1949---------	Iron

Manganese(III) Oxide, (partridgeite) Mn_2O_3 (cubic)

hkl	1928 Zachariasen Fe, 1.9373 A			1928 Drucker and Huttner Fe, 1.9373 A			1930 Wretblad Cr, 2.2909 A			1949 Morozov and Kuznecov Fe, 1.9373 A			1959 National Bureau of Standards Fe, 1.93597 A at 25° C		
	a	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A	A		A
200	------	------	------	------	------	------	------	------	------	------	------	------	4.70	2	9.41
211	3.86	15	9.46	3.75	vw	9.20	3.84	s	9.40	3.84	44	9.42	3.84	23	9.41
------	------	------	------	------	------	------	3.33	vw	------	------	------	------	------	------	------
------	------	------	------	------	------	------	2.98	s	------	------	------	------	------	------	------
222	2.72	100	9.43	2.70	s	9.34	2.72	vs	9.41	2.73	100	9.46	2.72	100	9.41
321	------	------	------	------	------	------	2.52	m	9.41	2.54	22	9.50	2.51	3	9.40
400	2.35	10	9.42	2.34	w	9.38	2.35	s	9.42	2.35	44	9.42	2.35	11	9.41
411	------	------	------	------	------	------	2.22	vw	9.40	------	------	------	2.22	<1	9.40
420	------	------	------	------	------	------	2.10	w	9.40	------	------	------	2.10	1	9.40
332	2.01	20	9.42	1.99	m	9.34	2.01	s	9.40	2.01	56	9.41	2.01	13	9.41
422	------	------	------	------	------	------	1.919	m	9.40	1.931	11	9.46	1.920	<1	9.40
431	1.842	30	9.39	1.836	m	9.36	1.845	s	9.41	1.850	67	9.43	1.845	13	9.41
521	------	------	------	1.710	vw	9.37	1.717	m	9.40	1.724	22	9.44	1.719	3	9.42
440	1.663	90	9.41	1.656	s	9.37	1.663	vs	9.41	1.664	89	9.42	1.664	32	9.41
433	------	------	------	------	------	------	1.614	m	9.41	1.614	11	9.40	1.615	1	9.42
600	------	------	------	------	------	------	1.567	w	9.40	1.563	11	9.39	1.566	<1	9.39
611	------	------	------	1.524	vw	9.40	1.525	m	9.40	1.530	33	9.43	1.527	4	9.41
620	------	------	------	------	------	------	1.487	w	9.40	1.489	22	9.42	1.487	1	9.40
541	1.453	20	9.42	1.449	m	9.39	1.4514	s	9.406	1.454	44	9.42	1.4524	8	9.413
622	1.419	60	9.41	1.414	s	9.38	1.4183	vs	9.408	1.421	67	9.43	1.4191	15	9.413
631	1.387	20	9.41	1.384	m	9.39	1.3873	m	9.409	1.388	44	9.41	1.3875	5	9.410
444	1.356	15	9.39	1.352	w	9.37	1.3583	m	9.411	1.361	33	9.43	1.3589	2	9.415
------	------	------	------	------	------	------	1.3306	w	------	1.325	11	------	------	------	------
640	------	------	------	1.302	vw	9.39	1.3044	m	9.406	1.304	22	9.40	1.3053	2	9.413
721	1.282	15	9.42	1.276	w	9.38	1.2802	m	9.408	1.285	44	9.42	1.2801	4	9.407
642	------	------	------	1.254	vw	9.38	1.2577	w	9.412	1.267	11	9.48	1.2583	2	9.416
------	------	------	------	1.233	vw	------	1.2355	w	------	------	------	------	------	------	------
732	1.195	5	9.41	1.189	w	9.36	1.1950	m	9.409	1.193	22	9.40	1.1949	2	9.409
800	1.177	15	9.42	1.174	w	9.39	1.1766	s	9.413	1.177	44	9.418	1.1764	2	9.411
811	1.159	15	9.42	1.153	w	9.37	1.1585	s	9.412	1.159	56	9.419	1.1582	3	9.409
821	1.144	15	9.43	------	------	------	------	------	------	1.141	44	9.413	1.1418	2	9.416
653	------	------	------	1.121	vw	9.38	------	------	------	1.124	44	9.410	1.1251	1	9.413
822	------	------	------	1.104	vw	9.37	------	------	------	1.111	11	9.420	1.1089	<1	9.409
831	------	------	------	------	------	------	------	------	------	1.094	11	9.416	1.0936	2	9.408
662	------	------	------	1.076	vw	9.38	------	------	------	1.080	56 [a]	9.416	1.0793	4	9.409
Average value of last five lines			9.42	------	------	9.38	------	------	9.411	------	------	9.415	------	------	9.411

[a] Four additional lines were omitted.

NBS sample. The sample of manganese sesquioxide was prepared at NBS by heating specially purified manganese dioxide contributed by Mallinckrodt Chemical Works at 850° C for 16 hr. Their spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of potassium and sodium; and 0.001 to 0.01 percent each of copper, lead, and molybdenum.

The sample was an opaque black powder.

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

Pattern	1	2	3
Zachariasen	222	440	622
Drucker and Hüttner	222	440	622
Wretblad	222	440	622
Morozov and Kuznecov	222	440	431
National Bureau of Standards	222	440	211

Structural data. Pauling and Shappell [5] in 1930 determined that manganese sesquioxide has the thallium oxide-type structure, the space group Ia3 No. 206) and 16(Mn_2O_3) per unit cell.

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

Lattice constants

		A
1928	Zachariasen [1]	9.43
1930	Wretblad [3]	9.410
1949	Morozov and Kuznecov [4]	9.42
1959	National Bureau of Standards	9.411 at 25° C

The density of manganese sesquioxide calculated from the NBS lattice constants is 5.031 g/cm³ at 25° C.

References

[1] W. H. Zachariasen, On the crystal structure of bixbyite and artificial Mn_2O_3, Z. Krist. **67**, 455–464 (1928).

[2] D. Drucker and R. Hüttner, Die Thermische Dissoziation des Mangandioxydes, Z. physik. Chem. **131**, 237–266 (1928).

[3] P. E. Wretblad, Röntgenographische Untersuchung der Systeme Fe_2O_3-Cr_2O_3 und Fe_2O_3-Mn_2O_3, Z. anorg. u. allgem. Chem. **189**, 329–336 (1930).

[4] I. S. Morozov and V. G. Kuznecov, The γ modification of manganese dioxide, Izvest. Akad. Nauk. SSSR Otdel. Khim. Nauk. #4, 343–353 (1949).

[5] L. Pauling and M. D. Shappell, The crystal structure of bixbyite and the C-modification of the sesquioxides, Z. Krist. **75**, 128–142 (1930).

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

ASTM cards

Card number	Index lines	Radiation	Source
5–0596	2.97 2.83 2.41	Copper	National Bureau of Standards [1] 1954.

The pattern reported on ASTM card No. 5–0596 has been reindexed to conform with the new cell size. The indexing on this card was based upon the unit cell and space group Pmmn proposed by Zachariasen [2]. More recent work by Aurivillius [3] with neutron diffraction indicates the "a" should be doubled and the space group should be Pnma. Eight lines of weak intensity have also been added.

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

Pattern	1	2	3
National Bureau of Standards	011	210	201

Structural data. Aurivillius [3] in 1956 determined that mercuric oxide has the space group Pnma (No. 62) and 4(HgO) per unit cell. The new unit-cell measurements are compared with the previous measurements reported.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1954	National Bureau of Standards [1]	3.304	5.518	3.519
1956	Aurivillius [3]	6.612	5.520	3.521
1959	National Bureau of Standards	6.608	5.518	3.519 at 25° C

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

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
	A	
200	3.302	1
101	3.101	2
011	2.967	100
210	2.834	81
020	2.759	58
201	2.408	67
211	2.206	2
220	2.117	<1
121	2.062	<1
221	1.814	49
002	1.759	11
400	1.651	11
031	1.630	15
230	1.607	13
131, 410	1.583	2
321	1.547	1
401, 212	1.495	25
022	1.484	12
411	1.443	18
420	1.417	11
040	1.379	4
421	1.315	1
402	1.204	5
241	1.1971	10
232	1.1866	9
431	1.1605	7
013	1.1475	4
203	1.1052	6
422	1.1039	8
042	1.0855	3
610	1.0801	3
440	1.0589	4
051	1.0532	4
601	1.0510	4
531, 223	1.0262	5
033	0.9890	3
621	.9823	4
630	.9450	5
413	.9425	3
612	.9202	4
442	.9072	3
252, 711	.8996	4

The density of mercuric oxide calculated from the NBS lattice constants is 11.209 g/cm³ at 25° C.

References

[1] National Bureau of Standards, Standard X-ray diffraction powder patterns, Nat. Bur. Standards Circ. 539 **III**, 35–37 (1954).

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

[3] K. Aurivillius, The crystal structure of mercury(II) Acta Cryst. **9**, 685–686 (1956).

