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VOLUME 10

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

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Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, Marlene I. Cook, Eloise H. Evans, and Johan H. deGroot

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Contents

*Not previously represented in the Powder Data File.

Errata

Vol. 9. Page 61, space group P4./nmc should be $P4_2/nmc$.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. 10—Data for 40 Substances

Howard E. Swanson, Marlene I. Cook,[1] Eloise H. Evans,[1] and Johan H. deGroot [1]

Forty standard X-ray diffraction powder patterns are presented Twenty-two are to replace thirty-five patterns already given in the X-ray Powder Data File, and eighteen are for substances not previously included. The X-ray Powder Data File is a compilation of diffraction patterns from most 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 substances: $AlPO_4$ (berlinite), $AlPO_4$, Sb_2O_3 (natural valentinite), Sb_2O_3 (synthetic valentinite), Sb_2O_4 (cervantite), Sb_2O_5, $BaCO_3$, $BeCr_2O_4$, Be_2GeO_4, $Ca_3Al_2(GeO_4)_3$, $Ca_3Cr_2(GeO_4)_3$, $Ca_3Cr_2(SiO_4)_3$ (uvarovite), $Ca_3Ga_2(GeO_4)_3$, $Ca_3Fe_2(GeO_4)_3$, $Ce_2Mg_3(NO_3)_{12}\cdot 24H_2O$, $CoAs_3$ (skutterudite), $CoAs_2$, $CoGa_2O_4$, Co_2GeO_4, $CoFeAs_4$ (safflorite), $CoCO_3$ (sperocobaltite), $Cu_3(OH)_2(CO_3)_2$ (azurite), $Cu_2(OH)_2(CO_3)$ (malachite), AuCN, $FeAs_2$ (loellingite), $MgGa_2O_4$, Mg_2GeO_4 (cubic), Mg_2GeO_4 (orthorhombic), $Mg_2SiO_4\cdot MgF_2$ (norbergite), MnSe, $NiAs_2$ (rammelsbergite), $NiFe_2O_4$ (trevorite), $NiGa_2O_4$, K_2RuCl_6, $K_4Ru_2Cl_{10}O\cdot H_2O$, SiO_2 (cristobalite), Ag_2S, (argentite), α-$Na_4P_4O_{12}\cdot 4H_2O$, TeO_2, paratellurite, Zn_2GeO_4.

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 40 compounds. This paper is the tenth of a series of "Standard X-ray Diffraction Patterns". These patterns are recommended to replace 35 cards now in the file. The patterns for 18 compounds not represented in the file have been added. These compounds are: barium carbonate (cubic), beryllium chromium oxide, calcium aluminum germanate, calcium chromium germanate, calcium gallium germanate, calcium iron germanate, cerium magnesium nitrate 24-hydrate, cobalt diarsenide, cobalt gallate, cobalt germanate, magnesium germanate (cubic), magnesium germanate (orthorhombic), manganese selenide, nickel gallate, potassium chlororuthenate (IV), potassium hydroxy-chlororuthenate, alpha sodium tetrametaphosphate tetrahydrate, tellurium(IV) oxide, paratellurite.

The experimental procedure and general plan of these reports have not changed from that of 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 1959 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 also 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

[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; Vol. 8, April 1959; and Vol. 9, February 1960.

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

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 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 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 ($K\alpha_1$) or cobalt radiation ($K\alpha_1$), having the wavelengths 1.5405 A, and 1.7889 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 given in the tables of *d*-values and intensities are in angstrom units, whereas the wavelengths listed under the first section of each report are the original work rather than that data reported on the ASTM cards.

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, using those *d*-values for which only one *hkl* could be assigned. 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 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 given 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.

Orthorhombic cell dimensions are presented 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. (1959).

[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, Remarks concerning the absolute value of Avogadro's number, Phys. Rev. **95,** 566 (1954).

Aluminum Orthophosphate (berlinite), $AlPO_4$ (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
3–0445, 3–0446	3. 32 1. 38 4. 27	Copper	Huttenlocher [1] 1935.

Additional published patterns. None.

NBS sample. The sample of aluminum orthophosphate was prepared by Alvin Perloff at the NBS in a Morey-type hydrothermal bomb [2] using aluminum metal and phosphoric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon and 0.001 to 0.01 percent iron.

The sample was colorless. The indices of refraction are $N_o=1.524$ and $N_e=1.530$ and it is optically positive.

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

Pattern	1	2	3
Huttenlocher	102	302	114
National Bureau of Standards	102	100	114

Structural data. Huttenlocher [1] in 1935 determined that the berlinite form of aluminum orthophosphate has the α-quartz-type structure, the space groups $P3_121$ (No. 152) or $P3_221$ (No. 154), and $3(AlPO_4)$ per unit cell. Other forms of aluminum orthophosphate which also parallel the silica system have been reported [3].

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

Lattice constants

		a	*c*
		A	A
1935	Huttenlocher [1]	4. 94	10. 96
1941	Strunz [4]	4. 983	10. 93
1948	Brill and De Brettеville [5]	4. 975	10. 84
1960	National Bureau of Standards	4. 942	10. 97 at 25° C.

hkl (hex.)	1935 Huttenlocher Cu, 1.5418 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		A	
100	4. 27	75	4. 28	23
101	3. 97	16	3. 984	5
003	-----	----	3. 661	2
102	3. 33	100	3. 369	100
110	2. 46	50	2. 471	10
111	-----	----	2. 404	<1
104	2. 30	50	2. 306	10
112	2. 25	16	2. 252	5
200	2. 14	50	2. 140	8
202	1. 98	33	1. 994	5
114	1. 82	83	1. 835	14
204	1. 68	58	1. 687	7
106			1. 679	4
115	1. 62	8	1. 639	1
210			1. 619	<1
211	-----	----	1. 600	<1
212	1. 54	83	1. 552	12
205	-----	----	1. 530	<1
213	-----	----	1. 479	<1
116	-----	----	1. 468	2
300	1. 42	33	1. 427	1
214	-----	----	1. 393	10
206	1. 38	8	1. 389	11
302	1. 37	100	1. 381	6
215	1. 30	42	1. 303	4
304, 207	1. 26	50	1. 2651	3
220	1. 23	25	1. 2359	1
216	1. 21	50	1. 2109	4
222	-----	----	1. 2054	2
305	1. 19	50	1. 1973	3
310	1. 185	50+	1. 1870	6
223	-----	----	1. 1701	<1
312	1. 155	33	1. 1603	2
306	1. 120	8	1. 1247	<1
314	1. 085	58	1. 0894	2
400	1. 067	16–	1. 0700	2
209	1. 059	25	1. 0605	1
402	-----	----	1. 0503	1
315	1. 042	33	1. 0447	3
226	1. 020	33	1. 0233	2
1·1·10	-----	----	1. 0010	2
404	-----	----	0. 9966	1
316	0. 994	33	. 9951	1
308	-----	----	. 9879	<1
320	. 979	16	. 9822	<1
1·0·11	-----	----	. 9722	<1
322	. 964	42	. 9666	3
323	-----	----	. 9483	<1
410	. 931	8	. 9341	<1
324	-----	----	. 9242	2

Aluminum Orthophosphate (berlinite), $AlPO_4$ (trigonal)—Continued

hkl (hex.)	1935 Huttenlocher Cu, 1.5418 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
406	-----	----	.9231	2
412	-----	----	.9207	1
228	.918	67	.9171	1
0·0·12	-----	----	.9148	2
2·1·10	.905	25	.9066	2
318, 325	.895	25	.8969	<1
414, 407	.883	25	.8841	1
229	.867	8	.8685	<1
500	.858	8	.8558	1
502	.846	8	.8459	1
2·0·12	.839	33	.8393	2
327, 416	.831	33	.8315	3
330	-----	----	.8238	2
2·2·10	.819	16	.8195	2
3·0·11, 504	.816	42	.8172	3
332	.810	25	.8148	1
420	.807	16—	.8090	2
409	.801	8	.8048	1
422	.798	42	.8003	1
328, 505	.796	16	.7979	4

The density of aluminum orthophosphate calculated from the NBS lattice constants is 2.618 g/cm ^{3} at 25° C.

References

[1] H. F. Huttenlocher, Kristallstruktur des Aluminiumorthophosphates, Z. Krist. **90A,** 508–516 (1935).
[2] Morey and Ingerson, Alterations and synthesis of silicates, Econ. Geol. **32,** 607 (1937).
[3] W. R. Beck, Crystallographic inversions of the aluminum orthophosphate polymorphs and their relation to those of silica, J. Am. Ceram. Soc. **32,** 147–151 (1949).
[4] H. Strunz, Isotypie von Berlinit mit Quarz, Z. Krist. **103A,** 228–229 (1941).
[5] R. Brill and A. De Bretteville, On the crystal structure of $AlPO_4$, Am. Min. **33,** 750 (1948).

Aluminum Orthophosphate, $AlPO_4$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
9–114	4. 08 2. 51 1. 62	Copper	Mooney [1] 1956.

Additional published patterns

Source	Radiation
Winkhaus [2] 1951	Copper

Strada [3] reports a pattern for tetragonal aluminum orthophosphate that is not comparable with these patterns.

NBS sample. The sample of aluminum orthophosphate was prepared at NBS by Alvin Perloff from aluminum metal and orthophosphoric acid. The sample was heated in a Morey-type hydrothermal bomb [4] at 1,200° C for 6½ days. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent iron.

The sample is colorless. The indices of refraction could not be determined by the oil immersion method because the sample was too fine-grained.

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

Pattern	1	2	3
Winkhaus	111	220	021, 201
Mooney	111	220, 202, 022	112
National Bureau of Standards	111	220	112

Structural data. Mooney [1] in 1956 determined that aluminum orthophosphate is ortho-

Aluminum Orthophosphate, $AlPO_4$ (orthorhombic)

hkl	1956 Mooney Cu, 1.5405 A		1951 Winkhaus Cu, 1.5418 A		1960 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A	[a]	*A*		*A*	
--------	-----	---	4. 294	vs	------	---
110	5. 02	<1	-----	----	5. 012	1
111	4. 08	100	4. 102	vvs	4. 077	100
020	3. 55	2	-----	----	3. 553	2
200	-----	---	-----	----	3. 539	3
002	3. 50	<1	-----	----	3. 496	2
021, 201	3. 17	12	3. 163	vs	3. 162	10
112	2. 87	15	2. 867	vs	2. 867	12
220	2. 51	24	2. 499	vvs	2. 506	18
202, 022	2. 50		------	----	2. 491	5
--------	2. 252	<1	-----	----	------	---
311, 131	2. 136	5	2. 123	m	2. 135	4
222	2. 041	3	2. 029	m	2. 038	3
203, 023	1. 949	7	1. 937	vs	1. 949	6
312, 132	1. 888	7	1. 876	vs	1. 888	5
040	1. 774	<1	------	----	1. 779	<1
400			------	----	1. 770	2
004	1. 752	2	1. 734	vvw	1. 749	2
223	1. 710	4	1. 699	s	1. 7072	3
114	1. 654	<1	-----	----	1. 6510	1
331	1. 625	7	------	----	1. 6250	5
133	1. 619		1. 616	vs	1. 6163	3
042	1. 584	1	1. 573	vvw	1. 5823	2
--------	1. 572	<1	-----	----	------	---
421	1. 547	4	1. 537	s	1. 5452	3
332	1. 509	5	1. 500	s	1. 5074	5
422	1. 445	3	-----	----	1. 4431	3
224	1. 436	2	1. 434	m	1. 4341	2
403	1. 412	2	1. 404	vw	1. 4101	1
134	1. 380	4	1. 374	m	1. 3789	2
511	1. 364	3	-----	----	1. 3630	1
333	-----	---	1. 354	w	1. 3582	1
115	1. 351	3	1. 342	w	1. 3474	2
423	1. 312	4	1. 305	s	1. 3104	2
512	1. 293	4	1. 287	s	1. 2913	2
440	1. 254	<1	-----	----	------	---
044, 404	1. 246	1	-----	----	1. 2443	<1
441	1. 234	2	1. 227	vw	1. 2333	1
225	1. 224	<1	-----	----	------	---
530	1. 216	2	1. 211	m	1. 2151	1
531	1. 199	7	------	----	1. 1977	<1
513	1. 195		------	----	1. 1936	1
315	1. 189		1. 189	w	1. 1866	1
--------	1. 182		------	----	------	---
442	1. 181		------	----	1. 1794	<1
244	1. 176		------	----	1. 1747	<1
601, 006	1. 164	<1	-----	----	1. 1644	<1
532	1. 150	<1	-----	----	1. 1480	<1

[a] Intensities based upon peak areas. Intensities reported on ASTM card #9-114 included Lorentz-polarization factor.

rhombic having the space group $C222_1$ (No. 20) with 4($AlPO_4$) per unit cell and not the small primitive tetragonal cell heretofore used for comparison with low-cristobalite. According to Beck [5] aluminum orthophosphate exhibits the same polymorphs as silica.

The "a" value reported by Winkhaus has been multiplied by the $\sqrt{2}$. The unit-cell measurements reported by Caglioti have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	c
		A	A	A
1935	Caglioti [6]*----	7. 149	-----	6.864
1951	Winkhaus [2]*--	7. 06	-----	6.90
1956	Mooney [1]-----	7. 099	7. 099	7.006
1960	National Bureau of Standards	7. 082	7. 098	6.993 at 25° C

*Based on tetragonal cell.

The density of aluminum orthophosphate calculated from the NBS lattice constants is 2.304 g/cm³ at 25° C.

References

[1] R. C. L. Mooney, The crystal structure of aluminum phosphate and gallium phosphate, low-cristobalite type, Acta Cryst. **9,** 728–734 (1956).

[2] B. Winkhaus, Die kristallchemischen Beziehungen zwischen Aluminum-orthophosphat $AlPO_4$ und Siliciumdioxyd SiO_2, Neues Jahrb. Mineral, Abhandl. **83,** 1–22 (1951).

[3] M. Strada, La struttura cristallina di alcuni fosfati ed arseniati di metalli trivalenti. I. Fosfato ed arseniato di alluminio, Gazz, chim. ital. **64,** 653–662 (1934).

[4] Morey-Ingerson, Alterations and synthesis of silicates, Econ. Geol. **32,** 607 (1937).

[5] W. R. Beck, Crystallographic inversions of the aluminum orthophosphate polymorphs and their relation to those of silica, J. Am. Ceram. Soc. **32,** No. 4, 147–151 (1949).

[6] V. Caglioti, Sulla struttura del fosfato ferrico, Rend. accad. nazl. Lincei (**6**) **22,** 146–149 (1935).

Antimony(III) Oxide (synthetic and natural) valentinite, Sb_2O_3 (orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
2–0585	3. 08 10. 85 1. 79	Copper	British Museum.
3–0530	3. 14 1. 80 4. 59	Molybdenum	Dow Chemical Co.

Additional published patterns. None.

NBS sample. The sample of synthetic antimony trioxide was prepared at NBS by melting antimony trioxide in an argon atmosphere. The liquid oxide was air quenched by pouring on a cool refractory tile. The small cakes that formed were composed of acicular crystals perpendicular to the cooling surface. Spectrographic analysis for the synthetic antimony trioxide showed the following impurities: 0.01 to 0.1 percent each of arsenic and lead; and 0.001 to 0.01 percent each of aluminum, copper, iron, magnesium, and silicon.

The sample of natural valentinite (Minas Geraes, Brazil) was obtained from the National Museum, #92516. Spectrographic analysis of the mineral showed the following impurities: 0.1 to 1.0 percent lead; 0.01 to 0.1 percent each of copper and silicon; and 0.001 to 0.01 percent each of aluminum, iron, and magnesium.

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

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

Pattern	1	2	3
British Museum----------	121, 040	---	161
Dow Chemical Co---------	121, 040	161	110
National Bureau of Standards (synthetic)---------	121	040	111
National Bureau of Standards (natural)----------	121	040	111

Structural data. Buerger [1] in 1936 determined that antimony trioxide has the space group Pccn (No. 56), and 4(Sb_2O_3) per unit cell. Antimony trioxide is used as a structure-type.

Roberts and Fenwick [2] in 1928 reported that antimony trioxide is dimorphous, namely cubic (senarmontite) and orthorhombic (valentinite). Senarmontite, Sb_2O_3 cubic, heated in air above 570° C oxidizes to Sb_2O_4, and if heated without oxygen forms valentinite. The unit-cell measurements reported by Buerger have been converted from kX to angstrom units for comparison with the NBS values.

The density of antimony trioxide calculated from the NBS lattice constants is 5.828 g/cm$_8$ (synthetic) and 5.832 g/cm³ (natural) at 25° C.

References

[1] M. J. Buerger, The crystal structure of valentinite, Am. Min. **21,** 206 (1936).

[2] E. J. Roberts and F. Fenwick, The antimony-antimony trioxide electrode and its use as a measure of acidity, J. Am. Chem. Soc. **50,** 2125–2147 (1928).

Antimony(III) Oxide (synthetic and natural) valentinite, Sb_2O_3 (orthorhombic)

hkl	---- British Museum mineral from Przibram, Bohemia Cu, 1.5418 A		1938 Dow Chemical Co. synthetic Mo, 0.7107 A		1960 National Bureau of Standards synethtic Cu, 1.5405 A at 25° C		1960 National Bureau of Standards mineral from Geraes, Brazil Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A	
--------	10. 85	80	------	----	------	----	------	----
--------	------	----	5. 40	4	------	----	------	----
110	4. 44	60	4. 59	25	4. 571	17	4. 56	17
111	3. 43	60	3. 50	20	3. 494	26	3. 494	23
130	------	----	------	----	3. 174	20	3. 173	20
121 }	3. 08	100	3. 14	100	{ 3. 142	100	3. 142	100
040 }					{ 3. 118	75	3. 117	80
131 }	2. 70	40	2. 72	8	{ 2. 738	9	2. 737	10
002 }					{ 2. 712	9	2. 710	9
012	2. 61	20	2. 64	8	2. 650	13	2. 648	13
200	2. 42	60	2. 45	12	2. 456	9	2. 456	9
141	------	----	------	----	2. 370	2	2. 371	3
032	------	----	2. 27	3	2. 271	2	2. 272	2
211	------	----	2. 21	2	2. 204	4	2. 203	4
221	2. 10	40	2. 09	2	2. 107	3	2. 107	4
151	2. 03	40	2. 05	12	2. 058	8	2. 058	9
042	1. 98	40	------	----	2. 046	8	2. 045	8
231	1. 95	40	1. 97	3	1. 971	5	1. 970	6
240	1. 91	70	1. 93	12	1. 9288	11	1. 929	11
142	------	----	1. 89	3	1. 8884	2	1. 888	1
052	------	----	1. 83	6	1. 8356	5	1. 835	5
241	------	----	------	----	1. 8178	4	1. 818	8
161	1. 79	80	1. 80	32	1. 8046	19	1. 804	20
170	1. 72	20	1. 67	16	1. 6745	8	1. 675	9
231, 251	1. 66	40	------	----	1. 6660	7	1. 666	8
310	1. 61	40	1. 62	3	1. 6239	3	1. 623	3
171	------	----	------	----	1. 6006	2	1. 6007	3
242, 133	------	----	1. 57	12	1. 5715	6	1. 5715	6
080	1. 55	40B	------	----	1. 5577	3	1. 5589	3
261	------	----	1. 52	12	1. 5226	11	1. 5230	7
321	1. 51	70	------	----	1. 5201	8	1. 5203	6
072	------	----	------	----	1. 4882	3	1. 4882	3
252, 331	1. 46	40	------	----	1. 4696	4	1. 4683	2
223	1. 41	20	------	----	1. 4169	3	1. 4161	2
341	------	----	------	----	1. 4011	4	1, 4013	4
312	1. 39	40	------	----	1. 3937	4	1. 3937	4
350	1. 36	40	------	----	1. 3689	4	1. 3693	3
082	1. 35	20	------	----	1. 3515	2	1. 3512	2
190	------	----	------	----	1. 3337	1	1. 3339	1
351	------	----	------	----	1. 3270	1	1. 3264	2
280	1. 31	40	------	----	1. 3158	5	1. 3164	3
342, 281	------	----	------	----	1. 2784	<1	1. 2781	1
272	1. 27	40	------	----	1. 2732	<1	------	----
361	1. 25	40	------	----	1. 2515	2	1. 2514	2
092	------	----	------	----	1. 2335	<1	------	----
400	1. 22	40	------	----	1. 2282	2	------	----
144	1. 20	20	------	----	1. 2058	2	------	----
411	1. 19	40	------	----	1. 1923	4	------	----
1. 10. 1	------	----	------	----	1. 1796	2	------	----
291	1. 17	60	------	----	1. 1774	6	------	----
431	1. 15	60	------	----	1. 1507	1	------	----
440	------	----	------	----	1. 1428	2	------	----

		a	*b*	*c*
		A	*A*	*A*
1936	Buerger [1]	4. 93	12. 49	5. 43
1960	National Bureau of Standards (synthetic)	4. 914	12. 468	5. 421 at 25° C
1960	National Bureau of Standards (natural)	4. 913	12. 474	5. 416 at 25° C

Antimony(IV) Oxide (cervantite), Sb_2O_4 (orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–0818	3. 07 3. 44 1. 72	Molybdenum	New Jersey Zinc Co.
3–0575	3. 07 3. 44 2. 94	Molybdenum	Dow Chemical Co.