Neodymium Ethylsulfate Nonahydrate, $Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$ (hexagonal

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of neodymium ethylsulfate nonahydrate was prepared at NBS by E. L. Weise. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent magnesium; and 0.001 to 0.01 percent each of calcium, sodium, and silicon.

The color of the sample was light purple and it was optically positive. The indices of refraction are $N_o = 1.478$ and $N_e = 1.484$.

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

Pattern	1	2	3
National Bureau of Standards	201	211	111

Structural data. Ketelaar [1] in 1937 determined that neodymium ethylsulfate nonahydrate has the space group $P6_3/m$ (No. 176) with $2\{Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O\}$ per unit cell.

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

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C		*hkl*	1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*		*d*	*I*
	A				
100	12.17	56	332	1.954	19
110	7.02	18	601	1.945	15
101	6.14	76	520		
200	6.07	76			
111	5.00	90	313	1.940	19
			422	1.929	10
201	4.620	100	431	1.925	10
300	4.055	68	403	1.869	10
211	3.858	93	512	1.8606	10
002	3.556	32			
301	3.517	24	610	1.8524	15
			323	1.8064	14
310	3.372	25	611	1.7931	12
112	3.174	7	004	1.7797	8
221	3.146	26	104	1.7602	8
202	3.072	15			
311	3.047	20	432	1.7418	6
			700	1.7360	7
400	3.037	19	114	1.7238	5
212	2.813	50	204	1.7069	10
320	2.788	50	522		
302	2.673	28			
410	2.652	26	503	1.6972	10
			701	1.6857	12
321	2.595	38	423	1.6493	10
222	2.499	15	612	1.6428	12
312	2.447	11	621	1.6396	13
500	2.430	11			
330	2.339	16	304	1.6294	7
			710	1.6093	21
103	2.329	12	513	1.6058	18
402	2.310	8	224	1.5860	6
501	2.298	41	314	1.5729	10
420			442		
322	2.195	32			
			702	1.5596	5
421	2.185	39	630	1.5312	7
510			433	1.5276	7
412	2.127	47	622	1.5219	10
213	2.108	24	541	1.5194	12
511	2.087	39			
			324	1.5002	6
600	2.026	14	631	1.4962	8
502	2.008	5	801	1.4852	5
430	1.998	10	414	1.4775	7

Lattice constants

		a	*c*
		A	*A*
1937	Ketelaar [1]	14.020	7.08
1959	National Bureau of Standards	14.028	7.116 at 25° C

The density of neodymium ethylsulfate nonahydrate calculated from the NBS lattice constants is 1.867 g/cm³ at 25° C.

References

[1] J. A. A. Ketelaar, The crystal structure of the ethylsulfates of the rare earths and yttrium, Physica 4, 619–630 (1937).

Nickel Aluminate, $NiAl_2O_4$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–1299	1.42 2.43 2.01	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Holgersson [2] 1927	Iron

NBS sample. The sample of nickel aluminate was prepared at NBS by heating co-precipitated hydroxides at 1,300°C. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of sodium; 0.01 to 0.1 percent each of cobalt and silicon; 0.001 to 0.01 percent each of chromium, iron, and magnesium; and 0.0001 to 0.001 percent each of calcium and manganese.

The sample had a blue color. The index of refraction was 1.825.

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

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	440	311	400
Holgersson	311	400	511
National Bureau of Standards	311	400	440

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1927 Holgersson Fe, 1.9360 A			1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	----------	------	----------	----------	------	----------	4.650	22	8.053
220	----------	------	----------	----------	------	----------	2.846	22	8.049
311	2.43	75	8.06	2.43	s	8.06	2.427	100	8.049
400	2.01	75	8.04	2.016	s	8.06	2.013	63	8.051
422	----------	------	----------	1.642	w	8.04	1.6415	7	8.042
511	1.55	13	8.05	1.554	s	8.08	1.5485	29	8.046
440	1.423	100	8.05	1.422	s	8.04	1.4232	60	8.051
531	----------	------	----------	----------	------	----------	1.3601	<1	8.046
620	----------	------	----------	----------	------	----------	1.2739	<1	8.057
533	----------	------	----------	1.226	w	8.04	1.2274	8	8.049
622	----------	------	----------	----------	------	----------	1.2134	<1	8.049
444	----------	------	----------	1.159	w	8.03	1.1613	6	8.046
642	----------	------	----------	1.074	vw	8.04	1.0753	2	8.047
731	----------	------	----------	1.046	s	8.03	1.0476	11	8.047
800	----------	------	----------	1.005	w	8.04	1.0061	7	8.049
751	----------	------	----------	----------	------	----------	0.9291	7	8.046
840	----------	------	----------	----------	------	----------	.8998	6	8.048
844	----------	------	----------	----------	------	----------	.8214	15	8.048
Average value of last five lines			8.05	----------	------	8.04	----------	------	8.048

Structural data. Bragg [3] in 1915 determined the structure of the spinel group. Nickel aluminate has the spinel-type structure, the space group Fd3m (No. 227), and $8(NiAl_2O_4)$ per unit cell.

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

Lattice constants

		A
1927	Holgersson [2]	8.045
1934	Krause and Thiel [4]	8.07
1943	Vegard and Borlaug [5]	8.050
1959	National Bureau of Standards	8.048 at 25° C

The density of nickel aluminate, calculated from the NBS lattice constant is 4.501 g/cm³ at 25° C.

References

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

[2] S. Holgersson, Röntgenographische Untersuchung der Mineralien des Spinellgruppe, Acta Univ. Lundensis **23**, (1927).

[3] W. H. Bragg, The structure of magnetite and the spinels, Nature **95**, 561 (1915).

[4] O. Krause and W. Thiel, Ueber Keramischer Farbkörper, Ber. deut. keram. Ges. **15**, 100–110 (1934).

[5] L. Vegard and A. Borlaug, Röntgenstrallanalyse von mischkristallen innerhalb der spinellgruppe, Avhandl. Norske Videnskaps-Akad. Oslo, I. Mat. Naturv. Kl. **5**, 1–19 (1943).

Nickel Germinate, Ni_2GeO_4 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of nickel germanate was prepared at NBS by solid state reaction between nickel oxide and germanium oxide at 1,100° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, chromium, iron, and silicon; and 0.001 to 0.01 percent each of magnesium, molybdenum, and antimony.

The sample had a light green color. The index of refraction was too high to be measured by the usual oil immersion method.

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

Pattern	1	2	3
National Bureau of Standards	311	440	220

Structural data. Goldschmidt [1] showed that nickel germanate has the spinel structure, the space group Fd3m (No. 227) and $8(Ni_2GeO_4)$ per unit cell.

Goldschmidt's unit cell value has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1931	Goldschmidt	8.22
1959	National Bureau of Standards	8.221 at 26° C

The density of nickel germanate calculated from the NBS lattice constant is 6.072 g/cm³ at 26° C.

Nickel Germanate, Ni_2GeO_4 (cubic)

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 26° C		
	d	*I*	*a*
	A		*A*
220	2.908	44	8.225
311	2.479	100	8.222
222	2.374	8	8.223
400	2.0558	19	8.223
422	1.6786	17	8.223
511	1.5821	34	8.221
440	1.4533	45	8.221
620	1.3001	6	8.223
533	1.2536	11	8.220
622	1.2392	4	8.220
642	1.0985	7	8.220
731	1.0704	16	8.222
800	1.0277	7	8.222
822	0.9690	4	8.222
751	.9494	10	8.222
840	.9193	2	8.222
664	.8764	3	8.221
931	.8619	6	8.220
844	.8392	16	8.222
10·2·0	.8062	6	8.222
951	.7948	9	8.221
Average value of last five lines		--------	8.221

References

[1] V. M. Goldschmidt, Zur Kristallchemie des Germaniums, Nachr. Ges. Wiss. Göttingen, Math.-Physik. Kl. 184–190 (1931).

Potassium Borohydride, KBH_4 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
8–227	3.33 3.84 2.36	Copper	Banus, Bragdon, and Hinckley [1] 1954.

Additional published patterns. None.

NBS sample. The sample of potassium borohydride was obtained from Metal Hydrides Inc., Beverly, Mass. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent sodium; 0.01 to 0.1 percent strontium; and 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, lead, and silicon.

The sample is colorless. The index of refraction is 1.493.

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

Pattern	1	2	3
Banus, Bragdon, and Hinckley	200	111	220
National Bureau of Standards	200	220	111

Structural data. Abrahams and Kalnajs [2] in 1954 determined that potassium borohydride has sodium chloride-type structure, the space group Fm3m (No. 225) and 4(KBH_4) per unit cell.

Lattice constants

		A
1954	Abrahams and Kalnajs [2]	6.7272 at 25° C
1954	Ford and Powell [3]	6.722 at 20° C
1959	National Bureau of Standards	6.7287 at 25° C

Potassium Borohydride, KBH_4 (cubic)

hkl	1954 Banus, Bragdon, and Hinckley Cu, 1.542 A			1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	3.84	70	6.65	3.883	56	6.726
200	3.33	100	6.66	3.366	100	6.732
220	2.36	70	6.68	2.379	59	6.729
311	2.02	70	6.70	2.029	34	6.729
222	1.925	30	6.68	1.942	19	6.727
400	1.675	10	6.70	1.682	7	6.728
331	1.540	20	6.71	1.543	10	6.726
420	1.500	20	6.71	1.504	19	6.726
422	1.375	20	6.74	1.373	12	6.731
511	1.300	10	6.76	1.295	7	6.732
440	1.195	10	6.76	1.189	4	6.726
531	-----	---	-----	1.137	4	6.727
600	-----	---	-----	1.121	5	6.726
620	-----	---	-----	1.064	5	6.729
533	-----	---	-----	1.0261	2	6.7286
622	-----	---	-----	1.0143	3	6.7288
444	-----	---	-----	0.9712	2	6.7287
711	-----	---	-----	.9422	2	6.7287
640	-----	---	-----	.9331	3	6.7287
642	-----	---	-----	.8991	4	6.7283
731	-----	---	-----	.8760	4	6.7287
800	-----	---	-----	.8411	3	6.7288
733	-----	---	-----	.8220	1	6.7284
820	-----	---	-----	.8160	4	6.7289
822	-----	---	-----	.7930	4	6.7288
Average value of last five lines			6.74	------	---	6.7287

The density of potassium borohydride calculated from the NBS lattice constant is 1.176 g/cm³ at 25° C.

References

[1] M. B. Banus, R. W. Bragdon, and A. A. Hinckley, Potassium, rubidium, and cesium borohydrides, J. Am. Chem. Soc. **76**, 3848–3849 (1954).

[2] S. C. Abrahams and J. Kalnajs, The lattice constants of the alkali borohydrides and the low-temperature phase of sodium borohydride, J. Chem. Phys. **22**, No. 3, 434–436 (1954).

[3] P. T. Ford and H. M. Powell, The unit cell of potassium borohydride, KBH_4 at 90°K, Acta Cryst. **7**, 604–605 (1954).

Potassium Cobaltinitrite, $K_3Co(NO_2)_6$ (cubic)

ASTM cards. None.

Additional published patterns

Source	Radiation
Ferrari and Colla [1] 1933	Iron

NBS sample. The sample of potassium cobaltinitrite was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent nickel; 0.01 to 0.1 percent each of copper, lead, and rubidium; and 0.001 to 0.01 percent each of aluminum, barium, iron, sodium, silicon, and strontium.

The color of the sample is greenish yellow. The index of refraction is 1.72.

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

Pattern	1	2	3
Ferrari and Colla	422	642	400
National Bureau of Standards	400	422	220

Structural data. van Driel and Verweel [2] in 1936 determined that potassium cobaltinitrite has the space group Fm3 (No. 202), and $4[K_3Co(NO_2)_6]$ per unit cell. Potassium cobaltinitrite is used as a structure-type.

The unit-cell measurements reported by Ferrari and Colla and by van Driel and Verweel have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1933	Ferrari and Colla [1]	10.46
1936	van Driel and Verweel [2]	10.48
1959	National Bureau of Standards	10.512 at 25° C

Potassium Cobaltinitrite, $K_3Co(NO_2)_6$ (cubic)

hkl	1933 Ferrari and Colla Fe, 1.937 A			1958 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	-----	---	-----	6.07	31	10.514
200	-----	---	-----	5.257	35	10.514
220	-----	---	-----	3.718	59	10.516
222	-----	---	-----	3.035	26	10.514
400	2.614	s	10.46	2.628	100	10.512
331	-----	---	-----	2.412	12	10.514
420	2.345	s	10.48	2.352	44	10.518
422	2.134	vs	10.46	2.1464	75	10.515
511	2.009	w	10.43	2.0234	14	10.514
440	1.854	w	10.48	1.8585	17	10.513
-----	1.772	vw	-----	------	---	-------
620	1.658	m	10.48	1.6622	21	10.513
640	1.448	w	10.44	1.4576	11	10.511
642	1.397	vs	10.45	1.4046	32	10.511
800	1.308	w	10.46	1.3145	10	10.516
822	1.238	m	10.50	1.2390	8	10.513
840	1.171	m	10.47	1.1752	14	10.511
644	1.117	m	10.48	1.1204	20	10.510
-----	1.028	s	-----	------	---	-------
Average value of last five lines			10.47	------	---	10.512

The density of potassium cobaltinitrite calculated from the NBS lattice constant is 2.585 g/cm³ at 25° C.

References

[1] A. Ferrari and C. Colla, Richerche chimiche e cristallografiche sui cobaltinitriti di ammonio, di potassio, di rubidio, di cesio e di talli, Rend. Accad. Naz. Lincei (6) **17**, 390–398 (1933).

[2] M. van Driel and H. J. Verweel, Über die struktur der Tripelnitrite, Z. Krist. **95A**, 308–314 (1936).

Potassium Heptafluozirconate, K_3ZrF_7 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
3–0511	3.18 2.24 1.83	Molybde-num	Dow Chemical Co., Midland, Michigan.

Additional published patterns

Source	Radiation
Hampson and Pauling [1] 1938	Copper

NBS sample. The sample of potassium heptafluozirconate was contributed by the Titanium Alloy

Potassium Heptafluozirconate, K_3ZrF_7 (cubic)

hkl	[illegible] ---- Dow Chemical Co. Mo, 0.709 A			1938 Hampson and Pauling Cu, --------			1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	5.2	33	9.0	5.17	m-s	8.95	5.190	42	8.989
200	4.50	20	9.0	4.47	m	8.94	4.495	25	8.990
220	3.19	100	9.02	3.16	vvs	8.94	3.177	100	8.986
311	2.72	3	9.02	2.70	vw	8.95	2.710	8	8.988
400	2.24	50	8.96	2.24	s	8.96	2.247	51	8.988
331	2.05	1	8.94	2.05	vw	8.94	2.062	5	8.988
420	2.00	6	8.94	2.00	w	8.94	2.009	12	8.985
422	1.83	50	8.96	1.86	vs	9.11	1.835	48	8.990
511	1.73	10	8.99	1.72	m	8.96	1.729	13	8.984
440	1.59	13	8.99	1.58	m-s	8.96	1.589	15	8.989
531	1.52	3	8.99	1.52	w-m	8.99	1.519	7	8.986
600	1.50	3	9.00	1.50	w	9.00	1.498	5	8.988
620	1.42	13	8.98	1.42	m-s	8.98	1.421	12	8.987
533	1.37	1	8.98	1.37	vvw	8.98	1.371	3	8.990
622	----------	------	----------	----------	------	----------	1.355	1	8.988
444	1.29	3	8.94	1.30	vw	8.97	1.2971	6	8.987
711	1.26	1	9.00	1.26	vvw	9.00	1.2584	4	8.987
640	1.25	1	9.01	1.24	<vvw	8.96	1.2466	3	8.989
642	1.19	13	8.90	1.20	m-s	8.99	1.2011	12	8.988
731	1.17	4	8.99	1.17	vw	8.99	1.1702	5	8.988
800	----------	------	----------	1.12	vvw	8.98	1.1242	3	8.994
733	----------	------	----------	----------	------	----------	1.0981	2	8.988
820	----------	------	----------	1.09	vvw	9.00	1.0900	2	8.988
822	----------	------	----------	1.06	m	8.99	1.0594	5	8.989
751	----------	------	----------	1.04	vvw	8.97	1.0379	3	8.989
662	----------	------	----------	----------	------	----------	1.0308	3	8.986
840	----------	------	----------	1.003	w	8.97	1.0048	4	8.987
911	----------	------	----------	0.985	vw	8.97	0.9867	5	8.989
842	----------	------	----------	.979	vvw	8.97	.9807	2	8.988
664	----------	------	----------	.956	vvw	8.97	.9581	1	8.988
931	----------	------	----------	.942	vvw	8.98	.9422	3	8.988
844	----------	------	----------	.918	vw	8.99	.9173	3	8.988
933	----------	------	----------	.905	vw	9.00	.9033	3	8.988
10·2·0	----------	------	----------	.881	m-s	8.98	.8815	4	8.990
Average value of last five lines			8.97	----------	------	8.98	----------	------	8.988

Mfg. Division of the National Lead Co., Niagara Falls, N. Y. Their spectrographic analysis showed the following impurities: 0.01 to 0.05 percent each of aluminum, iron, hafnium, magnesium, and strontium; 0.004 percent titanium; and 0.0001 to 0.0002 percent each of copper and manganese.

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

Interplanar spacings and intensity measurements. The *d*-values reported by the Dow Chemical Co. were converted from kX to angstrom units and the *d*-values reported by Hampson and Pauling were calculated from Bragg angle data. The i dice of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Dow Chemical Co.	220	400	422
Hampson and Pauling	220	422	400
National Bureau of Standards	220	400	422

Structural data. Hampson and Pauling [1] in 1938 determined that potassium heptafluozirconate has the space group Fm3m (No. 225), and $4(K_3ZrF_7)$ per unit cell. The unit-cell measurement reported by Hampson and Pauling has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1938	Hampson and Pauling [1]	8.969 (8.98) [a]
1959	National Bureau of Standards	8.988 at 25° C

[a] Average of last five lines in table.