Additional published patterns. None.

NBS sample. The sample of antimony tetroxide was prepared at NBS by heating Mallinckrodt's antimony trioxide at 775° C. No analysis of the heated sample was made at NBS; however, Mallinckrodt's analysis showed the following impurities: 0.01 to 0.1 percent each of lead and silicon; 0.001 to 0.01 percent each of silver, arsenic, calcium, copper, iron, nickel, and tin.

The color of the sample was 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. and by the Dow Chemical Co. 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
New Jersey Zinc Co	112	111	116, 222
Dow Chemical Co	112	111	004
National Bureau of Standards	112	004	111

Structural data. Dihlström [1] in 1938 determined that antimony tetroxide was isomorphous with stibiotantalite, having the space group $Pna2_1$ (No. 33), and $4(Sb_2O_4)$ per unit cell. Antimony tetroxide had previously been reported as being cubic by Dehlinger [2] and by Natta and Baccaredda [3].

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

The density of antimony tetroxide calculated from the NBS lattice constants is 6.641 g/cm³ at 25° C.

hkl	---- New Jersey Zinc Co. Mo, 0.7107 A		1938 Dow Chemical Co. Mo, 0.7107 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
002	------	----	5. 90	1	5. 901	3
----------	------	----	5. 40	1	------	----
011	------	----	4. 42	6	4. 455	9
110	3. 50	1	------	----	3. 604	3
111	3. 45	33	3. 44	40	3. 445	35
112	3. 08	100	3. 07	100	3. 073	100
013	------	----	------	----	3. 033	4
004	2. 94	23	2. 94	25	2. 942	44
200	------	----	2. 72	3	2. 718	8
113	2. 66	17	2. 65	20	2. 651	23

Antimony(IV) Oxide (cervantite), Sb_2O_4 (orthorhombic)—Continued

hkl	---- New Jersey Zinc Co. Mo, 0.7107 A		1938 Dow Chemical Co. Mo, 0.7107 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
202	2. 46	3	2. 46	8	2. 470	7
020	2. 39	7	2. 40	12	2. 404	17
203	2. 22	1	2. 24	3	2. 235	10
212	------	----	------	----	2. 195	5
121	------	----	------	----	2. 162	3
015	------	----	------	----	2. 112	3
122	------	----	------	----	2. 062	2
213	------	----	------	----	2. 026	2
204	1. 99	2	1. 99	6	1. 998	5
115	------	----	1. 97	6	1. 971	5
123	------	----	1. 92	2	1. 917	4
024	1. 86	20	1. 86	20	1. 862	25
220	------	----	------	----	1. 801	6
221, 205	1. 78	17	1. 78	15	1. 781	22
116, 222	1. 72	27	1. 72	25	1. 723	19
310	1. 68	3	1. 69	9	1. 697	10
311	------	----	------	----	1. 679	5
223	1. 63	7	1. 64	12	1. 636	11
125	1. 59	1	------	----	1. 607	4
206	------	----	------	----	1. 591	2
313	------	----	------	----	1. 557	2
224, 130	1. 53	2	------	----	1. 536	3
131, 117	------	----	------	----	1. 524	4
126	------	----	------	----	1. 509	1
216, 132	1. 48	15	------	----	1. 487	12
314, 008	------	----	------	----	1. 469	10
133	1. 43	12	------	----	1. 431	9
315	1. 37	1	------	----	1. 377	2
231	------	----	------	----	1. 372	2
035, 226, 402	1. 32	9	------	----	1. 325	6
028	1. 25	8	------	----	1. 255	4
119, 227	1. 20	5	------	----	1. 229	2
136	------	----	------	----	1. 210	2
330	------	----	------	----	1. 201	1
414, 331	------	----	------	----	1. 195	1
209, 042	------	----	------	----	1. 178	1
141	------	----	------	----	1. 168	1
037, 422	1. 16	7	------	----	1. 160	6
1·1·10	------	----	------	----	1. 119	2
406	------	----	------	----	1. 116	1
334, 044	1. 11	15	------	----	1. 112	4
318	------	----	------	----	1. 109	2
241	------	----	------	----	1. 095	2
243, 510	1. 06	8	------	----	1. 059	4
238, 146	1. 01	3	------	----	1. 013	3
341, 408	1. 00	4	------	----	0. 9982	<1
245, 139	------	----	------	----	. 9958	1
0·0·12, 434	------	----	------	----	. 9779	2
427	------	----	------	----	. 9678	1
152	------	----	------	----	. 9350	3
516	------	----	------	----	. 9330	<1
048	------	----	------	----	. 9310	3

Lattice constants

		a	b	c
		A	A	A
1938	Dihlström [1]	5. 435	4. 814	11. 78
1960	National Bureau of Standards.	5. 436	4. 810	11. 76 at 25° C.

References

[1] K. Dihlström, Über den Bau des wahren Antimontetroxyds und des damit isomorphen Stibiotantalits, $SbTaO_4$, Z. anorg. u. allgem. Chem. **239,** 57–64 (1938).

[2] U. Dehlinger, The crystal structure of the antimony oxides, Z. Krist. **66,** 108–119 (1927).

[3] G. Natta and M. Baccaredda, Composti chimici interstiziali. Struttura del pentossido di antimonio idrato e di alcuni antimoniati, Gazz. chim. ital. **66,** 308–316 (1936).

Antimony(V) Oxide, Sb_2O_5 (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–0154	6. 0 3. 10 2. 97	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
2–1385	1. 54 1. 81 1. 17	Molybdenum	Natta and Baccaredda [2] 1936.
*2–1383	1. 55 1. 81 1. 18	Molybdenum	Natta and Baccaredda [2] 1936.
*2–1386	1. 54 1. 81 1. 14	Molybdenum	Natta and Baccaredda [2] 1936.

*These two patterns are listed as hydrates, but match the anydrous pattern.

Additional published patterns. None.

NBS sample. The sample of antimony pentoxide was prepared at NBS by dissolving antimony metal in hydrochloric acid. Nitric acid was used to precipitate an oxide which was rinsed and dried. An X-ray pattern was obtained after heating the oxide to 780° C for 30 min. Johnson, Matthey and Co.'s chemical analysis for antimony showed: 0.02 to 0.03 percent each of lead, arsenic, and copper, and less than 0.01 percent each of nickel, silicon, iron, silver, and bismuth.

The color of the sample was white. 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 Hanawalt, Rinn, and Frevel and those reported by Natta and Baccaredda have been converted from kX to angstrom units. The indices of the three strongest lines for each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	111	311	222
Natta and Baccaredda	622	440	840
Natta and Baccaredda	622	440	662
Natta and Baccaredda	622	440	662
National Bureau of Standards	222	400	622

Structural data. Dehlinger [3] in 1927 determined that antimony pentoxide has the space group Fd3m (No. 227) and $8(Sb_2O_5)$ per unit cell. The unit-cell measurements reported by Dehlinger have been converted from kX to angstrom units for comparison with the NBS value.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1936 Natta and Baccaredda Mo, 0.7107 A [a]			1936 Natta and Baccaredda Mo, 0.7107 A [b]			1936 Natta and Baccaredda Mo, 0.7107 A			1960 National Bureau of Standards Cu, 1.5405 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	6. 0	100	10. 4	5. 90	40	10. 2	----	--	----	5. 91	20	10. 2	5. 952	27	10. 309
311	3. 10	80	10. 3	3. 08	40	10. 2	3. 09	40	10. 3	----	--	----	3. 108	22	10. 309
222	2. 97	80	10. 3	2. 95	60	10. 2	2. 96	60	10. 3	2. 96	60	10. 3	2. 976	100	10. 309
400	2. 58	16	10. 3	2. 55	40	10. 2	2. 56	50	10. 2	2. 56	20	10. 2	2. 577	30	10. 309
331	2. 36	4	10. 3	----	--	----	----	--	----	----	--	----	2. 365	4	10. 308
-----	-----	--	----	2. 28	20	----	----	--	----	2. 29	20	----	-----	--	-----
422	-----	--	----	----	--	----	2. 08	20	10. 2	----	--	----	2. 102	2	10. 301
511	1. 98	16	10. 3	1. 98	50	10. 3	1. 97	20	10. 2	1. 97	50	10. 2	1. 983	6	10. 305
440	1. 82	50	10. 3	1. 81	80	10. 3	1. 81	80	10. 3	1. 81	80	10. 3	1. 821	24	10. 302
531	1. 73	16	10. 2	1. 73	70	10. 2	1. 73	50	10. 2	1. 73	60	10. 2	1. 741	8	10. 303

Antimony(V) Oxide, Sb_2O_5 (cubic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1936 Natta and Baccaredda Mo, 0.7107 A [a]			1936 Natta and Baccaredda Mo, 0.7107 A [b]			1936 Natta and Baccaredda Mo, 0.7107 A			1960 National Bureau of Standards Cu, 1.5405 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
620	-----	--	----	1. 62	20	----	----	--	----	1. 62	20	10. 2	1. 629	<1	10. 304
533	-----	--	----	----	--	----	----	--	----	----	--	----	1. 572	2	10. 308
622	1. 55	36	10. 3	1. 54	100	10. 3	1. 55	100	10. 3	1. 54	100	10. 3	1. 553	29	10. 305
444	1. 48	8	10. 3	1. 47	7	10. 2	1. 48	40	10. 3	1. 47	40	10. 2	1. 488	9	10. 305
711	1. 44	8	10. 3	1. 42	50	10. 1	1. 43	20	10. 2	1. 43	50	10. 2	1. 443	8	10. 305
-----	-----	--	----	----	--	----	----	--	----	1. 37	20	----	-----	--	-----
731	1. 34	12	10. 3	1. 33	50	10. 2	1. 33	60	10. 2	1. 33	60	10. 2	1. 342	6	10. 305
800	-----	--	----	1. 28	50	10. 2	1. 28	20	10. 2	1. 28	50	10. 2	1. 288	4	10. 304
733	-----	--	----	----	--	----	----	--	----	----	--	----	1. 259	1	10. 305
822	-----	--	----	----	--	----	----	--	----	----	--	----	1. 190	1	10. 306
662	1. 18	8	10. 3	1. 17	70	10. 2	1. 18	70	10. 3	1. 17	70	10. 2	1. 182	8	10. 305
840	1. 15	4	10. 3	1. 14	80	10. 2	1. 14	70	10. 2	1. 14	70	10. 2	1. 152	8	10. 305
911	-----	--	----	1. 12	50	10. 2	1. 12	50	10. 2	----	--	----	1. 131	4	10. 305
931	1. 08	4	10. 3	1. 07	40	10. 3	----	--	----	1. 09	20	10. 4	1. 081	3	10. 308
844	1. 05	4	10. 3	1. 04	70	10. 2	1. 05	60	10. 3	1. 05	70	10. 3	1. 052	6	10. 305
933	-----	--	----	1. 03	50	10. 2	----	--	----	1. 03	50	10. 3	1. 036	3	10. 307
951	-----	--	----	----	--	----	----	--	----	----	--	----	0. 9964	2	10. 307
10·2·2	0. 991	4	10. 3	----	--	----	----	--	----	----	--	----	. 9917	4	10. 306
953	-----	--	----	----	--	----	----	--	----	----	--	----	. 9611	3	10. 307
11·1·1	-----	--	----	----	--	----	----	--	----	----	--	----	. 9291	1	10. 304
880	-----	--	----	----	--	----	----	--	----	----	--	----	. 9108	2	10. 304
11·3·1	-----	--	----	----	--	----	----	--	----	----	--	----	. 9004	6	10. 306
11·3·3	-----	--	----	----	--	----	----	--	----	----	--	----	. 8741	6	10. 305
10·6·2	-----	--	----	----	--	----	----	--	----	----	--	----	. 8709	8	10. 305
12·0·0	-----	--	----	----	--	----	----	--	----	----	--	----	. 8588	6	10. 305
11·5·1	-----	--	----	----	--	----	----	--	----	----	--	----	. 8499	3	10. 304
11·5·3	-----	--	----	----	--	----	----	--	----	----	--	----	. 8277	2	10. 305
12·4·0	-----	--	----	----	--	----	----	--	----	----	--	----	. 8147	5	10. 305
991	-----	--	----	----	--	----	----	--	----	----	--	----	. 8072	2	10. 306
Average value of last five lines----------	10. 3			----	--	10. 2	----	--	10. 2	----	--	10. 3	-----	--	10. 305

[a] Listed as $Sb_2O_5 \cdot H_2O$.

[b] Listed as $Sb_2O_5 \cdot 3H_2O$.

Lattice constants

		A
1927	Dehlinger [3]----------	10.26
1960	National Bureau of Standards.----------	10.305 at 26° C

The density of antimony pentoxide calculated from the NBS lattice constant is 3.927 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] G. Natta and M. Baccaredda, Composti chimici interstiziali. Struttura del pentossido di antimonio idrato e di alcuni antimoniati, Gazz. chim. ital. **66,** 308–316 (1936).

[3] U. Dehlinger, The crystal structure of the antimony oxides, Z. Krist. **66,** 108–119 (1927).

Barium Carbonate, $BaCO_3$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of barium carbonate was supplied by Baker and Adamson. The X-ray pattern was made at 1,075° C. Thorium dioxide was used as an internal standard assuming 5.651 as the cell size at 1,075° C. The transformation of the $BaCO_3$ to cubic is given as 956° to 976° C [2]. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium and

strontium; and 0.001 to 0.01 percent each of aluminum, chromium, iron, sodium, and silicon.

The sample was colorless.

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	111	220

Structural data. Boeke [1] first showed that barium carbonate had a cubic high-temperature polymorph with the sodium chloride type structure, the space group Fm3m (No. 225), and 4($BaCO_3$) per unit cell.

Lattice constants

		a
		A
1949	Lander [2]	6.96 at 960° C
1960	National Bureau of Standards.	6.959 at 1,075° C

The density of barium carbonate calculated from the NBS lattice constant is 3.889 g/m³ at 1,075° C.

Barium Carbonate, $BaCO_3$ (cubic)

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 1,075° C		
	d	*I*	*a*
	A		*A*
111	4. 02	63	6. 96
200	3. 48	100	6. 96
220	2. 459	62	6. 955
311	2. 099	31	6. 961
222	2. 010	7	6. 962
331	1. 596	10	6. 955
420	1. 557	8	6. 962
Average value of last five lines			6. 959

References

[1] H. E. Boeke, Chem. Zentr. I, 1909 (1913).

[2] J. J. Lander, Polymorphism and anion rotational disorder in the alkaline earth carbonates, J. Chem. Phys. **17,** 892–901 (1949).

Beryllium Chromium Oxide, $BeCr_2O_4$ (orthorhombic)

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
	A	
101	4. 135	59
111	3. 337	100
301	2. 654	50
220	2. 452	48
311	2. 402	41
121	2. 335	50
002	2. 277	11
401	2. 157	42
212	1. 940	11
321	1. 936	
421, 511	1. 715	22
222	1. 668	94
412	1. 600	6
610	1. 568	4
331	1. 539	10
521	1. 519	16
103	1. 501	6
203	1. 450	7
040	1. 4159	28
620	1. 4140	

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
	A	
303	1. 3765	5
141	1. 3390	16
701	1. 3370	
123	1. 3258	7
531, 711	1. 3020	5
403	1. 2907	7
432	1. 2497	7
440	1. 2256	4
622	1. 2014	5
004	1. 1389	8
541, 333, 603	1. 1125	4
523	1. 1050	5
151	1. 0922	4
442	1. 0793	13
802	1. 0784	
812	1. 0595	5
351	1. 0422	3
224, 404	1. 0326	7
703	1. 0289	
921	0. 9910	8
343	. 9867	6
741	. 9720	7

ASTM cards. None.

Additional published patterns. None.

NBS sample. Two comparable samples of beryllium chromium oxide were prepared by C. E. Weir at NBS in solid state reaction; one at 1,950° C in a BeO crucible, the other being fuzed in a carbon arc. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, barium, magnesium, and silicon; 0.001 to 0.01 percent each of calcium, iron, manganese, nickel, antimony, titanium, and vanadium.

The color of the sample was green. The indices of refraction were 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 the NBS pattern are as follows:

Pattern	1	2	3
National Bureau of Standards	111	222	101

Structural data. Weir and Van Valkenburg [1] in 1960 determined that beryllium chromium oxide is isomorphous with chrysoberyl in which case it would have the space group Pnma (No. 62) and $4(BeCr_2O_4)$ per unit cell.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1960	National Bureau of Standards.	9. 792	5. 663	4.555 at 25° C

The density of beryllium chromium oxide calculated from the NBS lattice constants is 4.654 g/cm³ at 25° C.

References

[1] C. E. Weir and A. Van Valkenburg, Studies of beryllium chromite and other beryllia compounds with R_2O_3 oxides, J. Research NBS **64A** No. 1, 103–106 (1960).

Beryllium Germanate, Be_2GeO_4 (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
3–0496	3. 21 2. 24 1. 68	Iron	Schütz [1] 1936.

Additional published patterns. None.

NBS sample. The sample of beryllium germanate was prepared at the NBS by Charles E. Weir from beryllium oxide and germanium dioxide heated to 1,100° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent gallium and 0.001 to 0.01 percent each of aluminum, iron and magnesium.

The sample was colorless. The indices of refraction are N_o=1.720 and N_e=1.734 and it is optically positive.

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

Pattern	1	2	3
Schütz	220	303	404, 342
National Bureau of Standards	211	220	113

Structural data. Goldschmidt [2] in 1931 determined that beryllium germanate has the phenacite-type structure, the space group R3 (No. 148) and $18(Be_2GeO_4)$ per unit hexagonal cell or $6(Be_2GeO_4)$ per unit rhombohedral cell.

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

Lattice constants

		a	*c*
		A	*A*
1931	Goldschmidt [2]	12. 68	8.39
1936	Schütz [1]	12. 79	8.43
1960	National Bureau of Standards.	12. 756	8.425 at 25° C

The density of beryllium germanate calculated from the NBS lattice constants is 3.892 g/cm³ at 25° C.

References

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

[2] V. M. Goldschmidt, Zur Kristallchemie des Germaniums, Nachr. Ges. Wiss. Göttingen, Math-Phys. Klasse **1931,** 184–190 (1931).

Beryllium Germanate, Be_2GeO_4 (trigonal)

hkl (hex.)	1936 Schütz Fe, 1.9356 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		A	
110	-----	-----	6. 37	20
021	-----	-----	4. 619	6
012	3. 95	20	3. 939	39
211	3. 69	60	3. 740	100
300			3. 678	22
202	3. 35	20	3. 352	5
220	3. 20	100	3. 187	52
122	-----	-----	2. 967	27
131	-----	-----	2. 878	22
113	2. 57	80	2. 574	49
312	-----	-----	2. 479	3
410	2. 41	40	2. 410	43
042	-----	-----	2. 310	11
303	2. 24	100	2. 235	10
232	-----	-----	2. 177	5
330	2. 13	60	2. 125	10
223	-----	-----	2. 109	12
104	-----	-----	2. 073	9
241	-----	-----	2. 026	14
024	1. 97	40	1. 969	10
502			1. 957	20
214	-----	-----	1. 883	10
422	-----	-----	1. 870	5
600	1. 85	60	1. 840	4
413	-----	-----	1. 829	4
152	-----	-----	1. 794	10
431	1. 77	20	1. 774	14
520	-----	-----	1. 768	11
314	-----	-----	1. 737	<1
333	-----	-----	1. 695	20
404	1. 67	100	1. 6760	6
342			1. 6676	6
161	-----	-----	1. 6510	5
324	-----	-----	1. 6207	2
205	-----	-----	1. 6113	1
440	1. 598	20	1. 5988	1
612	-----	-----	1. 5650	10
701	1. 554	40	1. 5504	5
603	-----	-----	1. 5402	8
054	-----	-----	1. 5262	8
621	-----	-----	1. 5067	8
523	-----	-----	1. 4968	2
244	-----	-----	1. 4830	4
532	1. 478	100	1. 4782	5
710	1. 468	80	1. 4623	7
514	-----	-----	1. 4449	5
262	-----	-----	1. 4407	3
235, 006	1. 402	100	1. 4067	8
630	-----	-----	1. 3911	4
443	-----	-----	1. 3871	3

hkl (hex.)	1936 Schütz Fe, 1.9356 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		A	
434	1. 371	60	1. 3760	2
081	-----	-----	1. 3620	1
452	-----	-----	1. 3409	4
271	-----	-----	1. 3320	3
164	-----	-----	1. 3158	1
802	1. 313	20	1. 3128	3
713	-----	-----	1. 2977	22
722	-----	-----	1. 2866	3
550	-----	-----	1. 2752	1
704	-----	-----	1. 2634	<1
633	1. 251	20	1. 2471	10
624	-----	-----	1. 2392	1
182	-----	-----	1. 2362	2
900	-----	-----	1. 2272	3
642	1. 209	20	1. 2148	8
372	-----	-----	1. 1920	3
027, 544	1. 174	10	1. 1748	3
553	-----	-----	1. 1614	2
217	-----	-----	1. 1586	4
535	1. 150	10	1. 1528	2
191	-----	-----	1. 1470	<1
740	-----	-----	1. 1451	<1
265	-----	-----	1. 1342	4
903, 137	-----	-----	1. 1223	1
912, 606	1. 119	20	1. 1167	3
381	-----	-----	1. 1118	2
823	1. 105	40	1. 1079	3
814	-----	-----	1. 1013	2
327	-----	-----	1. 0864	2
921	-----	-----	1. 0794	2
734	-----	-----	1. 0707	1
0·10·2	-----	-----	1. 0687	1
743	-----	-----	1. 0607	2
292	1. 052	60	1. 0541	2
571	-----	-----	1. 0498	1
10·1·0	-----	-----	1. 0484	1
841	-----	-----	1. 0359	1
752	-----	-----	1. 0264	<1
185, 930	-----	-----	1. 0232	1
654	-----	-----	1. 0143	7
437	-----	-----	1. 0046	1
0·11·1	-----	-----	0. 9968	<1
663	-----	-----	. 9943	<1
384	-----	-----	. 9894	2
2·10·1	-----	-----	. 9868	<1
167, 10·0·4	-----	-----	. 9787	<1
761	-----	-----	. 9734	1
850, 238	-----	-----	. 9725	<1

Calcium Aluminum Germanate, $Ca_3Al_2(GeO_4)_3$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of calcium aluminum germanate was prepared at NBS by hydrothermal synthesis at 850° C and 17,000 psi from calcium carbonate, aluminum oxide and germanium oxide. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of sodium and strontium; and 0.001 to 0.01 percent each of iron, magnesium, manganese, and silicon.

The sample was colorless. The index of refraction was 1.787.

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	420	400	640

Structural data. The structure of calcium aluminum germanate has not been published. It is the germanium analogue of the garnet, grossularite, and therefore has the garnet structure, the space group Ia3d (No. 230), and $8[Ca_3Al_2(GeO_4)_3]$ per unit cell.

Lattice constants

		a
		A
1960	National Bureau of Standards	12.117 at 25° C

The density of calcium aluminum germanate calculated from the NBS lattice constant is 4.359 g/m³ at 25° C.

hkl	1960 Nat'l. Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*
	A		A
211	4. 95	17	12. 121
220	4. 283	8	12. 115
321	3. 239	16	12. 120
400	3. 030	38	12. 120
420	2. 709	100	12. 114
332	2. 584	23	12. 121
422	2. 474	29	12. 120
510	2. 373	11	12. 121
440	2. 143	8	12. 122
611	1. 9660	3	12. 119
631	1. 7872	6	12. 121
444	1. 7496	25	12. 121
640	1. 6808	36	12. 120
721	1. 6491	4	12. 118
642	1. 6192	34	12. 117
732	1. 5388	5	12. 116
800	1. 5147	15	12. 117
811	1. 4916	1	12. 117
653	1. 4485	3	12. 119
822	1. 4287	1	12. 122
752	1. 3721	3	12. 118
840	1. 3547	10	12. 117
842	1. 3221	23	12. 117
921	1. 3069	3	12. 120
664	1. 2912	8	12. 113
930	1. 2775	1	12. 119
941	1. 2242	2	12. 119
10·2·0	1. 1881	5	12. 116
10·3·1	1. 1551	2	12. 115
10·4·0	1. 1249	18	12. 116
10·4·2	1. 1060	9	12. 116
880	1. 0709	6	12. 116
11·3·2	1. 0467	1	12. 116
10·6·0	1. 0389	<1	12. 116
12·0·0	1. 0097	6	12. 116
12·2·0	0. 9960	10	12. 117
11·5·2	. 9894	2	12. 118
12·2·2	. 9828	16	12. 117
11·6·1	. 9639	1	12. 116
10·8·2	. 9348	<1	12. 116
13·2·1	. 9186	2	12. 117
12·4·4	. 9134	16	12. 118
12·6·0	. 9031	24	12. 116
12·6·2	. 8932	6	12. 116
13·4·1	. 8883	1	12. 115
13·4·2	. 8744	8	12. 116
14·1·1	. 8611	3	12. 117
14·2·0	. 8570	1	12. 120
14·3·1	. 8442	1	12. 117
12·8·0	. 8401	5	12. 116
14·4·0	. 8321	22	12. 116
14·3·3	. 8282	<1	12. 116
14·4·2	. 8244	22	12. 116
14·5·1	. 8132	<1	12. 116
12·8·4	. 8096	2	12. 117
14·5·3	. 7989	2	12. 116
14·6·0	. 7955	<1	12. 117
15·3·2	. 7854	2	12. 117
Average value of last five lines			12. 117

Calcium Chromium Germanate, $Ca_3Cr_2(GeO_4)_3$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of calcium chromium germanate was prepared at the NBS by reaction between calcium carbonate, chromium oxide, and germanium oxide in a sealed platinum tube at 1,400° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, barium, beryllium, manganese, sodium, and strontium; 0.001 to 0.01 percent each of iron, magnesium, silicon, and vanadium.

The color of the sample yellow-green. The index of refraction was 1.925.

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	420	642	422

Structural data. Tauber, et al., [1] in 1958 determined that calcium chromium germanate has the garnet structure, the space group Ia3d (No. 230), and 8[$Ca_3Cr_2(GeO_4)_3$] per unit cell.

Lattice constants

		a
		A
1958	Tauber, et al. [1]	12.275
1960	National Bureau of Standards.	12.262 at 25° C

The density of calcium chromium germanate calculated from the NBS lattice constant is 4.567 g/cm³ at 25° C.

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*
	A		*A*
211	5.01	12	12.27
321	3.278	11	12.265
400	3.066	44	12.264
420	2.743	100	12.266
332	2.614	17	12.259
422	2.504	45	12.267
510	2.406	8	12.269
440	2.168	2	12.264
611	1.9893	1	12.263
631	1.8081	4	12.263
444	1.7701	14	12.264
640	1.7001	32	12.260
721	1.6679	<1	12.257
642	1.6383	46	12.260
732	1.5568	3	12.258
800	1.5326	13	12.261
653	1.4656	<1	12.262
752	1.3892	<1	12.269
840	1.3707	11	12.260
842	1.3379	17	12.262
921	1.3218	3	12.258
664	1.3072	8	12.263
941	1.2388	1	12.263
10·1·1	1.2137	<1	12.258
10·2·0	1.2026	<1	12.264
10·4·0	1.1384	16	12.261
10·4·2	1.1193	10	12.261
880	1.0836	8	12.260
11·3·2	1.0592	1	12.261
12·0·0	1.0219	3	12.263
12·2·0	1.0080	3	12.263
12·2·2	0.9945	8	12.261
12·4·4	.9243	3	12.262
12·6·0	.9138	8	12.260
12·6·2	.9039	4	12.261
888	.8848	3	12.260
14·1·1	.8714	1	12.262
14·3·1	.8543	<1	12.262
12·8·0	.8502	1	12.262
14·4·0	.8422	6	12.263
14·4·2	.8343	9	12.262
14·5·1	.8231	<1	12.264
12·10·0	.7849	7	12.261
Average value of last five lines		-----	12.262

References

[1] A. Tauber, E. Banks, and H. Kedesdy, Acta Cryst. **11,** 893 (1958).

Calcium Chromium Silicate (uvarovite), $Ca_3Cr_2(SiO_4)_3$ (cubic)

hkl	---- Gillery [a] Cu, 1.542 A			1950 Hummel [b] Cu, 1.540 A			1959 Geller and Miller [b] Cr, 2.2909 A			1960 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	-----	--	-----	4. 20	25	11. 88	-----	----	-----	4. 239	14	11. 989
-------	-----	--	-----	4. 14	27	-----	-----	----	-----	------	--	------
321	-----	--	-----	3. 20	12	11. 97	3. 21	w	12. 01	3. 205	6	11. 993
400	2. 97	61	11. 88	2. 96	63	11. 84	3. 00	m-s	12. 00	2. 999	70	11. 994
411	2. 80	3	11. 88	----	--	-----	-----	----	-----	------	--	------
420	2. 65	100	11. 85	2. 65	100	11. 85	2. 68	s	11. 99	2. 684	100	12. 001
332	2. 52	15	11. 82	----	--	-- --	2. 56	vw	12. 01	2. 557	18	11. 994
422	2. 42	33	11. 86	2. 43	59	11. 90	2. 45	m	12. 00	2. 449	53	11. 999
431	2. 33	20	11. 88	2. 33	11	11. 88	2. 35	w	11. 98	2. 352	24	11. 994
521	2. 16	15	11. 83	2. 17	8	11. 89	2. 19	w	12. 00	2. 191	15	11. 999
---	2. 04	2	-----	----	--	-----	-----	----	-----	------	--	------
600	1. 97	2	11. 82	1. 96	3	11. 76	-----	----	-----	------	--	------
611	1. 93	38	11. 90	1. 93	21	11. 90	1. 95	w-m	12. 02	1. 946	21	11. 994
620	1. 87	5	11. 83	----	--	-----	1. 90	vw	12. 02	1. 896	12	11. 991
541	1. 83	2	11. 86	----	--	-----	-----	----	-----	1. 854	8	12. 014
444	1. 713	18	11. 87	----	--	-----	1. 731	vw	11. 99	1. 732	8	12. 002
640	1. 645	51	11. 86	1. 66	24	11. 97	1. 663	m	11. 99	1. 664	24	11. 996
642	1. 588	66	11. 88	1. 60	69	11. 97	1. 602	m-s	11. 99	1. 603	59	11. 997
732	1. 503	2	11. 83	----	--	-----	-----	----	-----	------	--	------
800	1. 486	13	11. 89	----	--	-----	1. 499	w	11. 99	1. 500	11	11. 999
741	-----	--	-----	----	--	-----	-----	----	-----	1. 477	6	11. 995
653	1. 415	4	11. 84	----	--	-----	-----	----	-----	1. 432	8	11. 982
822	-----	--	-----	----	--	-----	-----	----	-----	1. 414	5	11. 997
840	1. 327	20	11. 87	1. 34	4	11. 99	1. 341	w-m	11. 99	1. 341	16	11. 998
842	1. 296	37	11. 88	1. 31	7	12. 01	1. 309	m	12 00	1. 309	15	11. 997
921	-----	--	-----	----	--	-----	1. 294	w	12. 00	------	--	------
664	1. 266	17	11. 88	----	--	-----	1. 279	w-m	12. 00	1. 279	13	11. 996
844	1. 208	2	11. 84	----	--	-----	-----	----	-----	1. 211	7	11. 992
941	1. 197	6	11. 85	----	--	-----	-----	----	-----	------	--	------
10·2·0	1. 166	3	11. 89	----	--	-----	-----	----	-----	------	--	------
10·4·0	1. 102	18	11. 87	----	--	-----	-----	----	-----	1. 1142	16	12. 000
10·4·2	1. 085	16	11. 89	----	--	-----	-----	----	-----	1. 0955	13	12. 001
880	1. 049	13	11. 87	----	--	-----	-----	----	-----	1. 0607	7	12. 000
12·0·0	0. 989	6	11. 87	----	--	-----	-----	----	-----	1. 0001	14	12. 001
12·2·0	. 976	7	11. 87	----	--	-----	-----	----	-----	0. 9862	4	11. 998
12·2·2	. 963	18	11. 87	----	--	-----	-----	----	-----	. 9734	12	12. 000
11·6·3	-----	--	-----	----	--	-----	-----	----	-----	. 9319	2	12. 007
12·4·4	. 895	6	11. 87	----	--	-----	-----	----	-----	------	--	------
12·6·0	. 885	15	11. 87	----	--	-----	-----	----	-----	. 8943	8	11. 998
12·6·2	. 873	8	11. 84	----	--	-----	-----	----	-----	. 8846	3	12. 000
888	. 857	7	11. 87	----	--	-----	-----	----	-----	. 8661	9	12. 001
12·8·0	. 823	6	11. 87	----	--	-----	-----	----	-----	. 8320	6	11. 999
14·4·0	. 815	21	11. 87	----	--	-----	-----	----	-----	. 8240	4	11. 998
14·4·2	. 808	28	11. 88	----	--	-----	-----	----	-----	. 8164	15	11. 999
Average value of last five lines---		--	11. 87	----	--	11. 98	-----	----	12. 00	------	--	11. 999

[a] Natural mineral, high aluminum content, intermediate garnet, closer to grossularite.
[b] Synthetic.

ASTM cards

Card number	Index lines	Radiation	Source
7–70	2. 65 1. 59 2. 97	Copper	Gillery [1].

Additional published patterns

Source	Radiation
Hummel [2] 1950	Copper
Geller and Miller [3] 1959	Chromium

NBS sample. The sample of uvarovite was prepared at NBS by solid state synthesis at 1,400° C from chromium oxide, calcium carbonate, and silicic acid. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of beryllium; 0.01 to 0.1 percent each of aluminum, sodium, and vanadium; and 0.001 to 0.01 percent each of antimony, barium, cobalt, lead, manganese, nickel, silver, strontium, and titanium.

The color of the sample was yellow-green. The index of refraction could not be determined by the usual liquid grain immersion method.

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

Pattern	1	2	3
Gillery (a)	420	642	400
Hummel (b)	420	642	400
Geller and Miller (b)	420	400	642
National Bureau of Standards (b)	420	400	642

Structural data. Menzer [4] in 1928 determined that uvarovite has the garnet structure, the space group Ia3d (No. 230), and $8[Ca_3Cr_2(SiO_4)_3]$ per unit cell. The unit cell measurement of Menzer has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1928	Menzer [4][c]	11.97
----	Gillery [1][a]	11.87
1959	Geller and Miller [3][b]	12.00
1960	National Bureau of Standards [b]	11.999 at 26° C

[a] Natural mineral, high aluminum content, intermediate garnet, closer to grossularite.
[b] Synthetic.
[c] Natural mineral; largest impurity is 1.93% Al_2O_3.

The density of uvarovite calculated from the NBS lattice constant is 3.848 g/cm³ at 26° C.

References

[1] Gillery, at College of Mineral Industries, Pennsylvania State University.
[2] F. A. Hummel, Synthesis of uvarovite, Am. Min. **35,** 324 (1950).
[3] S. Geller and C. E. Miller, The synthesis of uvarovite, Am. Min. **44,** Nos. 3 and 4, 445 (1959).
[4] G. Menzer, Die Kristallstruktur der Granate, Z. Krist. **69,** 300 (1928).

Calcium Gallium Germanate, $Ca_3Ga_2(GeO_4)_3$ (cubic)

ASTM cards. None.
Additional published patterns. None.
NBS sample. The sample of calcium gallium germanate was prepared at NBS by hydrothermal reaction of calcium carbonate, gallium oxide and germanium oxide at 850° C and 15,000 psi. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, copper, chromium, magnesium, nickel, silver, sodium, and strontium.

The sample was colorless. The index of refraction was 1.814.

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	420	400	422

Structural data. No published structure of calcium gallium germanate was found. It is a garnet with the space group Ia3d (No. 230), and $8[Ca_3Ga_2(GeO_4)_3]$ per unit cell.

Lattice constant

		a
1960	National Bureau of Standards.	12.251 at 26° C

The density of calcium gallium germanate calculated from the NBS lattice constant is 4.835 g/cm³ at 26° C.

Calcium Gallium Germanate, $Ca_3Ga_2(GeO_4)_3$ (cubic)

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 26° C		
	d	I	a
	A		A
211	4. 995	13	12. 24
220	4. 331	7	12. 25
321	3. 273	13	12. 25
400	3. 062	66	12. 25
420	2. 738	100	12. 24
332	2. 611	19	12. 24
422	2. 500	66	12. 25
431	2. 402	8	12. 25
611	1. 986	2	12. 24
620	1. 937	5	12. 25
541	1. 889	1	12. 24
631	1. 8067	4	12. 253
444	1. 7685	11	12. 253
640	1. 6989	32	12. 251
721	1. 6670	3	12. 250
642	1. 6374	55	12. 253
732	1. 5556	4	12. 249
800	1. 5314	18	12. 251
653	1. 4644	2	12. 252
752	1. 3881	2	12. 259
840	1. 3698	12	12. 252
842	1. 3367	14	12. 251
921	1. 3209	3	12. 250
664	1. 3060	9	12. 251
941	1. 2376	2	12. 252
10·3·1	1. 1680	1	12. 250
10·4·0	1. 1375	13	12. 251
10·4·2	1. 1182	13	12. 249
880	1. 0829	8	12. 252
11·3·2	1. 0585	1	12. 253
12·0·0	1. 0211	5	12. 253
12·2·0	1. 0071	5	12. 252
12·2·2	0. 9936	10	12. 251
13·2·1	. 9285	1	12. 247
12·4·4	. 9234	2	12. 250
12·6·0	. 9131	7	12. 250
12·6·2	. 9032	4	12. 252
10·9·3	. 8886	1	12. 249
14·1·1	. 8707	<1	12. 252
14·2·0	. 8662	<1	12. 251
14·3·1	. 8534	1	12. 249
12·8·0	. 8494	5	12. 251
14·4·0	. 8414	7	12. 251
14·4·2	. 8336	16	12. 251
14·5·1	. 8221	<1	12. 249
13·8·1	. 8010	<1	12. 252
15·3·2	. 7942	2	12. 251
12·10·0	. 7843	7	12. 251
Average value of last five lines		-----	12. 251

Calcium Iron Germanate, $Ca_3Fe_2(GeO_4)_3$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of calcium iron germanate was prepared at NBS by hydrothermal synthesis at 850° C and 15,000 psi from calcium carbonate, iron oxide, and germanium oxide. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of magnesium, manganese, and silicon; and 0.001 to 0.01 percent each of aluminum, sodium, strontium, and titanium.