The density of potassium heptafluozirconate calculated from the NBS lattice constant is 2.209 g/cm³ at 25° C.

References

[1] G. C. Hampson and L. Pauling, The structure of ammonium heptafluozirconate and potassium heptafluozirconate and the configuration of the heptafluozirconate group, J. Am. Chem. Soc. **60**, 2705–2707 (1938)

Praseodymium Oxychloride, PrOCl (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of praseodymium oxychloride was prepared at the NBS by heating praseodymium chloride to 800° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of iron and silicon; and 0.001 to 0.01 percent each of aluminum, calcium, copper, magnesium, and nickel.

The sample has a pale green color. The indices of refraction are $N_o = 1.916$ and $N_e = 1.975$.

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

Pattern	1	2	3
National Bureau of Standards	102	101	110

Structural data. Zachariasen [1] in 1949 determined that praseodymium oxychloride has lead fluorochloride-type structure, the space group P4/nmm (No. 129), and 2(PrOCl) per unit cell.

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

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
	A	
001	6.80	32
101	3.48	90
002	3.397	12
110	2.864	81
102	2.605	100
003	2.266	8
112	2.189	28
200	2.024	41
103	1.977	7
201	1.941	7
113	1.778	22
211	1.751	29
004	1.7001	2
212	1.5985	37
104	1.5676	15
203	1.5100	8
114	1.4623	6
220	1.4322	12
301	1.3245	4
222	1.3204	5
310	1.2811	10
302	1.2547	7
214	1.2395	12
115	1.2290	3
223	1.2100	5

Praseodymium Oxychloride, PrOCl (tetragonal)

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
	A	
312	1.1987	8
205	1.1297	5
313	1.1158	8
321	1.1087	5
215	1.0875	3
322	1.0668	9
304	1.0574	6
116	1.0544	3
314	1.0235	4
400	1.0127	2
206	0.9894	5
225	.9865	4
411	.9723	5
330	.9555	4
107	.9443	5
412	.9437	8
324	.9373	5

Lattice constants

		a	*c*
		A	*A*
1949	Zachariasen [1]	4.053	6.800
1959	National Bureau of Standards	4.051	6.802 at 25° C

The density of praseodymium oxychloride calculated from the NBS lattice constants is 5.722 g/cm^3 at 25° C.

References

[1] W. H. Zachariasen, Crystal chemical studies of the 5f-series of elements. XII. New Compounds representing known structure types, Acta Cryst. **2**, 388–390 (1949).

gamma-Silver Iodide, γ-AgI (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0503	3.74 2.29 1.95	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Barth and Lunde [2] 1925	Copper

NBS sample. The sample silver iodide was made at the NBS by dissolving Ag_2O in HI. The sample was heated at 120°C for 24 hr to sharpen the diffraction pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon; and 0.001 to 0.01 percent each of aluminum, barium, calcium, copper, iron, magnesium, and sodium.

The color of the sample is bright yellow. The index of refraction is too high to be measured by the usual liquid immersion method.

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

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	220	311
Barth and Lunde	220	311	111
National Bureau of Standards	111	220	311

Structural data. Wilsey [3] in 1921 determined that gamma-silver iodide has the zinc sulfide, zincblende, type structure, the space group $F\bar{4}3m$ (No. 216), and 4(AgI) per unit cell.

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

gamma-Silver Iodide, γ-AgI (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1925 Barth and Lunde Cu, 1.539 A			1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	I	a	d	I	a	d	I	a
	A		A	A		A	A		A
111	3.75	100	6.50	3.76	60	6.51	3.75	100	6.49
220	2.29	75	6.48	2.30	100	6.50	2.30	58	6.50
311	1.95	40	6.47	1.97	90	6.53	1.959	31	6.498
400	1.62	5	6.48	1.63	10	6.52	1.623	4	6.494
331	1.485	8	6.473	1.493	30	6.508	1.490	6	6.494
422	1.321	8	6.472	1.324	40	6.486	1.326	7	6.496
511	1.247	5	6.480	1.254	30	6.516	1.250	5	6.496
440	1.145	3	6.477	1.154	20	6.528	1.148	3	6.494
531	1.096	3	6.484	1.099	50	6.502	1.098	3	6.496
620	----------	------	----------	1.026	20	6.489	1.027	2	6.495
-------	----------	------	----------	0.990	20	----------	----------	------	----------
-------	----------	------	----------	.943	10	----------	----------	------	----------
-------	----------	------	----------	.910	30	----------	----------	------	----------
642	----------	------	----------	----------	------	----------	0.868	2	6.496
Average value of last five lines			6.477	----------	------	6.504	----------	------	6.495

Lattice constants

		A
1922	Davey [4]	6.53
1925	Barth and Lunde [2]	6.504
1925	Wilsey [5]	6.506
1931	Block and Möller [6]	6.50
1934	Kolkmeijer and van Hengel [7]	6.49
1940	Wilman [8]	6.502
1948	Mehmel [9]	6.48
1950	Trillat and Laloeuf [10]	6.49
1959	National Bureau of Standards	6.495 at 25° C

The density of gamma-silver iodide calculated from the NBS lattice constant is 5.686 g/cm³ at 25° C.

References

[1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray di fraction, Ind. Eng. Chem., Anal. Ed. **10**, 451–512 (1938).

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

[3] R. B. Wilsey, The crystal structure of the silver halides, Phil. Mag. **42**, 262–263 (1921).

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

[5] R. B. Wilsey, X-ray analysis of some mixed crystals of the silver halides, J. Franklin Inst. **200**, 739–746 (1925).

[6] R. Block and H. Möller, Über die Modifikationen des Jodsilbers, Z. physik. Chem. **152A**, 245–268 (1931).

[7] N. H. Kolkmeijer and J. W. A. van Hengel, Über das regulare und das hexagonale Silberjodid, Z. Krist. **88**, 317–322 (1934).

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

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

[10] J. J. Trillat and A. Laloeuf, Etude par diffraction electronique, de la structure des fumees d'iodure d'argent et de chlorure d'ammonium, Rayons X et structure atomique, 19–29 (1950).

Silver Metaperiodate, $AgIO_4$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
4-0559	3.21 1.64 1.30	Iron	Birckenbach and Buschendorf [1] 1932.

Additional published patterns. None.

NBS sample. The sample of silver metaperiodate was prepared at the NBS from cold solutions of silver nitrate and sodium metaperiodate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum and silicon; and 0.001 to 0.01 percent each of beryllium, calcium, cobalt, chromium, iron, indium, magnesium, molybdenum, and nickel.

The color of the sample was tan. The indices of

refraction could not be determined because the sample was too fine-grained.

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

Pattern	1	2	3
Birckenbach and Buschendorf	303, 312	503, 512	103, 112
National Bureau of Standards	103, 112	204	004

Structural data. Birckenbach and Buschendorf [1] in 1932 determined that silver metaperiodate has scheelite-type structure, the space group $I4_1/a$ (No. 88) and $4(AgIO_4)$ per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1932	Birckenbach and Buschendorf	5.379	12.037
1959	National Bureau of Standards	5.374	12.094 at 25° C

The density of silver metaperiodate calculated from the NBS lattice constants is 5.68 g/cm³ at 25° C.

References

[1] L. Birckenbach and F. Buschendorf, Darstellung und Kristallstructur des normalen (meta-) Silberperiodats, Z. physik. Chem. **B16**, 102–112 (1932).

Silver Metaperiodate, $AgIO_4$ (tetragonal)

hkl	1932 Birckenbach and Buschendorf Fe, 1.937 A		1959 National Bureau of Standards Cu, 1.5305 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
101	----	----	4.91	9
103	3.22	vs	3.22	100
112				
004	3.02	vw	3.02	22
200	2.69	w	2.687	21
114	2.36	vvw	2.366	5
211			2.358	5
204	2.01	vs	2.007	30
220	1.90	s	1.899	14
116	1.778	vs	1.781	16
301				
215	----	----	1.703	3
303	1.637	vvs	1.635	20
312				
224	1.609	s	1.608	11
008	1.511	vvw	1.512	4
314	1.478	vvw	1.475	1
321				
118	----	----	1.403	3
400	----	----	1.343	2
208	1.317	w	1.318	6
316	1.299	vs	1.299	8
413	1.240	m	1.240	6
332				
404	1.229	s	1.228	8
420	1.201	s	1.202	6
228	1.181	s	1.183	5
1·1·10	1.148	vw	1.153	6
406	1.118	vs	1.119	7
424			1.117	7
309	1.073	w	1.074	4
336			1.0728	3
503	1.036	vvs	1.0384	6
512				
0·0·12	1.005	m	1.0048	5
408				
3·1·10	----	----	0.9856	3
440	----	----	.9505	3
2·0·12	----	----	.9438	5
428	----	----	.9408	5
419	----	----	.9341	6
516				
532	----	----	.9112	8
444	----	----	.9064	7
600	----	----	.8954	4
2·2·16	----	----	.8905	5
3·3·10	----	----	.8749	3
446	----	----	.8587	2
604				
620	----	----	.8496	7
622	----	----	.8425	4
1·1·14	----	----	.8407	1
536	----	----	.8381	3
541				
606	----	----	.8179	3
624				
4·0·12	----	----	.8062	3
448	----	----	.8043	3
5·1·10	----	----	.7945	4

Sodium Borohydride, $NaBH_4$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of sodium borohydride was obtained from T. B. Douglas at NBS. Chemical analysis indicated the following percentages of the theoretical: sodium, 99.9 percent; boron, 99.9 percent; and hydrogen, 99.4 percent.