The color of the sample was yellowish gray color. The index of refraction was 1.932.

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	420	422	642

Structural data. Tauber, et al., mention [1] that calcium iron germanate has the garnet type structure, the space group Ia3d (No. 230) and $8[Ca_3Fe_2(GeO_4)]$ per unit cell.

Lattice constants

		a
		A
1958	Tauber, et al. [1]	12.312
1960	National Bureau of Standards	12.325 at 25°C

The density of calcium iron germanate calculated from the NBS lattice constant is 4.552 g/cm³ at 25°C.

References

[1] A. Tauber, et al., Synthesis of germanate garnets, Acta Cryst. **11,** 893 (1958).

Calcium Iron Germanate, $Ca_3Fe_2(GeO_4)_3$ (cubic)

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*
	A		*A*
211	5.032	15	12.326
321	3.292	13	12.319
400	3.081	43	12.322
420	2.755	100	12.321
332	2.628	18	12.325
422	2.516	50	12.324
431	2.417	8	12.323
611	2.001	<1	12.333
631	1.8171	1	12.324
444	1.7791	14	12.326
640	1.7092	34	12.325
721	1.6771	5	12.324
642	1.6469	46	12.324
732	1.5654	5	12.326
800	1.5403	12	12.322
653	1.4737	1	12.329
840	1.3780	13	12.325
842	1.3452	17	12.328
921	1.3297	3	12.331
664	1.3142	9	12.328
941	1.2457	3	12.331

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*
	A		*A*
10·4·0	1.1445	19	12.327
10·4·2	1.1253	11	12.327
880	1.0896	10	12.327
12·0·0	1.0274	4	12.329
12·2·0	1.0132	4	12.326
12·2·2	0.9999	14	12.328
12·4·4	.9291	4	12.326
12·6·0	.9187	10	12.326
12·6·2	.9092	4	12.333
888	.8895	4	12.325
12·8·0	.8550	2	12.331
14·4·0	.8465	12	12.325
14·4·2	.8386	10	12.325
14·5·1	.8273	2	12.326
12·10·0	.7891	10	12.326
12·10·2	.7826	10	12.324
Average value of last five lines			12.325

Cerium Magnesium Nitrate 24-Hydrate, $Ce_2Mg_3(NO_3)_{12}\cdot 24H_2O$ (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cerium magnesium nitrate hydrate was prepared at NBS by Robert Kaeser from stoichiometric mixtures of cerous nitrate and magensium nitrate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, lanthanum, and silicon; 0.001 to 0.01 percent nickel; and 0.0001 to 0.001 percent each of calcium, chromium, and manganese.

The sample is colorless. The indices of refraction are N_e=1.517 and N_o=1.524 and it is optically negative.

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	012	116	104

Structural data. Culvahouse and Sapp [1] determined that cerium magnesium nitrate hydrate has the cerium zinc nitrate hydrate-type structure, the space group $R\bar{3}m$ (No. 166), and $1[Ce_2Mg_3(NO_3)_{12}\cdot 24H_2O]$ per unit rhombohedral cell or $3[Ce_2Mg_3(NO_3)_{12}\cdot 24H_2O]$ per unit hexagonal cell.

The unit-cell measurements reported by Powell, quoted by Cooke, Duffus, and Wolf [2] were converted from rhombohedral units. The "c" has been doubled for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1953	Powell [2]	10.88	34.44
1960	National Bureau of Standards.	11.030	34.65 at 25° C

The density of cerium magnesium nitrate hydrate calculated from the NBS lattice constants is 2.087 g/cm³ at 25° C.

References

[1] J. W. Culvahouse and R. C. Sapp, Structure of cerium zinc nitrate, Department of Physics and Astronomy, University of Kansas (1959) (progress report to sponsors).

[2] A. H. Cooke, H. J. Duffus and W. P. Wolf, Cerium magnesium nitrate I: The magnetic properties and specific heat about 1° K, Phil. Mag. 44, 623–629 (1953).

Cerium Magnesium Nitrate 24-Hydrate, $Ce_2Mg_3(NO_3)_{12} \cdot 24H_2O$ (trigonal)

hkl (hex.)	1960 Nat'l. Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
	A	
003	11. 56	5
101	9. 21	14
012	8. 37	100
104	6. 42	75
006	5. 78	15
015	5. 60	15
110	5. 52	50
113	4. 98	4
202	4. 604	5
107	4. 399	6
024	4. 183	50
116	3. 988	78
018	3. 948	15
009	3. 850	4
211	3. 590	1
122	3. 534	13
027	3. 438	4
214	3. 335	43
1·0·10	3. 257	1
208	3. 209	11
300	3. 182	11
303	3. 071	5
217	2. 916	4
0·0·12	2. 886	4
0·2·10	2. 806	24
306	2. 786	15
128	2. 773	61
131	2. 646	4
312	2. 620	46
1·1·12	2. 558	27
134	2. 531	10
2·1·10	2. 499	26
226	2. 489	41
309	2. 454	<1
0·1·14	2. 397	23
404	2. 302	7
045	2. 260	14
2·0·14	2. 198	4
232	2. 174	10
3·0·12	2. 139	36
324	2. 125	32
1·0·16	2. 112	14
1·3·10	2. 105	18
410	2. 086	13
1·2·14	2. 042	9
2·2·12, 0·1·17	1. 994	19
0·2·16	1. 972	14
4·0·10	1. 967	15
416	1. 960	30
238	1. 956	23
0·0·18	1. 924	4
2·1·16	1. 857	11
3·2·10	1. 852	9
330	1. 837	6
419	1. 835	5
1·1·18, 333	1. 817	8
422	1. 795	6
244	1. 767	3
336	1. 751	7
425	1. 748	6
0·1·20, 0·2·19	1. 705	1
4·1·12	1. 689	8
1·3·16	1. 677	8
155	1. 666	4
3·0·18	1. 647	7
2·0·20	1. 629	2
4·0·16	1. 603	1
2·4·10	1. 600	2
600	1. 591	2
1·2·20	1. 563	3
0·4·17	1. 550	5

Cobalt Arsenide (skutterudite), $CoAs_3$ (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
*2–1022	2. 56 1. 60 1. 83	Copper----	British Museum.
*2–0977	2. 61 1. 85 1. 62	Copper----	Oftedal [1] 1928.
2–1001	2. 60 1. 61 1. 84	Copper----	Oftedal [1] 1928.
2–0987	2. 60 2. 20 1. 84	Molybdenum.	General Electric Co., Wembley, England.

*Incorrectly named smaltite on card. See Holmes [2].

Additional published patterns

Source	Radiation
Harcourt [3] 1942----------	Copper.

NBS sample. The sample of skutterudite was prepared by E. H. Roseboom [4] of the Geophysical Laboratory in an evacuated sealed silica-glass tube at 800° C with solid arsenic in equilibrium with the vapor. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of aluminum and nickel; 0.01 to 0.1 percent

hkl	British Museum [a] Cu, 1.542 A			1928 Oftedal [a] Cu, 1.542 A			1928 Oftedal Cu, 1.542 A		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
110	5. 78	20	8. 17	------	----	------	------	----	------
200	4. 06	20	8. 12	4. 10	vvw	8. 20	4. 08	vvw	8. 16
211	3. 16	40	7. 74	3. 36	vw	8. 23	3. 33	vw	8. 16
220	2. 89	40	8. 17	2. 89	w	8. 17	2. 87	w	8. 12
310	2. 56	100	8. 10	2. 61	vs	8. 25	2. 60	vs	8. 22
------	2. 42	20	------	------	----	------	------	----	------
222	2. 36	20	8. 18	------	----	------	------	----	------
------	2. 26	20	------	------	----	------	------	----	------
321	2. 18	60	8. 16	2. 21	m	8. 27	2. 19	m	8. 19
400	2. 03	40	8. 12	------	----	------	------	----	------
411	1. 93	40	8. 19	1. 95	w	8. 27	1. 93	w	8. 19
------	------	------	------	------	----	------	------	----	------
420	1. 83	70	8. 18	1. 85	vs	8. 27	1. 84	s	8. 23
------	1. 78	40	------	------	----	------	------	----	------
332	1. 74	40	8. 16	1. 76	w	8. 26	1. 75	w	8. 21
422	1. 67	60	8. 18	1. 69	m	8. 28	1. 68	s	8. 23
510	1. 60	80	8. 16	1. 62	vs	8. 26	1. 61	vs	8. 21
530	1. 40	60	8. 16	1. 42	s	8. 28	1. 41	s	8. 22
600	1. 37	40	8. 22	1. 38	w	8. 28	1. 37	m	8. 22
611	1. 33	20	8. 20	1. 35	vw	8. 32	1. 34	w	8. 26
620	1. 29	40	8. 16	1. 31	w	8. 29	1. 30	w	8. 22
541	------	------	------	1. 27	vvw	8. 23	1. 26	vw	8. 17
622	1. 24	40	8. 23	1. 25	m	8. 29	1. 24	w	8. 23
631	1. 21	70	8. 21	1. 22	s	8. 27	1. 21	m	8. 21
444	1. 19	60	8. 24	1. 20	m	8. 31	1. 18	w	8. 18
710	1. 16	60	8. 20	1. 17	w	8. 27	1. 16	w	8. 20
640	1. 14	60	8. 22	1. 15	w	8. 29	1. 14	w	8. 22
721	1. 12	60	8. 23	1. 13	w	8. 30	1. 12	w	8. 23
642	------	------	------	1. 11	vvw	8. 31	1. 10	vvw	8. 23
730	1. 08	70B	8. 23	1. 09	s	8. 30	1. 08	m	8. 23
732	1. 04	60	8. 19	1. 05	m	8. 27	1. 04	m	8. 19
800	1. 03	20	8. 24	1. 04	w	8. 32	1. 03	vw	8. 24
811	1. 00	20	8. 12	1. 02	w	8. 29	1. 01	vw	8. 21
820	------	------	------	1. 00	m	8. 25	0. 994	w	8. 20
653	------	------	------	0. 988	w	8. 27	. 980	w	8. 20
822	------	------	------	. 975	m	8. 27	. 967	m	8. 21
831	------	------	------	. 962	s	8. 28	. 955	vs	8. 22
662	------	------	------	------	----	------	------	----	------
752	------	------	------	------	----	------	------	----	------
840	------	------	------	------	----	------	------	----	------
910	------	------	------	. 914	m	8. 27	. 905	m	8. 20
842	------	------	------	------	----	------	. 894	w	8. 19
921	------	------	------	. 891	w	8. 26	. 883	w	8. 19
932	------	------	------	------	----	------	------	----	------
941	------	------	------	------	----	------	------	----	------
950	------	------	------	------	----	------	------	----	------
10·3·1	------	------	------	------	----	------	------	----	------
Average value of last five lines			8. 20	------	----	8. 27	------	----	8. 20

[a] Probably $(Co,Ni)As_3$.
[b] Labeled chloanthite-smaltite.

$CoAs_3$ (cubic)

---- G. E., Wembley, England Mo, 0.711 A			1942 Harcourt [a, b] Cu, 1.5418 A			1942 Harcourt [a] Cu, 1.5418 A			1960 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
5. 84	40	8. 26	6. 0	11	8. 49	------	----	----	5. 80	14	8. 21
4. 14	20	8. 28	4. 2	22	8. 40	------	----	----	4. 10	11	8. 19
3. 37	50	8. 25	3. 4	11	8. 33	3. 40	5	8. 33	3. 35	16	8. 20
------	----	----	2. 9	22	8. 20	2. 90	5	8. 20	2. 898	2	8. 20
2. 61	100	8. 25	2. 64	100	8. 35	2. 64	100	8. 35	2. 592	100	8. 20
------	----	----	------	----	----	2. 45	2	8. 49	------	----	------
------	----	----	------	----	----	------	----	----	2. 368	2	8. 204
------	----	----	------	----	----	------	----	----	------	----	------
2. 20	60	8. 23	2. 22	33	8. 31	2. 21	20	8. 27	2. 193	34	8. 204
------	----	----	2. 07	6	8. 28	2. 08	2	8. 32	------	----	------
1. 94	30	8. 23	1. 95	11	8. 27	1. 96	3	8. 32	1. 934	10	8. 205
1. 87	20	----	------	----	----	------	----	----	------	----	------
1. 84	60	8. 23	1. 87	44	8. 36	1. 86	30	8. 32	1. 835	34	8. 206
------	----	----	------	----	----	------	----	----	------	----	------
1. 75	30	8. 21	1. 77	11	8. 30	1. 76	5	8. 26	1. 749	10	8. 205
1. 68	50	8. 23	1. 69	22	8. 30	1. 70	10	8. 33	1. 675	19	8. 204
1. 61	50	8. 21	1. 63	33	8. 31	1. 62	30	8. 26	1. 609	32	8. 205
1. 41	40	8. 22	1. 43	22	8. 34	1. 42	10	8. 28	1. 4071	14	8. 205
1. 37	20	8. 22	1. 38	11	8. 28	1. 38	2	8. 28	1. 3675	6	8. 205
------	----	----	------	----	----	------	----	----	1. 3312	2	8. 206
1. 30	10	8. 22	1. 31	6	8. 29	1. 32	2	8. 35	1. 2974	5	8. 206
------	----	----	------	----	----	------	----	----	1. 2660	1	8. 205
1. 24	20	8. 22	1. 25	3	8. 29	------	----	----	1. 2370	6	8. 205
1. 21	40	8. 21	1. 23	22	8. 34	1. 22	10	8. 27	1. 2098	14	8. 205
------	----	----	1. 20	11	8. 31	1. 20	2	8. 31	1. 1843	5	8. 205
------	----	----	1. 17	11	8. 27	------	----	----	1. 1603	5	8. 205
------	----	----	1. 15	11	8. 29	1. 142	2	8. 24	1. 1378	4	8. 205
------	----	----	1. 13	11	8. 30	1. 125	2	8. 27	1. 1166	6	8. 205
------	----	----	------	----	----	------	----	----	------	----	------
------	----	----	1. 09	22	8. 30	1. 085	10	8. 26	1. 0773	11	8. 204
------	----	----	1. 05	11	8. 27	1. 050	3	8. 27	1. 0420	9	8. 205
------	----	----	------	----	----	------	----	----	1. 0256	3	8. 205
------	----	----	------	----	----	------	----	----	1. 0099	2	8. 204
------	----	----	1. 005	11	8. 29	1. 005	2	8. 29	0. 9949	9	8. 204
------	----	----	0. 990	6	8. 28	------	----	----	. 9806	7	8. 204
------	----	----	------	----	----	0. 975	3	8. 27	. 9668	14	8. 204
------	----	----	------	----	----	. 965	3	8. 30	. 9537	18	8. 204
------	----	----	------	----	----	------	----	----	. 9412	1	8. 205
------	----	----	------	----	----	------	----	----	. 9290	<1	8. 204
------	----	----	------	----	----	------	----	----	. 9173	<1	8. 205
------	----	----	------	----	----	. 916	3	8. 29	------	----	------
------	----	----	------	----	----	------	----	----	------	----	------
------	----	----	------	----	----	------	----	----	------	----	------
------	----	----	------	----	----	. 855	10	8. 29	------	----	------
------	----	----	------	----	----	. 840	5	8. 32	------	----	------
------	----	----	------	----	----	. 805	2	8. 29	------	----	------
------	----	----	------	----	----	. 790	10	8. 29	------	----	------
------	----	8. 22	------	----	8. 29	------	----	8. 30	------	----	8. 204

each of calcium, chromium, and iron; and 0.001 to 0.01 percent each of copper, manganese, magnesium, and antimony.

The sample was a gray opaque powder.

Interplanar spacings and intensity measurements. The *d*-values reported by the British Museum and General Electric Co. were converted from kX to angstrom units. The *d*-values reported by Oftedal 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	310	510	420
Oftedal	310	420	510
Oftedal	310	510	420
General Electric Co	310	321	420
Harcourt	310	420	510
*Harcourt	310	420	321
National Bureau of Standards	310	321	420

*Labeled chloamthite-smaltite.

Structural data. Oftedal [1] in 1928 determined that skutterudite has the space group Im3 (No. 204) and 8($CoAs_3$) 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	*Oftedal	8.257
1928	Oftedal	8.206.
1960	National Bureau of Standards	8.204 at 25° C.

*Probably (Co,Ni)As_3.

The density of skutterudite calculated from the NBS lattice constant is 6.821 g/cm³ at 25° C.

References

[1] I. Oftedal, Die Kristallstruktur von skutterudite und Speiskobalt-Chloanthit, Z. Krist. **66,** 517 (1928).

[2] R. J. Holmes, Higher mineral arsenides of cobalt, nickel, and iron, Bull. Geol. Soc. Am. **58,** 375 (1947).

[3] G. A. Harcourt, Tables for the identification of ore minerals by X-ray powder patterns, Am. Min. **27,** 98 (1942).

[4] E. H. Roseboom, Jr., The $CoAs_2$-$NiAs_2$-$FeAs_2$-As system, Annual Report of the Director of the Geophysical Laboratory, 201 (1956–57).

Cobalt(II) Carbonate (spherocobaltite), $CoCO_3$ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–1020	2. 77 1. 71 3. 65	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Ferrari and Colla [2] 1929	Iron
Baccaredda [3] 1932	Iron

NBS sample. The sample of cobaltous carbonate was prepared at NBS by hydrothermal synthesis in a Morey-type bomb [4] from cobalt chloride hexahydrate, sodium bicarbonate and carbonic acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of molybdenum and nickel; and 0.001 to 0.01 percent each of barium, copper, magnesium, silicon, and silver.

The color of the sample was pink-purple. It was optically negative and the index of refraction N_o was 1.854; N_e could not be determined. The sample showed extremely high double refraction.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel; Ferrari and Colla; and Baccaredda 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	104	116	012
Ferrari and Colla	104	018	012
Baccaredda	104	018	134
National Bureau of Standards	104	012	116

Structural data. Baccaredda [3] in 1932 determined that cobaltous carbonate has the calcite-type structure, the space group $R\bar{3}c$ (No. 167) and 6($CoCO_3$) per hexagonal unit cell.