The sample is white. The indices of refraction could not be determined because the sample reacted violently with the index liquids.

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

Pattern	1	2	3
National Bureau of Standards	200	220	111

Structural data. Soldate [1] in 1947 determined that the location of the Na and B atoms is of the NaCl type, but the positions of the hydrogen atoms and hence the space group could not be settled. The lattice if face-centered cubic with $4(NaBH_4)$ assumed per unit cell.

Lattice constants

		A
1959	National Bureau of Standards	6.162 at 25° C

The density of sodium borohydride calculated from the NBS lattice constant is 1.074 g/cm³ at 25° C.

hkl	1959 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*
	A		A
111	3.55	25	6.16
200	3.082	100	6.163
220	2.181	48	6.168
311	1.857	19	6.160
222	1.778	13	6.160
400	1.540	4	6.161
331	1.414	3	6.164
420	1.3781	10	6.163
422	1.2577	7	6.161
511	1.1855	3	6.160
440	1.0895	2	6.163
531	1.0416	1	6.162
600	1.0270	3	6.162
620	0.9742	2	6.161
533	.9398	<1	6.163
622	.9289	2	6.162
444	.8893	<1	6.161
711	.8630	<1	6.163
640	.8543	2	6.161
642	.8234	3	6.161
Average value of last five lines			6.162

References

[1] A. M. Soldate, The crystal structure of sodium borohydride, J. Am. Chem. Soc. **69**, 987–988 (1947).

Strontium Zirconate, $SrZrO_3$ (orthorhombic)

ASTM cards

Card numbers[a]	Index lines	Radiation	Source
1–0937	2.90 1.67 2.04	Molybdenum	New Jersey Zinc Co.
2–1447	1.09 2.89 2.04	Copper	Hoffmann [1] 1935.
3–0684	2.90 1.68 1.10	——	Megaw.

[a] These cards are listed as cubic.

Additional published patterns

Source	Radiation
Zachariasen [2] 1928	Iron

NBS sample. The sample of strontium zirconate was prepared at NBS by R. S. Roth. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of hafnium, aluminum, silicon, calcium and barium; 0.01 to 0.1 percent each of iron, magnesium, and titanium; and 0.001 to 0.01 percent each of beryllium and nickel.

The color of the sample was pinkish-white. The indices of refraction were too high to be determined

by the usual liquid grain immersion method.

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

Pattern	1	2	3
New Jersey Zinc Co.	121, 002	321, 123, 042	202, 040
Hoffmann	521, 244, 125, 163	121, 002	202, 040
Megaw	121, 002	321, 123, 042	521, 244, 125, 163
Zachariasen	521, 244, 125, 163	321, 123, 042	121, 002
National Bureau of Standards	002	121	202, 040

Structural data. The structure of strontium zirconate has not been published. Megaw [3] in 1946 showed some of the perovskite-type compounds to be orthorhombic. Roth [4] in 1957 reported that the probable symmetry of strontium zirconate was orthorhombic. Bailey [5], as quoted by Megaw [6], used the $CaTiO_3$ space group, Pnma (No. 62), and $4(SrZrO_3)$ per unit cell.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1957	Roth [4]	5.818	8.189	5.792
1959	National Bureau of Standards	5.814	8.196	5.792 at 25° C

The density of strontium zirconate calculated from the NBS lattice constants is 5.458 g/cm³ at 25° C.

Strontium Zirconate, $SrZrO_3$ (orthorhombic)

hkl	---- New Jersey Zinc Co. Mo, ----		1935 Hoffmann Cu, ----		---- Megaw ----		1928 Zachariasen Fe, ----		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
020	----	----	----	----	----	----	----	----	4.096	5
111	----	----	----	----	----	----	----	----	3.666	5
121	2.91	100	2.90	90	2.91	100	2.90	50	2.900	67
002									2.895	100
210	----	----	----	----	----	----	----	----	2.735	1
201	----	----	----	----	----	----	----	----	2.598	2
102	----	----	----	----	----	----	----	----	2.590	2
112	----	----	----	----	----	----	----	----	2.469	4
031										
220	----	----	----	----	----	----	----	----	2.369	4
022	----	----	----	----	----	----	----	----	2.363	1
131	----	----	----	----	----	----	----	----	2.272	<1
221	----	----	----	----	----	----	----	----	2.191	<1
122										
202	2.04	40	2.04	80	2.05	70	2.04	40	2.050	41
040										
212	----	----	----	----	----	----	----	----	1.986	3
230										
231	----	----	----	----	----	----	----	----	1.880	3
132, 013										
301	----	----	----	----	----	----	----	----	1.837	3
222										
103	----	----	----	----	----	----	----	----	1.832	3
141										
311	----	----	----	----	----	----	----	----	1.792	2
321	1.67	67	1.67	80	1.68	80	1.67	70	1.676	22
123										
042									1.672	36
232	----	----	----	----	----	----	----	----	1.6388	<1
213	----	----	----	----	----	----	----	----	1.5785	<1

hkl	---- New Jersey Zinc Co. Mo, --------		1935 Hoffmann Cu, --------		---- Megaw --------		1928 Zachariasen Fe, --------		1959 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
331	--------	------	--------	------	--------	------	--------	------	1.5246	1
400	1.45	27	1.45	60	1.45	70	1.45	40	1.4527	6
242									1.4495	14
410	--------	------	--------	------	--------	------	--------	------	1.4306	1
233	--------	------	--------	------	--------	------	--------	------	1.3860	1
303										
341	--------	------	--------	------	--------	------	--------	------	1.3679	1
313	--------	------	--------	------	--------	------	--------	------	1.3489	<1
204	1.29	24	1.29	70	1.30	70	1.30	50	1.2966	12
412										
430	--------	------	--------	------	--------	------	--------	------	1.2830	1
214										
252	--------	------	--------	------	--------	------	--------	------	1.2799	1
333										
351	--------	------	--------	------	--------	------	--------	------	1.2230	1
440	1.18	3	1.18	40	1.18	50	1.18	20	1.1854	5
044									1.1826	5
432	--------	------	--------	------	--------	------	--------	------	1.1731	1
511	--------	------	--------	------	--------	------	--------	------	1.1289	1
521									1.0980	8
244	1.09	27	1.09	100	1.10	80	1.09	100		
125, 163									1.0951	13
531	--------	------	--------	------	--------	------	--------	------	1.0522	2
404	--------	------	1.02	60	--------	------	--------	------	1.0254	4
414										
452	--------	------	--------	------	--------	------	--------	------	1.0177	<1
503										
541	--------	------	--------	------	--------	------	--------	------	0.9962	<1
305										
145	--------	------	--------	------	--------	------	--------	------	.9940	<1
513	--------	------	--------	------	--------	------	--------	------	.9884	<1
523									.9675	4
325	--------	------	--------	------	0.967	70	--------	------		
363									.9665	8
533	--------	------	--------	------	--------	------	--------	------	.9359	2
551										
602	--------	------	--------	------	.917	70	--------	------	.9187	3
444									.9169	5
612	--------	------	--------	------	--------	------	--------	------	.9134	2
630										
640									.8756	3
165	--------	------	--------	------	.875	70	--------	------		
046									.8735	4
553	--------	------	--------	------	--------	------	--------	------	.8514	1
642									.8385	5
246	--------	------	--------	------	.837	70	--------	------		
084									.8364	3
711	--------	------	--------	------	--------	------	--------	------	.8181	2
721									.8062	4
406	--------	------	--------	------	.804	80	--------	------		
482									.8042	10

References

[1] A. Hoffmann, Untersuchungen über Verbindungen mit Perowskitstruktur, Z. physik Chem. **28B**, 65–67 (1935).
[2] W. H. Zachariasen, Untersuchungen über die Kristallstruktur von Sesquioxyden und Verbindungen ABO_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. No. 4 (1928).
[3] H. D. Megaw, Crystal structure of double oxides of the perovskite type, Proc. Phys. Soc. London **58**, 133–152 (1946).
[4] R. S. Roth, Classification of perovskite and other ABO_3-type compounds, J. Research Nat. Bur. Standards **58**, No. 2, 75–88 (1958).
[5] P. Bailey, Thesis, Bristol (1952).
[6] H. D. Megaw, Ferroelectricity and crystal structure. II, Acta Cryst. **7**, 187–194 (1954).

Sulfur, S (orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
8–247, 8–248	3.85 3.21 3.44	Copper	deWolff, Delft, Holland

Additional published patterns

Source	Radiation
Hanawalt, Rinn, and Frevel[a] [1]	Molybdenum
Das [2]	-------

[a] ASTM card deleted in 8th Ed. Card Index.

NBS sample. The sample of sulfur was purified by Meyer Waxman at NBS. The sample was ground and annealed at 85° C to sharpen the diffraction pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent sodium; 0.001 to 0.01 percent each of barium, magnesium, and silicon; and 0.0001 to 0.001 percent calcium.

The color of the sample was yellow and it was optically positive. The index of refraction, $N_\alpha = 1.957$; N_β and N_γ were too high to be determined by the usual liquid grain immersion method.

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

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	222	206, 040	313
Das	222	026	206, 040, 313
deWolff	222	206, 040	026
National Bureau of Standards	222	206, 040	026

Structural data. Mark and Wigner [3] in 1924 determined that alpha sulfur has the space group Fddd (No. 70) and 128(S) per unit cell. Sulfur is used as a structure-type.

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

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1924	Mark and Wigner [3]	10.63	12.89	24.61
1925	Bragg and Bragg [4]	10.48	12.89	24.51
1935	Warren and Burwell [5]	10.50	12.95	24.60
1937	Trillat and Oketani [6]	10.42	12.83	24.60
1951	Ventriglia [7]	10.48	12.92	24.55
1955	Abrahams [8]	10.437	12.845	24.369
1958	deWolff	10.45	12.84	24.46
1959	National Bureau of Standards	10.468	12.870	24.49 at 25° C

The density of sulfur calculated from the NBS lattice constants is 2.065 g/cm³ at 25° C.

References

[1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem., Anal. Ed. **10**, 457–512 (1938).
[2] S. R. Das, A study of sulfur allotropes by X-ray diffraction method, Indian J. Phys. **12**, 163–181 (1938).
[3] H. Mark and E. Wigner, Die Gitterstruktur des rhombischen Schwefel, Z. physik. Chem. **111**, 398–414 (1924).
[4] W. H. Bragg and W. L. Bragg, X-rays and Crystal Structure, Fifth Ed., London, Bell, 254–257 (1925).
[5] B. E. Warren and J. T. Burwell, The structure of rhombic sulfur, J. Chem. Phys. **3**, 6–8 (1935).
[6] J. J. Trillat and S. Oketani, Étude sur la structure du soufre au moyen des rayons cathodiques, Z. Krist. (A) **98**, 334–343 (1937).
[7] U. Ventriglia, Sulla struttura dello zolfo rombico, Periodico mineral. (Rome) **20**, 237–55 (1951).
[8] S. G. Abrahams, The crystal and molecular structure of orthorhombic sulphur, Acta Cryst. **8**, 661–671 (1955).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1938 Das ---		1958 deWolff Cu, 1.5405 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*d*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
111	---	---	---	---	7.69	6	7.72	9
113	---	---	---	---	5.76	14	5.78	17
022	5.8	31	5.67	ms	5.68	5	5.70	8
202	---	---	---	---	4.80	2	4.82	4
115	---	---	---	---	4.19	2	4.20	5
220	---	---	---	---	4.06	11	4.062	15
131	---	---	---	---	3.91	12	3.921	20
222	3.86	100	3.85	vs	3.85	100	3.859	100
133	---	---	---	---	3.57	8	3.571	11
026	3.46	31	3.46	s	3.44	40	3.450	42
224	---	---	---	---	3.38	3	3.387	4
311	---	---	---	---	3.33	25	3.336	23
206	3.22	50	3.15	s	3.21	60	3.220	50
040								
313	3.11	38			3.11	25	3.115	26
135	---	---	---	---	3.08	17	3.087	15
008	---	---	---	---	3.06	1	---	---
044	---	---	2.85	ms	2.842	18	2.848	23
331	---	---	---	---	2.688	2	2.690	3
242	---	---	---	---	2.673	1	2.673	1
137	2.64	20	2.65	w	2.621	13	2.624	14
400	---	---	---	---	2.614	4	2.618	9
333	---	---	---	---	2.569	8	2.570	4
244	2.51	18	---	---	2.501	7	2.502	10
151	---	---	---	---	---	---	2.487	4
317	2.43	20	2.41	vw	2.424	13	2.428	15
404	---	---	---	---	2.404	2	2.407	4
422	2.38	15	---	---	2.375	4	2.379	7
335					2.366	4	2.371	6
0·2·10	2.30	15	2.26	w	2.288	6	2.289	5
048	---	---	---	---	2.215	2	---	---
1·1·11	---	---	---	---	2.146	4	2.146	4
319	2.12	25	2.12	vw	2.112	10B	2.115	11
062							2.113	11
2·2·10	---	---	---	---	2.098	2	2.096	3
511	---	---	---	---	2.057	1	2.058	1
248	---	---	---	---	2.041	1	2.042	<1
0·0·12								
353	---	---	---	---	---	---	2.008	3
513	2.00	3	---	---	2.003	2	2.003	3
442								
408	---	---	1.98	vw	1.988	4	1.989	4
262	---	---	---	---	1.957	2	1.960	4
444	---	---	---	---	1.926	1	1.926	2
355	1.90	25	1.91	vvw	1.900	7B	1.908	6
515							1.904	9
3·1·11	---	---	---	---	1.856	1	1.857	<1
159	---	---	---	---	1.838	1	1.842	<1
2·2·12	1.83	18	---	---	1.823	4	1.823	2
357	1.78	20	1.79	vvw	1.781	11	1.782	10
535	---	---	---	---	1.754	7	1.756	6

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1938 Das ----		1958 deWolff Cu, 1.5405 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
602	1.73	18	1.74	vvw	1.725	8	1.727	10
4·2·10	----------	----------	----------	----------	----------	----------	1.723	7
175	----------	----------	----------	----------	1.698	7	1.698	7
268	1.66	10	----------	----------	1.665	2	1.665	3
357	----------	----------	----------	----------	1.658	2	1.657	2
359	----------	----------	----------	----------	1.647	5	1.648	5
462	----------	----------	----------	----------	----------	----------	1.644	3
624	----------	----------	----------	----------	1.622	6	1.623	7
371								
551	----------	----------	----------	----------	----------	----------	1.620	3
080	----------	----------	----------	----------	----------	----------	1.609	1
177	1.61	20	----------	----------	1.607	6	1.607	2
2·2·14								
1·1·15	----------	----------	----------	----------	1.601	2	1.601	1
464								
373	----------	----------	----------	----------	1.595	3	1.595	2
553								
4·4·10	----------	----------	----------	----------	1.563	2	1.563	1
4·2·12								
2·6·10	1.54	3	----------	----------	1.542	1	1.542	<1
555								
466	----------	----------	----------	----------	1.531	1	1.537	<1
5·1·11	----------	----------	----------	----------	1.515	1	----------	----------
1·5·13	----------	----------	----------	----------	1.504	1	1.504	1
284	----------	----------	----------	----------	1.490	1	1.4914	1
644	----------	----------	----------	----------	----------	----------	1.4875	1
628	1.48	3	----------	----------	1.475	2	1.4756	2
2·4·14								
377								
713	----------	----------	----------	----------	1.461	1	1.4617	1
286	1.44	10	----------	----------	1.439	3	1.4389	1
646	1.43	15	----------	----------	----------	----------	1.4359	1
2·6·12	----------	----------	----------	----------	1.424	3	1.4230	2
1·1·17	----------	----------	----------	----------	1.419	1	1.4194	3
4·2·14								
733	----------	----------	----------	----------	1.391	1	1.3911	1
6·2·10	----------	----------	----------	----------	----------	----------	1.3879	<1
480	----------	----------	----------	----------	----------	----------	1.3702	<1
573	1.36	13	----------	----------	1.362	1	1.3620	<1
482								
0·6·14	----------	----------	----------	----------	----------	----------	1.3561	1
660	[a]	----------	----------	----------	1.354	3	1.3536	2

[a] Two additional lines were omitted.

Tellurium(IV) Oxide, (tellurite), TeO_2 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0117	6.8 2.82 3.09	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of tellurite, U. S. National Museum #R 8861, was obtained originally from Cananea, Sonora, Mexico. Attempts to synthesize the orthorhombic form were unsuccessful. Spectrographic analysis obtained from the U. S. Geological Survey showed the following impurities: 0.5 percent silicon; 0.3 percent copper; 0.2 percent each of aluminum and barium; 0.1 percent each of calcium and magnesium; 0.08 percent iron; 0.05 percent each of bismuth and tin; 0.02 percent each of lead, manganese, and strontium; and 0.004 percent silver.