Several unit-cell measurements have been converted from kX to angstrom units. The "a" (9.293) reported by Ferrari and Colla was divided by 2 and the "c" (7.521) was multiplied by 2. for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1929	Ferrari and Colla [2]	4. 647	15.042
1932	Baccaredda [3]	4. 675	15.135
1960	National Bureau of Standards.	4. 659	14.957 at 26° C

Cobalt(II) Carbonate (spherocobaltite), $CoCO_3$ (trigonal)

hkl (hex.)	1929 Ferrari and Colla Fe, 1.9373 A		1932 Baccaredda Fe, 1.9373 A		1938 Hanawalt, Rinn and Frevel Mo, 0.7107 A		1960 National Bureau of Standards Cu, 1.5405 A at 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
012	3. 448	m	3. 514	m	3. 66	40	3. 551	40
104	2. 715	vs	2. 723	vs	2. 78	100	2. 743	100
110	2. 310	m	2. 307	m	2. 34	11	2. 330	22
113	2. 099	m	----------	--------	2. 12	11	2. 112	22
202	1. 492	m	1. 937	m	1. 96	11	1. 948	22
024	1. 774	w	1. 767	w	----------	--------	1. 776	10
116	----------	--------	----------	--------	1. 71	71	1. 702	31
018	1. 698	s	1. 696	vs	----------	--------	1. 697	27
211	----------	--------	----------	--------	----------	--------	1. 5174	3
122	1. 492	m	1. 486	m	1. 50	11	1. 4946	12
214	1. 413	m	1. 407	m	1. 421	11	1. 4122	11
1·0·10	----------	--------	----------	--------	----------	--------	1. 4026	3
208	----------	--------	1. 369	m	----------	--------	1. 3714	4
125	----------	--------	----------	--------	----------	--------	1. 3582	2
119	----------	--------	----------	--------	1. 361	6	1. 3531	4
300	1. 346	m	1. 341	m	----------	--------	1. 3448	10
0·0·12	1. 245	w	1. 250	w	----------	--------	1. 2468	4
0·2·10	----------	--------	1. 199	w	----------	--------	1. 2015	3
128	----------	--------	1. 180	m	----------	--------	1. 1818	6
220	----------	--------	----------	--------	----------	--------	1. 1647	2
312	----------	--------	1. 100	m	----------	--------	1. 1067	2
1·1·12	----------	--------	----------	--------	----------	--------	1. 0989	3
134	1. 070	m	1. 069	s	----------	--------	1. 0719	7
2·1·10	----------	--------	----------	--------	----------	--------	1. 0678	4
226	1. 057	m	1. 053	m	----------	--------	1. 0552	4
0·1·14	----------	--------	----------	--------	----------	--------	1. 0327	1
404	----------	--------	----------	--------	----------	--------	0. 9737	4
318	----------	--------	----------	--------	----------	--------	. 9600	6
2·0·14	----------	--------	----------	--------	----------	--------	. 9441	1
2·1·13	----------	--------	----------	--------	----------	--------	. 9184	6
3·0·12	----------	--------	----------	--------	----------	--------	. 9140	8
1·0·16	----------	--------	----------	--------	----------	--------	. 9120	4

The density of cobaltous carbonate calculated from the NBS lattice constant is 4.214 g/cm^3 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 (1938).

[2] A. Ferrari and C. Colla, Sulla struttura cristallina dei carbonati neutri di cobalto e di nichelio, Rend. accad. naz. Lincei **10,**, 594 (1929).

[3] M. Baccaredda, Sulla struttura della sferocobaltite, Rend. accad. naz. Lincei **16,** 248–252 (1932).

[4] Morey and Ingerson, Alterations and synthesis of silicates, Econ. Geol. **32,**, 607 (1937).

Cobalt Diarsenide, $CoAs_2$ (monoclinic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cobalt diarsenide was prepared by E. H. Roseboom of the Geophysical Laboratory. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, antimony, nickel, and sodium; and 0.001 to 0.01 percent each of barium, calcium, chromium, copper, iron, magnesium, manganese, silver, titanium, zinc, and zirconium.

The sample was a gray opaque powder.

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	120	$\bar{1}11$	111

Structural data. No published structure or space group was found. Roseboom [1] states that cobalt diarsenide appears to be monoclinic. The present pattern was indexed assuming that cobalt diarsenide is monoclinic and has cell constants and density close to those of cobalt iron diarsenide, and $2(CoAs_2)$ per unit cell.

The density of cobalt diarsenide calculated from the NBS lattice constants is 7.479 g/cm³ at 25° C.

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*
	A	
110	3. 83	8
020	2. 94	11
011	2. 76	18
$\bar{1}01$	2. 67	47
101	2. 65	44
-------	2. 60	<3
120	2. 54	100
$\bar{1}11$	2. 43	60
111	2. 41	52
210	2. 319	26
-------	2. 083	4
-------	2. 045	6
$\bar{1}21, \bar{2}01$	1. 974	6
121	1. 966	4
220	1. 913	10
$\bar{2}11$	1. 870	28
211	1. 856	28
---------	1. 829	16
130	1. 825	23
-------	1. 702	<3
031	1. 658	35
$\bar{2}21$	1. 637	13
221	1. 627	18
310	1. 618	18
$\bar{1}31$	1. 576	9
131	1. 574	13
002	1. 564	16
230	1. 546	5
-------	1. 522	3
$\bar{3}01$	1. 487	<3
301	1. 477	3
040	1. 468	<3
320	1. 460	<3
140	1. 410	<3
$\bar{2}02, \bar{1}22$	1. 334	12
041, 122	1. 329	12
321	1. 318	7
$\bar{2}12$	1. 303	3
240	1. 269	13

References

[1] E. H. Roseboom, Jr., The $CoAs_2$-$NiAs_2$-$FeAs_2$-As System, Annual Report of the Director of the Geophysical Laboratory (1956–57).

Lattice constants

		a	*b*	*c*	*β*
		A	*A*	*A*	
1960	National Bureau of Standards	5. 047	5. 872	3. 127	90°51′ at 25° C.

Cobalt Gallate, $CoGa_2O_4$ (cubic)

ASTM cards. None.
Additional published patterns. None.
NBS sample. The sample of cobalt gallate was prepared at NBS by solid state reaction at 1,400° C between cobalt hydroxide and gallium oxide. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of nickel and antimony; 0.001 to 0.01 percent each of aluminum, calcium, chromium, copper, manganese, magnesium, and silicon.

The color of the sample was deep blue. The index of refraction was 1.943.

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	311	220	440

Structural data. No published structure of cobalt gallate was found. It is a spinel with the space group Fd3m (No. 227), and $8(CoGa_2O_4)$ per unit cell.

Lattice constants

		a
		A
1960	National Bureau of Standards	8.325 at 25° C

The density of cobalt gallate calculated from the NBS lattice constant is 6.039 g/cm³ at 25° C.

hkl	1960 National Bureau of Standards Co, 1.7889 A at 25° C		
	d	*I*	*a*
	A		*A*
111	4. 809	12	8. 329
220	2. 944	33	8. 326
311	2. 5096	100	8. 324
222	2. 4033	13	8. 325
400	2. 0818	20	8. 327
422	1. 6998	12	8. 327
511	1. 6026	29	8. 327
440	1. 4720	31	8. 327
620	1. 3163	4	8. 325
533	1. 2699	9	8. 327
622	1. 2549	5	8. 324
444	1. 2016	3	8. 325
642	1. 1126	4	8. 326
731	1. 0839	16	8. 326
800	1. 0407	6	8. 326
822	0. 9811	3	8. 325
751	. 9613	13	8. 325
662	. 9550	3	8. 325
840	. 9308	5	8. 325
Average value of last five lines			8. 325

Cobalt Germanate, Co_2GeO_4 (cubic)

ASTM cards. None.
Additional published patterns. None.
NBS sample. The sample of cobalt germanate was prepared at NBS by reaction at 1,200° C between cobalt hydroxide and germanium oxide. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of nickel; 0.01 to 0.1 percent each of calcium, magnesium, manganese, sodium, and tin; 0.001 to 0.01 percent each of aluminum, copper, and iron.

The color of the sample was reddish purple. The index of refraction was too high to be measured by the oil immersion method.

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	311	220	440

Structural data. The structure of cobalt germanate has not been published. It has the spinel-type structure, the space group Fd3m (No. 227), and $8(Co_2GeO_4)$ per unit cell.

Cobalt Germanate, Co_2GeO_4 (cubic)

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*
	A		*A*
220	2. 940	55	8. 316
311	2. 508	100	8. 319
222	2. 402	10	8. 319
400	2. 0792	23	8. 317
422	1. 6979	22	8. 318
511	1. 6010	43	8. 319
440	1. 4706	52	8. 319
620	1. 3154	9	8. 319
533	1. 2686	15	8. 319
622	1. 2543	4	8. 320
444	1. 2003	2	8. 316
642	1. 1116	10	8. 318
731	1. 0829	32	8. 318
800	1. 0398	9	8. 318
822	0. 9803	7	8. 318
751	. 9605	19	8. 318
662	. 9542	2	8. 319
840	. 9298	3	8. 316
Average value of last five lines			8. 318

Lattice constants

		a
		A
1960	National Bureau of Standards	8.318 at 25° C

The density of cobalt germanate calculated from the NBS lattice constant is 5.872 g/cm³ at 25° C.

Cobalt Iron Arsenide (safflorite), $CoFeAs_4$ (monoclinic)

ASTM cards

Card numbers	Index lines	Radiation	Source
2–0986	2. 60 2. 37 1. 64	Cobalt	Harcourt [1] 1942.
*2–1317	1. 85 1. 65 1. 63	Copper	British Museum.

*Pattern on card 2–1317 does not agree with the safflorite pattern in comparison table.

Additional published patterns

Source	Radiation
De Jong [2] 1926	Iron

NBS sample. The sample of safflorite was prepared by E. H. Roseboom at the Geophysical Laboratory in an evacuated sealed silica-glass tube at 800° C. Spectrographic analysis indicated the following impurities: 0.1 to 1.0 percent each of nickel and silicon; 0.01 to 0.1 percent of aluminum; and 0.001 to 0.01 percent each of barium, beryllium, calcium, copper, magnesium, manganese, and antimony.

The sample was a gray opaque powder.

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

Pattern	1	2	3
De Jong	120	211	111
Harcourt	120	111	221
National Bureau of Standards	120	101	111

Structural data. Peacock [3] in 1944 determined that safflorite has the space group P2/m (No. 10) and 1($CoFeAs_4$) per unit cell. The unit cell measurements reported by De Jong have been converted from kX to angstrom units and the "c" (6.35) has been divided by 2 for comparison with the NBS values.

		a	*b*	*c*	*β*
		A	*A*	*A*	
1926	De Jong [2]	4. 87	5. 81	3. 18	
1944	Peacock [3]	5. 25	5. 97	2. 93	90°
1960	National Bureau of Standards	5. 232	5. 952	2. 957	90° at 25° C

Cobalt Iron Arsenide (safflorite), $CoFeAs_4$ (monoclinic)

hkl (ortho)	1926 De Jong Fe, 1.9373 A		1942 Harcourt Co, 1.7902 A		1960 National Bureau of Standards Co, 1.7889 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
110	------	------	------	------	3. 932	7
020	------	------	------	------	2. 975	7
------	------	------	2. 84	5	------	------
011	------	------	------	------	2. 648	18
120	2. 66	100	2. 60	100	2. 586	100
101	2. 59	70	------	------	2. 573	94
210	2. 47	40	------	------	2. 394	39
111	2. 38	80	2. 37	40	2. 361	91
------	2. 22	20	------	------	------	------
------	2. 09	10	------	------	------	------
220	2. 00	10	2. 04	3	1. 9648	13
121	1. 94	10	1. 94	5	1. 9475	10
211	1. 89	90	1. 87	30	1. 8614	51
130	------	------	------	------	1. 8555	37
310	------	------	------	------	1. 6739	23
031	------	------	------	------	1. 6476	37
221	------	------	1. 635	40	1. 6361	33
230	------	------	------	------	1. 5804	6
131	------	------	1. 565	10	1. 5716	13
301	------	------	1. 500	20	1. 5023	12
040	------	------	------	------	1. 4876	7
002	------	------	------	------	1. 4784	14
231	------	------	------	------	1. 3944	3
321	------	------	------	------	1. 3409	6
330	------	------	------	------	1. 3100	4
240	------	------	------	------	1. 2932	11
122	------	------	1. 275	10	1. 2837	18
410	------	------	------	------	1. 2773	7
212	------	------	------	------	1. 2582	8
150	------	------	1. 160	5	1. 1605	4
132	------	------	------	------	1. 1562	9
421	------	------	------	------	1. 1100	18
312	------	------	1. 100	10	1. 1080	21
051	------	------	------	------	1. 1045	5
250	------	------	------	------	1. 0834	5
151, 232	------	------	1. 075	10	1. 0803	13
341	------	------	------	------	1. 0570	22
042	------	------	1. 048	10	1. 0488	5
520, 501	------	------	------	------	0. 9867	9
332	------	------	------	------	. 9804	6
242, 511	------	------	0. 975	5	. 9733	15
412	------	------	. 965	5	. 9667	12
113	------	------	------	------	. 9557	6
161, 530	------	------	------	------	. 9255	8

The density of safflorite calculated from the NBS lattice constants is 7.471 g/cm³ at 25° C.

References

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

[2] W. F. De Jong, Bepaling van de absolute Aslengten van Markasit en darmee isomorfe Mineralen, Physica **6,** 325–332 (1926).

[3] M. A. Peacock, On Loellingite and Safflorite (Abstract), Trans. Roy. Soc. Can. **38,** 155 (1944).

Copper Carbonate, basic (azurite), $Cu_3(OH)_2(CO_3)_2$ (monoclinic)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–0564	3. 51 5. 1 2. 51	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
*2–0153	5. 20 3. 67 3. 53	Molybdenum.	Waldo 1935.
*3–0360	3. 50 5. 15 2. 53	Copper	British Museum.

*Deleted in 1959 powder data index.

Additional published patterns. None.

NBS sample. The sample of azurite was obtained from the National Museum, catalog #R8545. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent zinc; 0.001 to 0.01 percent each of aluminum, iron, magnesium, and silicon; and 0.0001 to 0.001 percent each of calcium, chromium, gallium, lead, and nickel.

The color of the sample was bright blue. It was optically positive and the indices of refrac-

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
002	5. 1	71	5. 15	54
011			5. 08	29
100	------	-----	4. 99	11
012	------	-----	3. 86	2
110	------	-----	3. 80	7
$\bar{1}02$	3. 69	23	3. 674	52
102	3. 52	100	3. 516	100
$\bar{1}12$	3. 03	23	3. 107	11
013	------	-----	2. 964	2
020	------	-----	2. 920	8
021	------	-----	2. 811	7
$\bar{1}13$	------	-----	2. 590	11
022	------	-----	2. 540	24

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
120	2. 52	51	2. 523	20
113			2. 510	36
$\bar{2}00$	------	-----	2. 503	28
$\bar{1}04$	------	-----	2. 336	17
$\bar{2}10$	------	-----	2. 299	12
$\bar{1}22$	------	-----	2. 287	35
$\bar{2}11$	2. 27	40	2. 265	25
211	------	-----	2. 224	72
$\bar{1}14$	------	-----	2. 168	14
114	2. 09	6	2. 104	7
$\bar{1}23$	------	-----	2. 057	2
123	------	-----	2. 015	3
$\bar{2}13$	1. 94	17	1. 948	21
220	------	-----	1. 900	7
$\bar{2}21$, 213	------	-----	1. 879	4
$\bar{2}21$	------	-----	1. 858	2
$\bar{2}04$	------	-----	1. 836	7
$\bar{1}24$	1. 82	11	1. 824	16
115	1. 79	6	1. 791	8
124	------	-----	1. 786	9
204	------	-----	1. 759	3
006, $\bar{1}32$	------	-----	1. 721	2
033	------	-----	1. 696	3
300	------	-----	1. 6678	1
016	------	-----	1. 6512	2
$\bar{1}33$, $\bar{3}11$	1. 59	17	1. 5953	15
$\bar{2}15$, 302	------	-----	1. 5678	5
034, $\bar{2}24$	------	-----	1. 5546	3
$\bar{2}31$	------	-----	1. 5265	7
231, 312	1. 52	17	1. 5140	10
215, 224	------	-----	1. 5076	8
$\bar{3}13$	1. 473	6	1. 4773	11
$\bar{2}06$	------	-----	1. 4473	2
017	1. 433	6	1. 4306	8
$\bar{2}33$, 035	------	-----	1. 4173	5
042	------	-----	1. 4059	3
$\bar{1}17$	------	-----	1. 3910	5
322	1. 383	6	1. 3817	3
$\bar{1}35$, 304	------	-----	1. 3746	4
$\bar{1}42$	------	-----	1. 3575	3
$\bar{3}23$, 135	1. 348	6	1. 3536	4
$\bar{2}26$	1. 298	6	1. 2971	16

Lattice constants

		a	*b*	*c*	*β*
		A	*A*	*A*	
1932	Brasseur [2]	4. 97	5. 84	10. 29	
1958	Gattow and Zemann [3]	5. 00	5. 85	10. 35	92. 33
1960	National Bureau of Standards	5. 008	5. 844	10. 336	92. 45 at 25° C

tion were N_α=1.729 and N_β=1.758. N_γ could not be determined because the sample reacted with the liquids above 1.82.

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	102	002	113
National Bureau of Standards	102	211	002

Structural data. Brasseur [2] in 1932 determined that azurite has the space group $P2_1/c$ (No. 14) and $2[Cu_3(OH)_2(CO_3)_2]$ per unit cell. The unit-cell measurements reported by Brasseur have been converted from kX to angstrom units for comparison with the NBS values.

The density of azurite calculated from the NBS lattice constants is 3.786 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,** 485 (1938).

[2] H. Brasseur, Sur les structures de l'Azurite et de la Malachite, Z. Krist. **82,** 195–209 (1932).

[3] G. Gattow and J. Zemann, Neubestimmung der Kristallstruktur von Azurit $Cu_3(OH)_2(CO_3)_2$, Acta Cryst. **11,** 866–872 (1958).

Copper Carbonate, basic, (malachite) $Cu_2(OH)_2(CO_3)$ (monoclinic)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–0959	2. 86 3. 68 5. 1	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
2–0345	3. 67 2. 84 5. 00	Molybdenum	Waldo [2] 1935.

Additional published patterns. None.

NBS sample. The sample of malachite was crystallized from reagent grade basic copper carbonate and carbonic acid in a Morey bomb at 300° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent nickel; 0.001 to 0.01 percent each of aluminum, iron, magnesium, and silicon; 0.0001 to 0.001 percent each of beryllium, calcium, and lead.

The color of the sample was deep green. The indices of refraction were not determined because the sample reacted with the index liquids.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel, and by Waldo 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	140	220	120
Waldo	220	140	240
National Bureau of Standards	140	220	120

Structural data. Brasseur [3] in 1932, using data of Goldschmidt, determined that malachite has the space group $P2_1/a$ (No. 14), and $4[Cu_2(OH)_2(CO_3)]$ per unit cell.

Lattice constants

		a	*b*	*c*	*β*
		A	*A*	*A*	
1932	Brasseur [3]	9. 40	11. 97	3. 19	91°3′
1950	Ramsdell and Wolfe [4]	9. 49	12. 00	3.24	98°42′
1951	Wells [5]	9. 48	12. 03	3. 21	98°
1960	National Bureau of Standards	9. 502	11. 974	3. 240	98°45′ at 25°C

Copper Carbonate, basic, (malachite) $Cu_2(OH)_2(CO_3)$ (monoclinic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1935 Waldo Mo, 0.709 A		1960 National Bureau of Standards Cu, 1.5405A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
110	------	-----	------	-----	7. 41	10
020	6. 0	35	5. 91	40	5. 993	54
120	5. 1	40	5. 01	80	5. 055	77
200	------	-----	------	-----	4. 699	12
220	3. 69	50	3. 68	100	3. 693	87
310	------	-----	------	-----	3. 028	17
040	------	-----	------	-----	2. 988	16
$\bar{2}01$, 140, 186	2. 87	100	2. 85	100	2. 857	100
111, 021	------	-----	------	-----	2. 823	37
320, $\bar{2}11$	------	-----	2. 77	80	2. 778	43
240	2. 50	25	2. 51	86	2. 520	56
201	------	-----	------	-----	2. 477	29
330	------	-----	2. 46	40	2. 464	32
211	------	-----	2. 41	40	2. 425	18
400, 131	------	-----	------	-----	2. 349	13
$\bar{2}31$	2. 31	5	2. 32	40	2. 316	17
221	------	-----	2. 29	40	2. 289	16
$\bar{3}21$	------	-----	2. 23	20	2. 252	6
041, 420, $\bar{1}41$	2. 16	5	2. 17	60	2. 186	19
340	------	-----	------	-----	2. 160	7
250	------	-----	2. 12	40	2. 129	19
$\bar{3}31$	------	-----	2. 06	60	2. 076	16
311	2. 04	5	------	-----	2. 054	9
430	------	-----	------	-----	2. 022	4
060	------	-----	------	-----	1. 991	10
321	------	-----	1. 96	20	1. 969	16
160	1. 94	5	------	-----	1. 947	15
$\bar{4}21$	------	-----	------	-----	1. 941	9
$\bar{1}51$, 241	------	-----	1. 90	40	1. 911	16
350	------	-----	------	-----	1. 899	13
510	------	-----	------	-----	1. 855	3
$\bar{2}51$	------	-----	------	-----	1. 833	9
411	1. 78	5	1. 78	20	1. 759	10
421, 061	------	-----	------	-----	1. 696	8
$\bar{1}61$	------	-----	------	-----	1. 691	22
450	1. 67	10	1. 68	80	1. 678	12
$\bar{2}61$	------	-----	1. 64	40	1. 640	11
431	------	-----	1. 61	40	1. 616	16
012, 540	1. 59	5	1. 59	60	1. 589	17
351	------	-----	1. 56	40	1. 571	13
102	------	-----	------	-----	1. 541	6
112	------	-----	------	-----	1. 531	12
180	------	-----	------	-----	1. 480	4
$\bar{6}01$	1. 51	5	1. 50	20	1. 498	12
171, $\bar{2}32$, 550	1. 48	5	------	-----	1. 476	17
$\bar{3}22$, 521	------	-----	------	-----	1. 472	10
451, $\bar{3}32$, 531	1. 42	5	1. 42	40	1. 422	7
$\bar{4}12$	------	-----	------	-----	1. 418	15
$\bar{2}42$, $\bar{5}51$	------	-----	1. 38	20	1. 406	4
640	------		------	-----	1. 386	9
232	------	-----	------	-----	1. 362	2
380	------	-----	1. 35	40	1. 352	9
302	------	-----	------ [a]	-----	1. 349	10

[a] Eight additional lines were omitted.