The sample is colorless and optically positive. The refractive indices are too high to be measured by the usual liquid immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The mineral has a platy cleavage which has been identified with the 010 plane. If intensity measurements are obtained from a pressed sample the 040 reflection will dominate the pattern, being considerably stronger than any other line. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	020	131, 200	040
National Bureau of Standards	121	111	040

Structural data. Ito and Sawada [2] in 1939 determined that tellurite has the space group Pbca (No. 61) and 8(TeO_2) per unit cell. Tellurite is used as a structure-type.

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

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
020	6.81	100	6.01	5
021	4.27	13	4.05	10
111	3.89	10	3.723	94
-------	3.42	44	--------	--------
121	3.24	50	3.280	100
040	3.10	63	3.008	47
131	2.83	75	2.800	24
200				
002				
210	--------	--------	2.730	44
041	--------	--------	2.636	4
102	--------	--------	2.453	9
221	2.29	31	2.298	24
230				
-------	2.17	3	--------	--------
-------	2.12	5	--------	--------
240	2.07	3	2.050	21
151				
042	--------	--------	2.023	20
212	1.93	8	1.930	26
061	--------	--------	1.883	2
250	1.83	20	1.826	8
161	1.78	15	1.785	17
232	--------	--------	1.759	21
311	1.73	20	1.750	16
113			1.714	9
321	--------	--------	1.696	17
123	164	8	1.666	8
062				
331			1.6168	6
133	1.58	10	1.5903	7
171	1.55	3	1.5734	2
252	1.51	13	1.5176	10
213				
080			1.5021	2
143	--------	--------		
270	1.440	4	1.4662	9
351	--------	--------	1.4246	5
173	1.407	13	1.4093	6
181	--------	--------	1.4026	7
361	1.359	3	1.3267	8
082	1.315	3	1.3184	6
313			1.2946	11
124	--------	--------		
253	1.281	3	1.2885	5
281				
440	--------	--------	1.2708	7
191	--------	--------	1.2650	3
402	--------	--------	1.2489	6
044	--------	--------	1.2434	5
1·10·1	--------	--------	1.1504	7

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1939	Ito and Sawada	5.60	11.77	5.51
1959	National Bureau of Standards	5.607	12.034	5.463 at 25° C

The density of tellurite calculated from the NBS lattice constants is 5.75 g/cm³ at 25° C.

References

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

[2] T. Ito and H. Sawada, The crystal structure of tellurite (TeO_2), Z. Krist. **102A**, 13–25 (1939).

Thulium(III) Oxide, Tm_2O_3 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
2–0631	3.02 1.85 1.58	Copper	Bommer [1] 1939.

Additional published patterns. None.

NBS sample. The sample of thulium sesquioxide was prepared by the Lindsay Chemical Co., West Chicago, Ill. Their analysis showed the following impurities: a total of less than 0.1 percent of erbium and ytterbium oxides and a trace of lutecium oxide. The sample was annealed at 1,100° C for a period of 16 hr.

The sample was colorless. The index of refraction was not determined because the sample was too fine-grained.

Interplanar spacings and intensity measurements. Bragg angle data reported by Bommer was converted to *d*-values in angstroms. The indices of the three strongest lines of each pattern are as follows:

hkl	1939 Bommer Cu, 1.5418 A			1959 National Bureau of Standards Co, 1.7889 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
211	------	---	------	4.28	16	10.491
222	3.02	vs	10.47	3.028	100	10.490
321	2.809	vvw	10.51	2.803	4	10.487
400	2.617	s	10.47	2.622	41	10.489
411	2.468	w	10.47	2.472	8	10.487
420	2.342	vvw	10.47	2.3452	3	10.488
332	------	---	------	2.2368	5	10.492
422	2.138	vvw	10.48	2.1401	2	10.484
431	2.055	m	10.48	2.0570	10	10.489
521	1.912	vw	10.47	1.9147	4	10.487
440	1.850	vs	10.46	1.8534	40	10.484
433	1.795	vw	10.47	1.7989	4	10.489
600	1.744	vvw	10.46	1.7478	1	10.487
611	1.698	m	10.47	1.7019	6	10.491
620	1.656	vw	10.47	1.6588	1	10.491

hkl	1939 Bommer Cu, 1.5418 A			1959 National Bureau of Standards Co, 1.7889 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
541	1.616	w-m	10.47	1.6184	4	10.488
622	1.578	vs	10.46	1.5810	29	10.487
631	1.544	m	10.47	1.5467	6	10.490
444	1.512	m-s	10.48	1.5141	7	10.490
543	1.482	w	10.48	1.4835	3	10.490
640	1.455	vw	10.49	1.4550	1	10.492
721	1.425	w	10.47	1.4281	3	10.494
642	------	---	------	1.4016	2	10.489
732	1.331	w	10.48	1.3322	2	10.490
800	1.309	w-m	10.47	1.3114	4	10.491
811	------	---	------	1.2917	4	10.494
820	1.270	vw	10.47	1.2722	2	10.491
653	1.252	w	10.47	1.2538	2	10.490
822	1.235	vw	10.48	1.2362	2	10.490
831	1.216	w-m	10.46	1.2195	4	10.490
662	1.202	m-s	10.48	1.2034	8	10.491
840	1.170	m-s	10.47	1.1727	7	10.489
833	1.157	w	10.47	1.1582	1	10.488
842	1.143	w	10.48	1.1445	1	10.490
921	1.129	m	10.47	1.1312	2	10.490
851	1.103	w-m	10.47	1.1058	3	10.490
932	1.0803	w-m	10.474	1.0820	2	10.490
844	1.0693	m-s	10.477	1.0706	6	10.490
941	------	---	------	1.0596	3	10.490
10·0·0	------	---	------	1.0489	2	10.489
10·1·1	------	---	------	1.0386	1	10.489
10·2·0	1.0277	m	10.481	1.0286	4	10.490
943	------	-	------	1.0189	1	10.490
10·2·2	1.0082	m-s	10.478	1.0094	5	10.490
10·3·1	------	---	------	1.0002	3	10.490
871	------	---	------	0.9824	3	10.489
10·4·0	------	---	------	.9739	4	10.489
10·3·3	------	---	------	.9655	2	10.488
10·4·2	------	---	------	.9574	4	10.488
954	------	---	------	.94957	3	10.4883
11·2·1	------	---	------	.93432	4	10.4877
880	------	---	------	.92700	2	10.4878
10·4·4	------	---	------	.91289	2	10.4883
11·3·2	------	---	------	.90602	2	10.4879
Average value of last five lines		---	10.476	------	---	10.4880

Pattern	1	2	3
Bommer	222	440	622
National Bureau of Standards	222	400	440

Structural data. Pauling and Shappell [4] in 1930 determined that thulium sesquioxide has the thalliumoxide type structure (rare earth type C), the space group Ia3 (No. 206) and 16 (Tm_2O_3) per unit cell.

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

Lattice constants

		A
1925	Goldschmidt, Barth, and Lunde [3]	10.54
1927	Zachariasen [2]	10.54
1939	Bommer [1]	10.48
1954	Templeton and Dauben [5]	10.488
1959	National Bureau of Standards	10.488 at 25° C

The density of thulium sesquioxide calculated from the NBS lattice constant is 8.884 g/cm³ at 25° C.

References

[1] H. Bommer, Die Gitterkonstanten der C-Formen der Oxyde der seltenen Erdmetalle, Z. anorg. u. allgem. Chem. **241**, 273–280 (1939).

[2] W. 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 (1927).

[3] V. M. Goldschmidt, T. Barth, and G. Lunde, Isomorphie und Polymorphie der Sesquioxide, die Lanthaniden-Kontraktion und ihre Konsequenzen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. No. **7**, 1–59 (1925).

[4] L. Pauling and M. D. Shappell, The crystal structure of Bixbyite and the C-modification of the sesquioxides, Z. Krist. **75**, 128–142 (1930).

[5] D. H. Templeton and C. H. Dauben, Lattice parameters of some rare earth compounds and a set of crystal radii, J. Am. Chem. Soc. **76**, 5237–5239 (1954).

Titanium(III) Oxide, $TiO_{1.515}$ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
2–1359	1.68 1.85 1.47	Copper	Halla [1] 1929.

Additional published patterns

Source	Radiation
Zachariasen [2] 1928	Copper

NBS sample. The sample of titanium sesquioxide was obtained from Linde Speedway Laboratory, Indianapolis, Ind. Spectrographic analysis showed the following impurities. 0.01 to 0.1 percent each of aluminum, cobalt, chromium, iron, and silicon; and 0.001 to 0.01 percent each of barium and copper. Andersson, Collén, Kuylenstierna, and Magnélí [3] reported a homogeneity range in Ti_2O_3 of $TiO_{1.49}$ to $TiO_{1.51}$ Our chemical analysis showed this sample to have $TiO_{1.515}$.

The sample is a black opaque powder.

Interplanar spacings and intensity measurements. The *d*-values reported by Halla and by Zachariasen

hkl	1929 Halla Cu, 1.5418 A		1928 Zachariasen Cu, 1.5418 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
012	-----	---	3.71	40	3.732	26
104	2.73	w	2.69	50	2.712	52
110	2.57	w	2.57	50	2.572	58
006	-----	---	-----	---	2.277	7
113	2.23	vw	2.24	40	2.238	36
202	-----	---	2.118	10	2.116	10
024	1.869	m	1.858	50	1.865	35
116	1.696	w	1.696	100	1.704	100
-------	1.688	s	1.668	10	------	-----
122	1.632	vw	1.641	20	1.634	11
018	-----	---	-----	---	1.592	3
214	1.494	w	1.508	40	1.510	31
300	1.481	m	1.484	60	1.483	45
119	1.305	w	1.299	30	1.306	24
220	-----	---	1.287	30	1.2849	16
306	1.241	vw	1.241	30	1.2432	10
223	-----	---	-----	---	1.2365	6
312	-----	---	1.219	10	1.2146	6
0·2·10	1.166	m	-----	---	1.1643	6
134	-----	---	1.161	30	1.1613	16
0·0·12	-----	---	-----	---	1.1386	7
226	1.123	m	1.118	40	1.1192	26
042	-----	---	-----	---	1.0982	4
2·1·10	1.067	m	-----	---	1.0603	10
404	-----	---	1.058	40	1.0578	16

hkl	1929 Halla Cu, 1.5418 A		1928 Zachariasen Cu, 1.5418 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
1·1·12	-----	---	-----	---	1.0407	10
232	-----	---	-----	---	1.0098	4
324	0.984	w	-----	---	0.9783	10
140	-----	---	-----	---	.9713	10
0·1·14	.962	vw	-----	---	.9533	3
0·2·13	-----	---	-----	---	.9502	2
1·3·10	.927	w	-----	---	.9158	20
3·0·12	.906	s	-----	---	.9030	16
2·0·14	-----	---	-----	---	.8934	30
416						
4·0·10	.873	w	-----	---	.8626	12
054	-----	---	-----	---	.8612	10
330	-----	---	-----	---	.8566	17
2·2·12	-----	---	-----	---	.8520	10
1·2·14	.844	w	-----	---	.8439	6
1·0·16	-----	---	-----	---	.8384	8
419	.828	m	-----	---	.8179	16
3·2·10						
244	-----	---	-----	---	.8168	14
336	-----	---	-----	---	.8016	12
0·2·16	-----	---	-----	---	.7970	10

have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Halla	---	3·0·12	024
Zachariasen	116	300	104
National Bureau of Standards	116	110	104

Structural data. Lunde [4] in 1927 determined that titanium sesquioxide has alpha aluminum oxide-type structure, the space group $R\bar{3}c$ (No. 167), and $2(Ti_2O_3)$ per unit rhombohedral cell or $6(Ti_2O_3)$ per unit hexagonal cell.

Two unit-cell measurements reported in the literature have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1927	Lunde [4]	5.144	13.642
1928	Zachariasen [2]	5.16	13.59
1957	Andersson, Collén, Kuylenstierna, and Magnélf [3]	[a] 5.160	13.60
1957	Andersson, Collén, Kuylenstierna, and Magnélf [3]	[b] 5.147	13.64
1959	National Bureau of Standards	[c] 5.139	13.659 at 25° C

[a] $TiO_{1.49}$
[b] $TiO_{1.51}$
[c] $TiO_{1.515}$

The density of titanium sesquioxide calculated from the NBS lattice constants is 4.585 g/cm³ at 25° C.

References

[1] F. Halla, Reaktionen des Titansesquioxyds mit Eisenoxyder, Z. anorg. Chem. **184**, 421–427 (1929).
[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] S. Anderssen, B. Collén, U. Kuylenstierna, and A. Magnélí, Phase analysis on the titanium-oxygen system, Acta Chem. Scand. **11**, 1641–1652 (1957).
[4] G. Lunde, Über Titansesquioxyd, Z. anorg. u. allgem. Chem. **164**, 341–344 (1927).

Zinc Iodide, ZnI_2 (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0575	3.49 6.5 2.11	Molybdenum	Hanawalt, Rinn, and Frevel [1], 1938.

Additional published patterns. None.

NBS sample. The sample of zinc iodide was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent phosphorous; 0.01 to 0.1 percent calcium; and 0.001 to 0.01 percent each of aluminum, barium, iron, magnesium, and silicon.

The sample was colorless. The indices of refraction were not measured because the sample reacted with the index liquids.

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

Zinc Iodide, ZnI_2 (tetragonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1959 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
-------	6.5	20B	--------	--------
-------	5.7	20B	--------	--------
-------	4.5	12	--------	--------
-------	3.99	12	--------	--------
102	3.50	100	3.49	100
110	3.07	8	3.068	21
004	2.94	3	2.945	4
112	2.76	3	2.756	5
104	--------	--------	2.441	3
200	2.17	16	2.169	21
114	2.11	28	2.125	39
105	--------	--------	2.053	4
212	1.84	20	1.843	33
106	1.79	8	1.789	10
204	1.74	4	1.746	12
220	1.53	4	1.534	9
008	--------	--------	1.473	4
302	--------	--------	1.405	8
216	1.378	4	1.380	13
310	--------	--------	1.373	6
224	--------	--------	1.360	3
118	--------	--------	1.3282	3
314	1.242	4	1.2442	10
208	--------	--------	1.2196	5
322	--------	--------	1.1793	5
306	--------	--------	1.1653	6
1·0·10	--------	--------	1.1379	4
219	--------	--------	1.0855	3
228	--------	--------	1.0622	5
2·0·10	--------	--------	1.0358	4
326	--------	--------	1.0263	7
332 / 2·1·10	--------	--------	1.0072	4
334	--------	--------	0.9661	4
1·1·12	--------	--------	.9355	4
416	--------	--------	.9287	3
407	--------	--------	.9114	3

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	102	114	212
National Bureau of Standards	102	114	212

Structural data. Balconi [2] in 1948 determined that zinc iodide has mercuric iodide-type structure, the space group P4./nmc (No. 137), and (ZnI_2) per unit cell.

Two other forms of zinc iodide have been reported in the literature. One form has the cadmium iodide-type structure, according to Yamaguchi [3]; the other has cadmium chloride-type structure, according to Pinsker, Tatarinova, and Novikova [4].

The unit-cell measurements reported by Balconi are compared with the NBS lattice constants.

Lattice constants

		a	*c*
		A	*A*
1948	Balconi	4.27	11.80
1959	National Bureau of Standards	4.338	11.788 at 25° C

The density of zinc iodide calculated from the NBS lattice constants is 4.777 g/cm³ at 25° C.

References

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

[2] M. Balconi, La struttura dello ZnI_2, Rend. soc. mineralog. ital. **5**, 46–51 (1948).

[3] S. Yamaguchi, Determining the crystal structure of hygroscopic substances by electron diffraction, Sci. Papers Inst. Phys. Chem. Research (Tokyo) **39**, 357–359 (1942).

[4] Z. G. Pinsker, L. I. Tatarinova, and V. A. Novikova, Electronographic determination of the structure of zinc iodide, Zhur. Fiz. Khim. SSSR **20**, 1401–1402 (1946)

CUMULATIVE INDEX TO VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, AND 9[6]

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

THE NATIONAL BUREAU OF STANDARDS

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

WASHINGTON, D.C.

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

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

Heat. Temperature Physics. Thermodynamics. Cryogenic Physics. Rheology. Molecular Kinetics. Free Radicals Research.

Atomic and Radiation Physics. Spectroscopy. Radiometry. Mass Spectrometry. Solid State Physics. Electron Physics. Atomic Physics. Neutron Physics. Radiation Theory. Radioactivity. X-ray. High Energy Radiation. Nucleonic Instrumentation. Radiological Equipment.

Chemistry. Organic Coatings. Surface Chemistry. Organic Chemistry. Analytical Chemistry. Inorganic Chemistry. Electrodeposition. Molecular Structure and Properties of Gases. Physical Chemistry. Thermochemistry. Spectrochemistry. Pure Substances.

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

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

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

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

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

Applied Mathematics. Numerical Analysis. Computation. Statistical Engineering. Mathematical Physics.

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

● Office of Basic Instrumentation.

● Office of Weights and Measures.

BOULDER, COLORADO

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

Radio Propagation Physics. Upper Atmosphere Research. Ionosphere Research. Regular Prediction Services. Sun-Earth Relationships. VHF Research. Radio Warning Services. Airglow and Aurora. Radio Astronomy and Arctic Propagation.

Radio Propagation Engineering. Data Reduction Instrumentation. Radio Noise. Tropospheric Measurements. Tropospheric Analysis. Propagation-Terrain Effects. Radio-Meteorology. Lower Atmosphere Physics.

Radio Standards. High-Frequency Electrical Standards. Radio Broadcast Service. Radio and Microwave Materials. Electronic Calibration Center. Microwave Circuit Standards.

Radio Communication and Systems. Low Frequency and Very Low Frequency Research. High Frequency and Very High Frequency Research. Modulation Systems. Antenna Research. Navigation Systems. Systems Analysis. Field Operations.