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

The density of malachite calculated from the NBS lattice constants is 3.983 g/cm^3 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] A. W. Waldo, Identification of the copper ore minerals by means of X-ray powder diffraction patterns, Am. Min. **20,** 583 (1935).

[3] H. Brasseur, Contribution to the structure of malachite, Z. Krist. **81,** 111–126 (1932).

[4] L. Ramsdell and C. Wolfe, The unit cell of malachite, Am. Min. **35,** 119–121 (1950).

[5] A. F. Wells, Malachite: Re-examination of crystal structure, Acta Cryst. **4,** 200–203 (1951).

Gold(I) Cyanide, AuCN (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0910	2. 95 2. 55 5. 1	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of gold cyanide was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of silver, copper, palladium, and silicon; and 0.001 to 0.01 percent each of calcium, iron, magnesium, nickel, and lead.

The color of the sample was yellow. The indices of refraction were too high to be determined by the oil immersion method.

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	100	101, 002	001
National Bureau of Standards	001	100	101, 002

Structural data. Zdhanov and Shugam [2] in 1945 determined that gold cyanide has the space group P6mm (No. 183) or P6/mmm (No. 191) and 1(AuCN) per unit cell. The unit-cell measurements reported by Zdhanov and Shugam have been converted from kX to angstrom units for comparison with the NBS values.

The density of gold cyanide calculated from the NBS lattice constants is 7.301 g/cm^3 at 25° C.

Lattice constants

		a	*c*
		A	*A*
1945	Zdhanov and Shugam [2]	3. 41	5.10
1960	National Bureau of Standards.	3. 395	5.080 at 25° C

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
001	5. 1	60	5. 078	100
100	2. 96	100	2. 941	98
101, 002	2. 56	100	2. 542	70
102	1. 92	40	1. 921	23
110	1. 69	16	1. 698	18
003			1. 693	5
111	1. 61	12	1. 610	12
200	1. 47	20	1. 470	12
103			1. 468	15
201	1. 413	16	1. 412	11
112			1. 408	12
202	1. 274	4	1. 273	3
004			1. 2702	5
113	1. 202	4	1. 1985	3
104	1. 167	4	1. 1659	4
210	1. 112	4	1. 1112	13
211	1. 088	4	1. 0855	4
212	1. 020	4	1. 0183	4
005			1. 0160	4
300	------	-----	0. 9794	3
301, 204	0. 963	4	. 9611	3
105			. 9602	3

References

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

[2] H. Zhdanov and E. Shugam, The crystal structure of cyanides. III Structure of the gold cyanide, Acta Physicochim. URSS **20,** 253–258 (1945).

Iron Arsenide (loellingite), $FeAs_2$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
5–0650	2. 60 2. 34 1. 85	Iron	Volker, Geol. Min. Museum Leiden, Holland.

Additional published patterns

Source	Radiation
De Jong [1] 1926	Iron.
Peacock [2] 1941	Iron.
Harcourt [6] 1942	Iron.
Pehrman [3] 1950	Copper.

NBS sample. The sample of loellingite was prepared by E. H. Roseboom at the Geophysical Laboratory in an evacuated sealed silica-glass tube at 800° C. Spectrographic analysis indicated the following impurities: 0.01 to 0.1 percent each of aluminum, chromium, titanium, and tungsten; and 0.001 to 0.01 percent each of silver, barium, beryllium, cobalt, copper, magnesium, nickel, and antimony.

The sample was a gray opaque powder.

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

Pattern	1	2	3
Volker	120, 011	111	211
De Jong	120, 011	211	111
Peacock	120, 011	111	101
Harcourt	210	120, 011	211
Pehrman	120, 011	-----	221
National Bureau of Standards	120	111	101

Structural data. Buerger [4] in 1932 determined that loellingite has the marcasite structure, the space group Pnnm (No. 58) and $2(FeAs_2)$ per unit cell. Several unit cell measurements have been converted from kX to angstrom units for comparison with the NBS values. The "c" (6.35) reported by De Jong has been divided by 2.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1922	Huggins [5]	4. 72	5. 11	3. 83
1926	De Jong [1]	4. 87	5. 81	3. 18
1932	Buerger [4]	5. 26	5. 93	2. 86
1941	Peacock [2]	5. 29	5. 98	2. 88
1960	National Bureau of Standards.	5. 300	5. 983	2. 882 at 25° C

hkl	---- T. Volker Fe, 1.9373 A		1926 De Jong Fe, 1.9373 A		1941 Peacock Fe, 1.9373 A		1942 Harcourt Fe, 1.9373 A		1950 Pehrman Cu, 1.5405 A		1960 National Bureau of Standards Co, 1.78890 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*	
110	-----	-----	----	-----	----	----	----	----	----	-----	3. 97	3
-----	-----	-----	----	-----	----	----	3. 46	12	----	-----	-----	----
020	2. 98	10	----	-----	----	----	----	----	----	-----	2. 989	5
-----	2. 88	20	----	-----	----	----	2. 84	12	2. 85	90	-----	----
-----	2. 81	10	----	-----	----	----	----	----	----	-----	-----	----
200	-----	-----	----	-----	----	----	----	----	----	-----	2. 651	6
120	2. 61	100	2. 67	100	2. 60	vs	2. 67	25	2. 57	100	2. 605	100
011											2. 599	58
101	2. 55	60	2. 61	60	2. 53	s	2. 55	5	----	-----	2. 532	59
210	2. 40	40	2. 47	50	2. 41	m	2. 43	100	----	-----	2. 421	32
111	2. 34	80	2. 39	80	2. 32	vs	2. 196	5	2. 33	70	2. 331	64
-----	2. 04	10	2. 08	20	----	----	2. 096	5	----	-----	-----	----
220	1. 972	20	2. 01	10	1. 978	w	2. 029	12	1. 999	50	1. 984	9
121	1. 935	10	1. 92	10	1. 925	vw	----	----	----	-----	1. 932	7
130	-----	-----	----	-----	1. 861	m	----	----	----	-----	1. 867	21

Iron Arsenide (loellingite), $FeAs_2$ (orthorhombic)—Continued

hkl	---- T. Volker Fe, 1.9373 A		1926 De Jong Fe, 1.9373 A		1941 Peacock Fe, 1.9373 A		1942 Harcourt Fe, 1.9373 A		1950 Pehrman Cu, 1.5405 A		1960 National Bureau of Standards Co, 1.78890 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		A	
211	1. 858	80	1. 89	90	1. 850	m	1. 810	25	1. 854	70	1. 8543	32
-----	1. 808	10	----	-----	----	----	----	----	----	-----	-----	----
310	1. 681	40	----	-----	1. 692	s	----	----	1. 682	20	1. 6945	24
031	-----	-----	----	-----	----	----	----	----	----	-----	1. 6401	25
221	1. 639	70	----	-----	1. 633	s	1. 631	5	1. 637	80	1. 6344	33
230	1. 584	10	----	-----	1. 592	vw	----	----	----	-----	1. 5934	6
131	1. 567	20	----	-----	1. 562	vw	----	----	----	-----	1. 5669	11
301	1. 503	10	----	-----	1. 501	w	----	----	----	-----	1. 5059	8
040	1. 490	10	----	-----	----	----	----	----	----	-----	1. 4960	6
002	1. 456	30	----	-----	1. 439	m	----	----	1. 438	20	1. 4413	9
-----	-----	-----	----	-----	1. 393	w	----	----	----	-----	-----	----
321	1. 343	20	----	-----	1. 345	w	1. 343	8	----	-----	1. 3454	7
330	1. 314	10	----	-----	1. 323	vw	----	----	1. 321	10	1. 3224	5
240	1. 298	30	----	-----	1. 303	w	----	----	----	-----	1. 3030	7
410	1. 284	20	----	-----	1. 296	vw	----	----	----	-----	1. 2942	8
202	1. 271	30	----	-----	----	----	----	----	----	-----	1. 2660	3
122	1. 246	20	----	-----	1. 260	m	----	----	1. 266	30	1. 2612	11
212	1. 226	10	----	-----	1. 239	w	1. 217	5	----	-----	1. 2388	6
420	1. 221	20	----	-----	1. 211	vw	----	----	----	-----	1. 2116	<3
241	-----	-----	----	-----	----	----	----	----	----	-----	1. 1870	5
411	-----	-----	----	-----	1. 179	vw	----	----	----	-----	1. 1802	5
150	-----	-----	----	-----	1. 168	w	----	----	----	-----	1. 1671	6
222	1. 163	10	----	-----	----	----	----	----	----	-----	1. 1659	6
340 / 132	1. 146	20	----	-----	1. 141	w	----	----	----	-----	1. 1407	8
421	-----	-----	----	-----	1. 117	m	----	----	----	-----	1. 1167	8
051	1. 112	50	----	-----	1. 106	m	----	----	----	-----	1. 1052	6
430	-----	-----	----	-----	----	----	----	----	----	-----	1. 1036	5
312	1. 101	50	----	-----	1. 097	m	----	----	1. 099	20	1. 0977	8
250	1. 085	20	----	-----	1. 090	w	----	----	----	-----	1. 0906	5
151	1. 080	30	----	-----	1. 082	m	----	----	----	-----	1. 0820	7
232	-----	-----	----	-----	----	----	----	----	----	-----	1. 0687	4
341	1. 058	70	----	-----	1. 061	s	----	----	1. 058	30	1. 0615	12
042	-----	-----	----	-----	----	----	----	----	----	-----	1. 0378	5
142	-----	-----	----	-----	----	----	----	----	----	-----	1. 0186	4
520	-----	-----	----	-----	----	----	----	----	----	-----	0. 9989	7
060	-----	-----	----	-----	----	----	----	----	----	-----	. 9974	5
501	-----	-----	----	-----	----	----	----	----	----	-----	. 9948	7
440	-----	-----	----	-----	----	----	----	----	----	-----	. 9918	<3
511	-----	-----	----	-----	----	----	----	----	----	-----	. 9812	<3
160	-----	-----	----	-----	----	----	----	----	----	-----	. 9800	6
332	-----	-----	----	-----	----	----	----	----	----	-----	. 9743	6
242	-----	-----	----	-----	----	----	----	----	----	-----	. 9663	7
412	-----	-----	----	-----	----	----	----	----	----	-----	. 9626	6
013	-----	-----	----	-----	----	----	----	----	----	-----	. 9485	<3
103	-----	-----	----	-----	----	----	----	----	----	-----	. 9452	<3
441	-----	-----	----	-----	----	----	----	----	----	-----	. 9379	<3
530	-----	-----	----	-----	----	----	----	----	----	-----	. 9360	10
113	-----	-----	----	-----	----	----	----	----	----	-----	. 9336	7
161	-----	-----	----	-----	----	----	----	----	----	-----	. 9278	9

The density of loellingite calculated from the NBS lattice constants is 7.472 g/cm³ at 25° C.

References

[1] W. F. De Jong, Bepaling van de absolute Aslengten van Markasit en daarmee isomorfe Mineralen, Physica **6,** 325–332 (1926).

[2] M. A. Peacock, Identification of ore minerals by X-Rays, Trans. Roy. Soc. Can. 3rd Ser. IV **35,** 105–113 (1941).

[3] G. Pehrman, Löllingit von Kuortane, Acta Acad. Aboensis, Math. et Phys. **17,** 1–8 (1950).

[4] M. J. Buerger, The crystal structure of löllingite—$FeAs_2$, Z. Krist. **82,** 165–187 (1932).

[5] M. L. Huggins, The crystal structure of marcasite (FeS_2), arsenopyrite (FeAsS), and loellingite ($FeAs_2$), Phys. Rev. **19,** 369 (1922).

[6] G. A. Harcourt, Tables for the identification of ore minerals by X-Ray Powder Patterns, Am. Min. **27,** 63–113 (1942).

Magnesium Gallate, $MgGa_2O_4$ (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
2–1057	2. 50 1. 47 1. 61	Molybdenum	Machatschki [1] 1932.
3–1158	1. 47 0. 85 2. 50	Copper	Hauptmann and Novak [2] 1932.

Additional published patterns. None.

NBS sample. The sample of magnesium gallate was prepared at NBS by solid state reaction at 1,400° C between magnesium carbonate and gallium oxide. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of tin; 0.01 to 0.1 percent each of calcium, cobalt, germanium, sodium, and nickel; and 0.001 to 0.01 percent each of aluminum, bismuth, chromium, copper, iron, lead, and silicon.

hkl	1932 Machatschki Mo, 0.709 A			1932 Hauptmann and Novak Cu, 1.5418 A			1960 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. 76	4	8. 24	-----	---	----	4. 779	5	8. 277
220	2. 94	30	8. 32	2. 93	80	8. 29	2. 927	44	8. 279
311	2. 50	100	8. 29	2. 50	90	8. 29	2. 495	100	8. 276
222	2. 38	10	8. 24	2. 39	15	8. 28	2. 390	7	8. 280
400	2. 08	30	8. 32	2. 07	60	8. 28	2. 070	21	8. 277
422	1. 73	30	8. 48	1. 69	60	8. 28	1. 6900	16	8. 279
511	1. 61	60	8. 37	1. 60	80	8. 31	1. 5935	38	8. 280
440	1. 47	90	8. 32	1. 47	100	8. 32	1. 4633	45	8. 278
531	----	---	----	-----	---	----	1. 3994	1	8. 279
620	1. 32	10	8. 35	1. 31	40	8. 29	1. 3092	6	8. 280
533	----	---	----	1. 27	65	8. 33	1. 2627	12	8. 280
622	1. 25	20	8. 29	1. 25	30	8. 29	1. 2481	4	8. 279
444	1. 19	10	8. 24	-----	---	----	1. 1949	3	8. 279
642	1. 11	20	8. 31	1. 11	60	8. 31	1. 1063	7	8. 279
731	1. 09	50	8. 37	1. 08	80	8. 30	1. 0779	18	8. 280
800	1. 04	20	8. 32	1. 04	60	8. 32	1. 0348	8	8. 278
822	----	---	----	0. 978	50	8. 30	0. 9758	5	8. 280
751	----	---	----	. 958	80	8. 30	. 9561	12	8. 280
662	----	---	----	-----	---	----	. 9497	2	8. 279
840	----	---	----	. 928	40	8. 30	. 9258	3	8. 281
931	----	---	----	. 870	70	8. 30	. 8680	2	8. 280
844	----	---	----	. 847	100	8. 30	. 8451	10	8. 280
10·2·0	----	---	----	-----	---	----	. 8119	6	8. 280
951	----	---	----	-----	---	----	. 8004	15	8. 279
10·2·2	----	---	----	-----	---	----	. 7967	2	8. 280
Average value of last five lines			8. 31	-----	---	8. 30	---------	-----	8. 280

The color of the sample was bluish-white. The index of refraction was 1.879.

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

Pattern	1	2	3
Machatschki	311	440	511
Hauptmann and Novak	440	844	311
National Bureau of Standards	311	440	220

Structural data. Barth and Posnjak [3] in 1931 determined that magnesium gallate has spinel-type structure, the space group Fd3m (No. 227), and $8(MgGa_2O_4)$ per unit cell.

The unit-cell measurements reported by Barth and Posnjak, and Hauptmann and Novak have been converted from kX to angstrom units for comparison with the NBS value.

The density of magnesium gallate calculated from the NBS lattice constant is 5.328 g/cm^3 at 25° C.

Lattice constants

		a
		A
1932	Barth and Posnjak [4]	8. 28
1932	Machatschki [1]	8. 30
1932	Hauptmann and Novak [2]	8. 296
1960	National Bureau of Standards	8. 280 at 25° C

References

[1] F. Machatschki, Der Magnesium-Gallium Spinell, Z. Krist. **82,** 348–354 (1932).

[2] H. Hauptmann and J. Novak, Gitterkonstanten einiger Verbindungen vom Spinelltypus, Z. physik. chem. (B) **15,** 365–372 (1932).

[3] T. F. W. Barth and E. Posnjak, The Spinel Structure: an example of variate atom equipoints, J. Wash. Acad. Sci., 255–258 (1931).

[4] T. F. W. Barth and E. Posnjak, Spinel Structures: with and without variate atom equipoints, Z. Krist. **82,** 325–341 (1932).

Magnesium Germanate, Mg_2GeO_4 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of magnesium germanate was prepared at NBS by hydrothermal synthesis at 800° C and 10,000 psi from magnesium oxide and germanium oxide. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, sodium, and silicon; and 0.001 to 0.01 percent each of aluminum, cobalt, copper, iron, and antimony.

The sample was colorless. The index of refraction was 1.769.

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	311	220	440

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*
	A		*A*
111	4. 764	25	8. 251
220	2. 917	76	8. 251
311	2. 488	100	8. 251
222	2. 383	2	8. 254
400	2. 063	8	8. 252

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*
	A		*A*
331	1. 8926	7	8. 250
422	1. 6842	29	8. 251
511	1. 5876	35	8. 250
440	1. 4582	50	8. 249
531	1. 3937	4	8. 245
620	1. 3042	11	8. 248
533	1. 2578	11	8. 248
711	1. 1547	2	8. 246
642	1. 1020	12	8. 247
731	1. 0736	19	8. 246
800	1. 0308	6	8. 246
733	1. 0075	<1	8. 247
822	0. 9719	6	8. 247
662	. 9462	10	8. 249
911	. 9051	2	8. 246
664	. 8790	3	8. 246
931	. 8644	6	8. 246
844	. 8417	17	8. 247
933	. 8287	1	8. 245
10·2·0	. 8085	9	8. 245
951	. 7972	19	8. 246
Average value of last five lines			8. 246

Structural data. Goldschmidt [1] in 1931 showed that cubic magnesium germanate has the spinel type structure, the space group Fd3m (No. 227), and 8(Mg_2GeO_4) per unit cell.

Lattice constants

		a
		A
1931	Goldschmidt [1]	8.3
1954	Roy and Roy [2]	8.255
1960	National Bureau of Standards	8.246 at 25° C

The density of magnesium germanate calculated from the NBS lattice constant is 4.387 g/cm³ at 25° C.

References

[1] V. M. Goldschmidt, Zur Kristallchemie des Germaniums, Nachr. Ges. Wiss. Göttingen, Math.-physik. Kl., Fachgruppen: IV, Bd. **1,** 184 (1931).

[2] D. M. Roy and R. Roy, Formation and properties of synthetic serpentines, Am. Min. **39,** Nos. 11 and 12, 968 (1954).

Magnesium Germanate, Mg_2GeO_4 (orthorhombic)

ASTM cards. None.

Additional published patterns

Source	Radiation
Robbins and Levin [1] 1959	Copper

NBS sample. The sample of magnesium germanate was prepared at NBS by reaction at 1,400° C from magnesium oxide and germanium oxide. Spectrographic analysis showed the follow-

hkl	1959 Robbins and Levin Cu, 1.5405 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
200	5.15	21	5.16	27
101	4.42	38	4.44	42
210	3.91	100+	3.92	100
011	3.80	32	3.81	27
201	3.55	31	3.55	20
211	3.06	10	3.06	8
020	3.01	58	3.02	36
-----	2.96	3	-----	----
301	2.81	46	2.82	31
400	2.57	10	2.575	12
311	2.55	100+	2.552	88
121	2.49	100+	2.494	78
002	2.45	10	2.456	7
102	2.39	22	2.389	12
410	2.37	37	2.369	19
221	2.29	20	2.301	12
401	2.28	21	2.283	11
112	2.22	61	2.222	20
411	-----	----	2.135	1
212	2.08	16	2.081	7

hkl	1959 Robbins and Levin Cu, 1.5405 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		*A*	
302	1.99	22	1.999	10
420	1.96	17	1.960	8
022	1.90	42	1.904	10
501	-----	----	1.901	16
122, 230	1.87	26	1.872	10
421	-----	----	1.819	1
222	1.78	35	1.786	13
231	1.75	8	1.750	1
600	1.72	5	1.717	1
412	1.70	40	1.705	11
322	1.66	23	1.666	8
610	1.65	16	1.652	8
331	1.64	56	1.636	14
430	1.585	18	1.585	7
013	1.580	19	1.581	7
203	1.561	13	1.561	5
132	1.539	16	1.538	7
422	1.532	15	1.531	5
512	1.528	29	1.527	12
040, 431	1.508	49	1.508	16
620	1.493	52	1.492	24
303	1.478	5	1.478	1
240	1.448	3	1.448	1
313	1.435	16	1.435	8
123	1.425	23	1.425	7
701	1.411	14	1.410	5
223	1.396	49	1.386	14
403	1.382	45	1.382	13
711	1.374	11	1.373	4
612	1.371	8	1.370	4
413	1.347	15	1.347	4
432	1.332	12	1.332	3
341	1.329	11	1.329	5

ing impurities: 0.01 to 0.1 percent each of platinum and silicon; 0.001 to 0.01 percent each of aluminum, antimony, calcium, chromium, and nickel.

The sample was colorless. The indices of refraction were $N\alpha=1.698$, $N\beta=1.717$, $N\gamma=1.765$, and $2V=\sim 65°$.

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

Pattern	1	2	3
Robbins and Levin	210	311	121
National Bureau of Standards	210	311	121

Structural data. Goldschmidt [2] in 1931 determined that orthorhombic magnesium germanate has the olivine type structure, the space group Pnma (No. 62), and $4(Mg_2GeO_4)$ per unit cell.

		a	*b*	*c*
		A	*A*	*A*
1954	Roy and Roy [3].	10. 295	6. 020	4. 915
1960	National Bureau of Standards.	10. 304	6. 032	4. 913 at 25° C

The density of magnesium germanate calculated from the NBS lattice constants is 4.028 g/cm³ at 25° C.

References

[1] C. R. Robbins and E. M. Levin, The system magnesium oxide-germanium dioxide, Am. J. Sci. **257,** 63–70 (1959).

[2] V. M. Goldschmidt, Zur Kristallchemie des Germaniums, Nachr. Ges. Wiss. Göttingen, Math. physik. Kl., Fachgruppen IV **Bd. 1,** 184 (1931).

[3] D. M. Roy and R. Roy, An experimental study of the formation and properties of synthetic serpentines and related layer silicate minerals, Am. Min. **39,**, Nos. 11 and 12, 968 (1954).

Magnesium Silicate Fluoride (norbergite), $Mg_2SiO_4 \cdot MgF_2$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
2–1345	1. 74 3. 08 2. 26	Copper	British Museum.

Additional published patterns

Source	Radiation
Sahama [1] 1953	Copper

NBS sample. The sample of norbergite was prepared by A. Van Valkenburg at NBS from magnesium oxide, magnesium fluoride, and silicic acid. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent iron; 0.01 to 0.1 percent each of aluminum and calcium; and 0.001 to 0.01 percent each of boron, chromium, manganese, nickel, strontium, and titanium.

The color of the sample was tan. It is optically positive with indices of refraction of $N\alpha=1.548$, $N_\beta=1.552$, and $N_\gamma=1.570$.

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

Pattern	1	2	3
British Museum	402	121	401
Sahama	121	311	231
National Bureau of Standards	121	231	311

Structural data. Taylor and West [2] in 1929 determined that norbergite has the space group Pnma (No. 62) and $4(Mg_2SiO_4 \cdot MgF_2)$ per unit cell.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1929	Taylor and West [2]	10. 2	8. 74	4. 71
1960	National Bureau of Standards	10. 271	8. 727	4. 709 at 25° C.

The density of norbergite calculated from the NBS lattice constants is 3.194 g/cm³ at 25° C.

References

[1] Th. G. Sahama, Mineralogy of the humite group, Ann. Acad. Sci. Fennicae Ser. A., III. Geologia-Geographica No. **31,** 1–50 (1953).

[2] W. H. Taylor and J. West, The structure of norbergite, Z. Krist. **70,** 461–474 (1929).

Magnesium Silicate Fluoride (norbergite), $Mg_2SiO_4 \cdot MgF_2$ (orthorhombic)

hkl	British Museum Cu, 1.5418 A		1953 Sahama Cu, 1.5405 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
200	5. 2	40	5. 13	m	5. 145	18
----------	4. 8	40	--------	------	--------	------
210	4. 41	50	--------	------	4. 428	10
020	--------	------	4. 38	w	4. 371	28
101	--------	------	4. 27	vw	4. 283	12
011	--------	------	4. 14	vw	4. 149	20
220	3. 37	60	3. 32	m	3. 327	22
211	--------	------	3. 22	m	3. 227	27
121	3. 08	80	3. 06	vs	3. 058	100
----------	2. 94	40	--------	------	--------	------
301	2. 77	40	2. 76	vw	2. 771	14
221	--------	------	2. 72	vw	2. 716	12
311	2. 66	70	2. 63	s	2. 639	73
410	2. 52	60	2. 46	w	2. 466	15
131	2. 42	40	2. 41	m	2. 408	36
321	2. 35	40	2. 34	m	2. 337	34
102	--------	------	2. 29	w	2. 296	16
401	2. 26	80	2. 25	m	2. 255	68
231	--------	------	2. 23	s	2. 230	80
112	--------	------	--------	------	2. 214	8
411	--------	------	--------	------	2. 184	8
122	2. 03	20	2. 03	vw	2. 0320	10
240, 331	--------	------	--------	------	2. 0068	5
141	1. 94	60	1. 948	vw	1. 9442	14
430	--------	------	--------	------	1. 9243	6
222	--------	------	--------	------	1. 9201	5
241	1. 86	20	--------	------	1. 8472	8
511	1. 81	20	1. 838	vw	1. 8408	9
322	--------	------	--------	------	1. 7733	4
402	1. 74	100	1. 733	m	1. 7357	32
232	1. 74	20	1. 723	s	1. 7241	48
341	--------	------	1. 721	m	1. 7125	5
412	--------	------	1. 699	vw	1. 7022	14
250	1. 65	50	--------	------	1. 6529	10
151	1. 60		--------	------	1. 6160	7
332, 422	--------	------	--------	------	1. 6125	10
042	--------	------	--------	------	1. 6004	9
620	--------	------	1. 592	vw	1. 5938	10
611, 142	--------	------	--------	------	1. 5808	6
441	--------	------	--------	------	1. 5678	4
103	--------	------	--------	------	1. 5518	2
502, 013	1. 54	20	--------	------	1. 5450	2
242, 113	--------	------	--------	------	1. 5280	6
432	--------	------	1. 480	w	1. 4890	16
213, 351	1. 49	80	1. 475	m	1. 4763	45
123	1. 47	40	1. 471	w	1. 4621	6
522	--------	------	1. 460	w	1. 4582	6
060	--------	------	--------	------	1. 4547	20
450	--------	------	--------	------	1. 4435	6
301	--------	------	--------	------	1. 4265	4
313, 631	1. 41	40	--------	------	1. 4080	7
701, 260	[a]	------	1. 398	vw	1. 3990	6

[a] Eight additional lines were omitted.

Manganese Selenide, MnSe (cubic)

ASTM cards. None.

Additional published patterns

Source	Radiation
Broch [1] 1927	Copper

NBS sample. The sample of manganese selenide was prepared at NBS from manganese and selenium in an evacuated fused silica tube at 600° C. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of aluminum; 0.01 to 0.1 percent each of silver and iron; and 0.001 to 0.01 percent each of calcium, chromium, copper, magnesium, nickel, and tin.

The sample was a deep brown opaque powder.

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

Pattern	1	2	3
Broch	200	220	420
National Bureau of Standards	200	220	222

Structural data. Goldschmidt [2] in 1927 determined that manganese selenide has the NaCl type structure, the space group Fm3m (No. 225), and 4(MnSe) per unit cell. Baroni [3] has also shown MnSe to exist as a sphalerite and as a wurtzite structure.

Lattice constants

		a
		A
1927	Broch [1]	5.46
1927	Goldschmidt [2]	5.464
1938	Baroni [3]	5.45
1960	National Bureau of Standards.	5.462 at 25° C

The density of the manganese selenide calculated from the NBS lattice constants is 5.456 g/cm^3 at 25° C.

References

[1] E. Broch, Prazisionsbestimmungen der Githerkonstanten der Verbindungen MgO, MgS, MgSe, MnO, MnSe, Z. physik. Chem. **127,** 446–54 (1927).

[2] V. M. Goldschmidt, G. V. VIII Untersuchungen über Baucend Eigenschaften von Krystallen, Skrifter Norske Videnskaps Akad Oslo. I. Mat. Naturv. Kl., **1927,** No. 8, 1–139 (1927).

[3] A. Baroni, Sul polymorfismo di MnSe, Z. Krist. **99,** 336–39 (1938).

hkl	1927 Broch Cu, 1.539 A			1960 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	------	----	------	3. 152	11	5. 459
200	2. 728	vvs	5. 456	2. 732	100	5. 464
220	1. 927	vvs	5. 450	1. 931	57	5. 461
311	------	----	------	1. 646	5	5. 460
222	1. 574	vs	5. 452	1. 577	20	5. 463
400	1. 363	s	5. 454	1. 366	10	5. 464
420	1. 219	vvs	5. 450	1. 221	20	5. 461
422	1. 113	vvs	5. 453	1. 115	15	5. 463
440	0. 964	m	5. 453	0. 9651	6	5. 460
600	------	----	------	. 9105	11	5. 463
620	------	----	------	. 8637	10	5. 462
622	------	----	------	. 8232	11	5. 460
Average value of last five lines			5. 452	------	----	5. 462

Nickel Arsenic 1:2 (rammelsbergite), $NiAs_2$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
7–319	2. 57 2. 84 2. 48	Copper	Kaiman [1] 1946.

Additional published patterns

Source	Radiation
Peacock and Dadson [2] 1940	Copper
Harcourt [3] 1942	Copper

NBS sample. The sample of rammelsbergite was prepared by E. H. Roseboom [4] of the Geophysical Laboratory in an evacuated sealed silica-glass tube at 800° C with solid arsenic and nickel in equilibrium with the vapor. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, cobalt, iron, titanium, and zirconium; and 0.001 to 0.01 percent each of magnesium, lead, and antimony.

The sample was a gray opaque powder.

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

Pattern	1	2	3
Peacock and Dadson	101	111	120
Harcourt	211	111	101
Kaiman	111	101	120
National Bureau of Standards	111	120	101

Structural data. Peacock and Dadson [2] in 1940 determined that rammelsbergite has the space group Pnnm (No. 58) and $2(NiAs_2)$ per unit cell.

The unit-cell measurements of Peacock and Dadson have been converted from kX to anstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1940	Peacock and Dadson [2].	4. 79	5. 79	3. 54
1960	National Bureau of Standards.	4. 759	5. 797	3. 539 at 25° C

The density of rammelsbergite calculated from the NBS lattice constants is 7.091 g/cm³ at 25° C.

References

[1] S. Kaiman, The crystal structure of rammelsbergite, $NiAs^2$, Univ. Toronto Studies. Geol. Ser. **51,** 49–58 (1946).

[2] M. A. Peacock and A. S. Dadson, On rammelsbergite and pararammelsbergite, Am. Min. **25,** 561–577 (1940).

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

[4] E. H. Roseboom, Jr., The $CoAs_2$–$NiAs_2$–$FeAs_2$–As system. Annual Report of the Director of the Geophysical Laboratory, 201 (1956–57).

hkl	1940 Peacock and Dadson Cu, 1.5418 A		1942 Harcourt Cu, 1.5418 A		1946 Kaiman Cu, 1.5418 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
110	3. 69	m	3. 61	4	3. 69	10	3. 679	11
011	3. 03	vw	------	-----	3. 02	5	3. 023	13
020	------	-----	2. 91	6	------	-----	2. 901	9
101	2. 86	s	2. 77	50	2. 84	80	2. 843	63
111	2. 56	s	2. 490	62	2. 57	100	2. 552	100
120	2. 47	s	2. 420	38	2. 48	80	2. 476	87
200	2. 40	vw	2. 325	4	2. 39	5	2. 382	10
210	2. 21	w	2. 170	12	2. 21	8	2. 202	10
121	2. 02	w	1. 989	12	2. 03	8	2. 030	12
211	1. 875	s	1. 837	100	1. 876	70	1. 870	56

Nickel Arsenic 1:2 (rammelsbergite), $NiAs_2$ (orthorhombic)—Continued

hkl	1940 Peacock and Dadson Cu, 1.5418 A		1942 Harcourt Cu, 1.5418 A		1946 Kaiman Cu, 1.5418 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A	
220	------	-----	------	-----	1. 803	5	1. 840	10
130	1. 780	w	------	-----	------	-----	1. 790	22
002	1. 767	m	1. 733	12	1. 764	15	1. 771	23
031	1. 693	m	1. 673	38	1. 696	30	1. 696	32
221	1. 638	m	1. 613	12	1. 638	8	1. 632	15
131, 112	1. 596	m	1. 581	25	1. 596	15	1. 597	16
310	1. 533	m	1. 518	25	1. 538	8	1. 530	10
230	------	-----	------	-----	1. 509	3	1. 500	4
301	------	-----	------	-----	------	-----	1. 448	20
122	1. 442	s	1. 425	50	1. 442	20	1. 440	7
202	------	-----	------	-----	------	-----	1. 420	6
311	------	-----	------	-----	1. 414	3	1. 405	7
320	------	-----	------	-----	------	-----	1. 392	8
231, 212	1. 376	vw	1. 350	12	1. 378	5	1. 380	6
321, 141	------	-----	1. 283	6	1. 298	3	1. 295	2
222	------	-----	1. 268	6	1. 279	3	1. 276	4
132	------	-----	1. 244	6	1. 257	3	1. 259	4
240	1. 238	m	1. 230	38	1. 242	10	1. 238	10
400	------	-----	------	-----	1. 195	3	1. 190	2
241, 410	------	-----	------	-----	------	-----	1. 166	4
331, 312, 013	1. 159	m	1. 159	50	1. 158	10	1. 158	10
103, 232	------	-----	------	-----	1. 146	3	1. 144	4
150	------	-----	1. 134	2	1. 124	5	1. 126	3
113	1. 123	w	------	-----	------	-----	1. 124	4
042	------	-----	------	-----	------	-----	1. 121	3
051, 420	------	-----	1. 114	25	1. 103	3	1. 102	5
322	1. 098	w	1. 094	25	1. 093	3	1. 094	5
151	1. 073	w	1. 068	38	1. 073	8	1. 073	6
421	1. 054	w	1. 048	38	1. 055	5	1. 051	6
213	1. 039	w	1. 032	12	1. 040	5	1. 040	5
341	1. 026	m	1. 022	38	1. 025	8	1. 024	7
242	1. 013	m	1. 010	50	1. 017	10	1. 014	8
332, 033	------	-----	1. 001	6	1. 003	3	1. 007	5
223	0. 990	vw	------	-----	0. 991	3	0. 994	3
402	------	-----	0. 989	12	------	-----	. 9878	5
133	------	-----	------	-----	------	-----	. 9856	5
431, 412	. 975	w	. 974	50	. 977	5	. 9742	4
060	------	-----	------	-----	------	-----	. 9662	4
152	------	-----	------	-----	------	-----	. 9504	3
160	. 948	w	. 949	50	------	-----	. 9471	5
510	------	-----	------	-----	------	-----	. 9391	<1
313, 422	------	-----	. 936	6	------	-----	. 9348	3
440	. 921	w	. 922	38	------	-----	. 9192	4
161	------	-----	------	-----	------	-----	. 9143	<1
351, 520	------ [a]	-----	------	-----	------	-----	. 9050 [b]	4

[a] Six additional lines were omitted.
[b] Two weak lines (*d* values 2.910 and 2.567) were omitted from the NBS pattern because they did not index.

Nickel Ferrite (trevorite), $NiFe_2O_4$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
3–0875	2. 51 1. 48 1. 60	Molybdenum	Dow Chemical Company

Additional published patterns

Source	Radiation
Passerini and Bruni [1] 1929	Iron

NBS sample. The sample of trevorite was prepared at NBS by solid state reaction at 1,400° C in an oxidizing atmosphere between co-precipitated hydroxides of ferric iron and nickel. Spectrographic analysis showned the following impurities: 0.01 to 0.1 percent each of silver, aluminum, arsenic, calcium, magnesium, platinum, and zinc; 0.001 to 0.01 percent each of barium, cobalt, manganese, molybdenum, antimony, and strontium.

The sample was a black opaque powder.

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

Pattern	1	2	3
Dow Chemical Company	311	440	511
Passerini and Bruni	440	800	311
National Bureau of Standards	311	440	511

hkl	---- Dow Chemical Co. Mo, 0.709 A			1929 Passerini and Bruni Fe, 1.9356 A			1960 National Bureau of Standards Co, 1.7889 A at 25° C.		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
111	4. 82	7	8. 35	-----	---	----	4. 82	18	8. 34
220	2. 95	20	8. 34	2. 88	11	8. 15	2. 948	29	8. 339
311	2. 51	100	8. 32	2. 48	29	8. 22	2. 513	100	8. 335
222	2. 41	5	8. 35	2. 37	6	8. 22	2. 408	7	8. 340
400	2. 08	23	8. 32	2. 06	20	8. 26	2. 085	23	8. 340
331	1. 92	1	8. 37	1. 90	2	8. 28	1. 9125	2	8. 336
422	1. 70	13	8. 33	1. 69	12	8. 30	1. 7025	7	8. 341
511	1. 60	33	8. 31	1. 60	19	8. 30	1. 6051	31	8. 340
440	1. 48	53	8. 37	1. 471	100	8. 32	1. 4760	40	8. 349
531	----	---	----	1. 408	3	8. 33	1. 4100	1	8. 342
620	1. 32	4	8. 35	1. 317	10	8. 33	1. 3187	5	8. 340
533	1. 27	9	8. 33	1. 270	15	8. 33	1. 2706	8	8. 332
622	----	---	----	1. 254	9	8. 32	1. 2573	3	8. 340
444	1. 21	3	8. 38	1. 201	16	8. 32	1. 2036	4	8. 339
711	----	---	----	1. 155	8	8. 25	1. 1676	<1	8. 338
642	1. 11	3	8. 31	1. 114	16	8. 34	1. 1145	4	8. 340
731	1. 09	13	8. 37	1. 087	25	8. 35	1. 0857	14	8. 339
800	1. 04	4	8. 32	1. 044	35	8. 35	1. 0424	5	8. 339
822	0. 982	1	8. 33	-----	---	----	0. 9827	1	8. 338
751	. 962	5	8. 33	-----	---	----	. 9630	9	8. 340
662	----	---	----	-----	---	----	. 9566	1	8. 339
840	----	---	----	-----	---	----	. 9324	7	8. 340
911	----	---	----	-----	---	----	. 9152	1	8. 338
Average value of last five lines			8. 33	-----	---	8. 33	--------	-----	8. 339

Lattice constants

		a
		A
1927	Holgersson [3]	8.431
1929	Passerini and Bruni [1]	8. 357
1934	Krause and Thiel [4]	8. 357
1948	Bulgakova et al. [5]	8. 33
1960	National Bureau of Standards	8.339 at 25° C

Structural data. Bragg [2] in 1915, determined the structure of the spinel group. Trevorite has the spinel-type structure, the space group Fd3m (No. 227), and 8($NiFe_2O_4$) per unit cell.

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

The density of trevorite, calculated from the NBS lattice constant is 5.368 g/cm³ at 25° C.

References

[1] L. Passerini and S. G. Bruni, Ricerche sugli spinelli, Ren. accad. naz. Lincei **9,** 338–343 (1929).

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

[3] S. Holgersson, Rontgenographische Untersuchung der Mineralien der Spinellgruppe, Acta Univ. Lundensis **23,** 22–112 (1927).

[4] O. Krause and W. Thiel, Ueber Keramische Farbkorper I, Ber. deut. keram. Ges. **15,** 101–110 (1934).

[5] T. I. Bulgakova et al., Issledovanie Reaktsii Obrazovaneya Ferritov Kovalta I Nikelya, Zhur. Obshchei Khim. **18,** 154–164 (1948).

Nickel Gallate, $NiGa_2O_4$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of nickel gallate was prepared at NBS by solid state reaction at 1,300° C between nickel oxide and gallium oxide. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, iron, magnesium, molybdenum, lead, and silicon.

The color of the sample was light blue. The index of refraction was too high to be measured by the oil immersion method. It was estimated at 2.005.

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	311	440	220

Structural data. The structure of nickel gallate has not been published. It has spinel-type structure, the space group Fd3m (No. 227), and 8($NiGa_2O_4$) per unit cell.

Lattice constants

		a
		A
1960	National Bureau of Standards.	8.262 at 25° C

The density of nickel gallate calculated from the NBS lattice constant is 6.173 g/cm³ at 25° C.

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C		
	d	*I*	*a*
	A		*A*
111	4. 771	8	8. 264
220	2. 923	37	8. 267
311	2. 491	100	8. 262
222	2. 386	12	8. 265
400	2. 0651	20	8. 260
422	1. 6862	16	8. 261
511	1. 5898	31	8. 261
440	1. 4605	47	8. 262
620	1. 3060	5	8. 260
533	1. 2601	12	8. 263
622	1. 2455	5	8. 262
444	1. 1926	3	2. 863
642	1. 1041	5	8. 262
731	1. 0757	16	8. 263
800	1. 0328	5	8. 262
822	0. 9737	2	8. 262
751	. 9540	9	8. 262
662	. 9477	2	8. 262
840	. 9236	2	8. 261
664	. 8808	1	8. 263
931	. 8661	7	8. 262
844	. 8432	14	8. 262
10·2·0	. 8102	4	8. 262
951	. 7987	9	8. 262
10·2·2	. 7950	1	8. 262
Average value of last five lines			8. 262

Potassium Chlororuthenate(IV), K_2RuCl_6 (cubic)

ASTM cards. None.

Additional published patterns

Source	Radiation
Adams and Mellor [1] 1952	Cobalt

NBS sample. The sample of potassium chlororuthenate was prepared at NBS by R. B. Johannesen using the Charonnant method [2]. Chemical analysis showed:

hkl	1952 Adams and Mellor Co, 1.7889 A			1960 National Bureau of Standards Cu, 1.5405 A at 26° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
111	5.69	vs	9.85	5.65	100	9.79
200	4.86	m+	9.72	4.89	41	9.79
220	3.44	s	9.72	3.46	42	9.79
311	2.93	m+	9.71	2.951	51	9.79
222	2.83	s	9.81	2.826	57	9.79
400	2.43	vs	9.73	2.447	71	9.788
331	2.23	w	9.72	2.244	17	9.778
420	2.17	w+	9.72	2.188	26	9.785
422	1.98	w+	9.72	1.996	19	9.778
511	1.87	m	9.73	1.883	27	9.784
440	1.72	s	9.73	1.730	48	9.786
531	1.65	m	9.74	1.654	24	9.785
600	1.62	w	9.72	1.631	16	9.786
620	1.54	w	9.74	1.547	8	9.784
533	1.49	vw	9.74	1.492	9	9.784
622	1.47	w	9.73	1.475	11	9.784
444	1.41	m	9.74	1.412	20	9.783
711	1.36	m	9.75	1.370	14	9.784
640	1.352	vw	9.75	1.357	9	9.785
642	1.303	w	9.75	1.307	9	9.781
731	1.269	w+	9.75	1.273	11	9.778
800	1.219	w	9.75	1.223	7	9.784
820	1.182	w	9.75	1.186	6	9.780
822	1.149	w	9.75	1.153	4	9.784
751	1.126	w	9.75	1.130	5	9.786
------	1.119	vw	------	------	----	------
840	1.091	m	9.76	1.094	14	9.785
911	1.071	w	9.76	1.074	6	9.785
842	1.065	vw	9.76	1.067	6	9.779
664	------	----	------	1.043	5	9.784
931	------	----	------	1.026	4	9.787
844	------	----	------	0.9986	6	9.784
933	------	----	------	.9830	4	9.781
10·0·0	------	----	------	.9780	4	9.780
10·2·0	------	----	------	.9593	4	9.783
951	------	----	------	.9458	5	9.783
953	------	----	------	.9121	5	9.781
10·4·0	------	----	------	.9082	3	9.782
10·4·2	------	----	------	.8930	2	9.782
11·1·1	------	----	------	.8819	1	9.781
880	------	----	------	.8646	5	9.782
11·3·1	------	----	------	.8546	5	9.781
10·4·4	------	----	------	.8513	3	9.781
Average value of last five lines		----	9.76	------	----	9.781

	Observed (average) %	Theoretical %
Ru	25. 804	25. 901
Cl_2	54. 21	54. 18

The sample is a black opaque powder.

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

Pattern	1	2	3
Adams and Mellor	111	400	220
National Bureau of Standards	111	400	222

Structural data. Adams and Mellor [1] in 1952 determined that potassium chlororuthenate is isomorphous with potassium chloroplatinate (IV), and has the space group Fm3m (No. 225) and $4(K_2RuCl_6)$ per unit cell.

Lattice constants

		A
1952	Adams and Mellor	9.738
1960	National Bureau of Standards	9.781 at 26° C

The density of potassium chlororuthenate calculated from the NBS lattice constant is 2.782 g/cm³ at 26° C.

References

[1] C. S. Adams and D. P. Mellor, The crystal structure of potassium hexachlororuthenate (IV), Australian J. Sci. Research **5,** 577–578 (1952).

[2] R. Charonnat, Recherches sur les Combinaisons Complexes du Ruthénium, Ann. chim. **16,** 5–121 (1931).

Potassium Hydroxy-Chlororuthenate, $K_4Ru_2Cl_{10}O \cdot H_2O$ (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium hydroxy-chlororuthenate was prepared at NBS by R. B. Johannesen. Potassium chloride solution was added to a hot solution of chlororuthenic acid, H_2RuCl_6, saturated with hydrochloric acid and chlorine. The salt obtained also contained some potassium hexachlororuthenate. Spectrographic analysis showed the following impurities: 0.1 to 0.01 percent each of barium, nickel, and zirconium; and 0.01 to 0.001 percent each of aluminum, cesium, sodium, and silicon.

The sample had a dark brown color. It is optically positive with the index of refraction $N_o = 1.820$; N_e could not be determined because the sample showed high absorption in that direction.

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.	101	220	204

Structural data. Mathieson, Mellor, and Stephenson [1] in 1952 determined that potassium hydroxy-chlororuthenate has the space group I4/mmm (No. 139) and $2(K_4Ru_2Cl_{10}O \cdot H_2O)$ per unit cell.

The density of potassium hydroxy-chlororuthenate calculated from the NBS lattice constants is 1.510 g/cm³ at 25° C.

Lattice constants

		a	*c*
		A	A
1952	Mathieson, Mellor, and Stephenson.	7. 10	16. 95
1960	National Bureau of Standards.	7. 1098	17. 073 at 25° C

References

[1] A. McL. Mathieson, D. P. Mellor, and N. C. Stephenson, The structure of potassium hydroxy-chlororuthenate, $K_4Ru_2Cl_{10}O \cdot H_2O$, Acta Cryst **5,** 185–186 (1952).

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C.	
	d	*I*
	A	
002	8. 51	7
101	6. 568	100
110	5. 023	16
103	4. 444	17
004	4. 271	25
200	3. 554	13
114	3. 253	47
211	3. 125	31
105	3. 077	27
006	2. 845	16

hkl	1960 National Bureau of Standards Cu, 1.5405 A at 25° C.	
	d	*I*
	A	
213	2. 778	8
204	2. 732	49
220	2. 514	69
116	2. 476	16
301	2. 351	5
215	2. 326	12
224	2. 167	9
008	2. 134	19
314	1. 990	1
321	1. 960	13
226	1. 884	11
323	1. 864	5
109, 208	1. 833	10
400	1. 778	18
316	1. 764	7
411	1. 716	8
325	1. 708	11
307, 403	1. 698	3
330, 209	1. 671	<1
413	1. 649	3
219, 228	1. 628	18
1·1·10	1. 616	2
334	1. 561	3
415	1. 540	2
406	1. 508	3
424	1. 490	3
309	1. 481	<1
336	1. 444	1
501	1. 417	5
2·2·10	1. 412	3
417	1. 409	3
510	1. 3946	<1
408	1. 3663	11
3·1·10	1. 3593	2
514	1. 3256	3
2·0·12	1. 3209	4
505	1. 3127	3
419	1. 2763	2
506	1. 2725	1
440	1. 2567	2
516	1. 2526	2
4·0·10	1. 2312	2
530	1. 2194	2
600	1. 1848	1
534	1. 1725	<1
611	1. 1663	<1
4·1·11	1. 1534	<1
446	1. 1496	1
509	1. 1376	2
620	1. 1237	4
541	1. 1078	1
2·2·14	1. 0970	4
543	1. 0905	<1
448	1. 0831	1
5·1·10	1. 0803	<1
2·1·15	1. 0716	2
4·2·12	1. 0599	1
631	1. 0572	1

Silicon Dioxide (low or α-cristobalite), SiO_2 (tetragonal)

ASTM cards. The following pattern is essentially the same pattern shown on ASTM card 4–0379 prepared in 1953 by National Bureau of Standards [1]. Eight new weak lines brought out by slower scanning have been included in the front portion of the pattern. The pattern has been extended to include the full range of 2θ to 160°.

Additional published patterns

Source	Radiation
Tokuda [2] 1957	Copper

NBS sample. The sample of cristobalite was prepared at NBS by S. Zerfoss at 1,700° C from silica gel. Spectrographic analysis shows the following impurities: 0.01 to 0.1 percent each of aluminum and copper; 0.001 to 0.01 percent each of iron and titanium; and 0.0001 to 0.001 percent each of silver, magnesium, and tin.

The sample was colorless. The indices of refraction were $N_e = 1.484$ and $N_o = 1.486$.

Interplanar spacings and intensity measurements. The 3.53 A spacing does not fit the calculated value as closely as it should. This was true of measurements from two patterns. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
National Bureau of Standards	101	200	102
Tokuda	101	102	200
National Bureau of Standards	101	200	102

Silicon Dioxide (low or α-cristobalite), SiO_2 (tetragonal)

hkl	1953 Swanson and Tatge Cu, 1.5405 A		1957 Tokuda Cu, 1.5405 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
101	4. 04	100	4. 04	100	4. 05	100
110	-------	------	3. 515	2	3. 53 [a]	3
111	3. 138	12	3. 134	25	3. 135	11
102	2. 845	14	2. 843	30	2. 841	12
200	2. 489	18	2. 485	30	2. 485	19
112	2. 468	6	2. 466	9	2. 465	5
201	2. 342	<1	2. 340	1	2. 340	1
-------	------	----	2. 2	0. 2	------	----
211	2. 121	4	2. 118	7	2. 118	4
202	2. 024	3	2. 020	6	2. 019	3
113	1. 932	4	1. 930	10	1. 929	5
212	1. 874	4	1. 872	13	1. 870	6
220	1. 756	1	1. 758	1	1. 757	<1
004	1. 736	1	1. 730	1. 5	1. 730	1
203	1. 692	3	1. 691	6	1. 690	3
104	1. 642	1	1. 634	1	1. 634	1
301	1. 612	5	1. 613	10	1. 612	4
213	1. 604	2	1. 603	3	1. 600	2
310	1. 574	1	1. 570	1	1. 571	<1
222	------	----	--------	----	1. 567	<1
311	1. 535	2	1. 534	5	1. 533	3
302	1. 495	3	1. 495	6	1. 494	4
312	1. 432	2	1. 432	5	1. 431	3
204	1. 423	1	1. 421	2	1. 419	2
223	1. 401	1	1. 398	2	1. 398	2
320	------	----	--------	----	1. 379	<1
214	1. 368	1	1. 365	4	1. 365	2
321	1. 353	1	1. 352	2	1. 352	2
303	1. 345	1	1. 346	1	1. 346	<1
105	1. 336	1	1. 333	3	1. 333	3
313	1. 301	2	1. 299	4	1. 299	3
322	1. 282	2	1. 281	5	1. 281	3
400	------	----	--------	----	1. 242	<1
224	1. 235	<1	1. 2341	1	1. 233	1
401	1. 224	<1	1. 2243	2	1. 223	2
205	------	----	--------	----	1. 210	2
410	1. 207	1	1. 2064	3	1. 206	2
411	------	----	--------	----	1. 188	1
323	1. 1842	2	1. 1846	3	1. 183	1
215	1. 1762	1	1. 1759	3	1. 175	2
330	------	----	--------	----	1. 172	1
314	1. 1659	1	1. 1643	1	1. 163	<1
331	1. 1556	<1	1. 1565	0. 8	1. 155	<1
412	------	----	--------	----	1. 138	<1
332	1. 1112	1	1. 1107	1. 0	1. 110	<1
421	1. 0989	3	1. 0968	4. 0	1. 097	3
116	------	----	--------	----	1. 095	3
225	------	----	1. 0883	0. 2	1. 086	<1
324	------	----	1. 0793	0. 4	1. 0776	<1
413	------	----	1. 0699	0. 2	1. 0687	<1
422	------	----	1. 0591	0. 9	1. 0582	<1
333	------	----	1. 0455	0. 4	1. 0445	<1
315	------	----	1. 0396	0. 5	1. 0384	<1
--------	------	----	1. 0101	0. 2	------	----
423	------	----	1. 0021	0. 7	1. 0015	<1

hkl	1953 Swanson and Tatge Cu, 1.5405 A		1957 Tokuda Cu, 1.5405 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
430	------	----	0. 99493	0. 8	0. 9941	<1
414	------	----	. 98986	2. 0	. 9890	1
501	------	----	. 98503	0. 8	. 9841	<1
--------	------	----	. 97745	0. 3	------	----
334, 107	------	----	. 97069	0. 9	. 9696	<1
511	------	----	. 96636	0. 8	. 9654	<1
502	------	----	. 95622	1. 2	. 9555	<1
--------	------	----	. 95268	0. 1	------	----
306	------	----	. 94736	0. 4	. 9467	<1
424	------	----	. 93603	0. 2	. 9350	<1
316	------	----	. 93067	0. 5	. 9298	<1
405	------	----	. 92561	0. 3	. 9244	<1
207	------	----	. 91920	0. 3	. 9185	<1
503	------	----	. 91363	1. 0	. 9129	<1
--------	------	----	. 90975	0. 4	------	----
217	------	----	. 90375	1. 0	. 9032	1
513	------	----	. 89860	0. 4	. 8979	<1
522	------	----	. 89239	0. 6	. 8919	<1
326	------	----	. 88520	0. 4	. 8845	<1
425	------	----	. 86719	0. 8	. 8664	<1
504	------	----	. 86226	1. 0	. 8618	<1
523	------	----	. 85778	0. 2	. 8569	<1
530	------	----	. 85281	0. 5	. 8524	<1
442	------	----	. 85210	0. 8	. 8518	<1
531	------	----	. 84660	0. 2	. 8463	<1
317	------	----	. 83726	0. 4	. 8366	<1
--------	------	----	. 82885	0. 04	------	----
601	------	----	. 82297	1. 0	. 8226	<1
610	------	----	. 81757	1. 0	. 8172	<1
505	------	----	. 80778	0. 3	. 8072	<1
602, 218	------	----	. 80642	1. 5	. 8060	1
426	------	----	. 80061	0. 7	. 8002	<1
--------	------	----	. 79863	0. 3	------	----
515	------	----	. 79732	2. 0	. 7969	2
621	------	----	. 78123	1. 0	. 7809	2
--------	------	----	. 78005	0. 2	------	----

• Calculated value=3.5149.

Structural data. Nieuwenkamp [3] in 1935 determined that cristobalite has a tetragonal structure, the space group $P4_12$ (No. 92) or $P4_32$ (No. 96), and $4(SiO_2)$ per unit cell.

Lattice constants

		a	*c*
		A	*A*
1953	National Bureau of Standards [1].	4. 973	6. 95
1957	Tokuda [2]----------	4. 9733	6. 9262
1960	National Bureau of Standards.	4. 971	6. 918 at 25° C

The density of cristobalite calculated from the NBS lattice constants is 2.334 g/cm³ at 25° C.

References

[1] H. E. Swanson and E. Tatge, Standard X-ray diffraction patterns, NBS Circ. 539 **1,** 39–41 (1953).

[2] T. Tokuda, X-ray spacings of synthetic cristobalites especially in back reflection region, J. Chem. Soc. Japan **79** No. 9, 1063–1067 (1957).

[3] W. Nieuwenkamp, The crystal structure of low cristobalite, Z. Krist. **A 92,** 82 (1935).

Silver Sulfide (argentite), Ag_2S (monoclinic)

ASTM cards. The name argentite is well established for this most common ore mineral of silver. A cubic phase, shown to exist above approximately 180° C, has occasionally in cooling contributed cubic faces to monoclinic Ag_2S and has been responsible for the mineral being considered as isometric.

Even though the mineral is now described as

hkl	1949 Graham Cu, 1.5418 A		1958 Djurle Cu, 1.5418 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
--------	------	----	4.09	vw	------	----
$\bar{1}01$	------	----	3.96	w	3.96	10
$1\bar{1}0$	------	----	3.57	vw	3.571	5
$\bar{1}11$	3.45	10	3.419	m	3.437	33
012	3.38	5	3.383	w	3.383	21
111	3.09	30	3.079	m	3.080	57
$\bar{1}12$	2.85	40	2.838	m	2.836	74
$1\bar{2}0$	2.67	20	2.662	m	2.664	47
$\bar{1}21$	2.60	100	2.606	s	2.606	100
022	------	----	2.585	m	2.583	68
112	2.45	80	2.455	w	2.456	72
121	------	----	2.438	m	2.440	82
013	------	----	2.421	w	2.421	57
$\bar{1}03$	2.38	50	2.382	m	2.383	76
031	2.22	30	2.213	w	2.213	47
122	2.09	40	2.094	vw	2.093	15
200	------	----	2.083	m	2.083	47
023	------	----	2.070	vw	2.072	16
$1\bar{0}3$	2.04	5	2.047	w	2.047	16
$\bar{1}31$	2.00	5	1.994	w	1.995	15
$\bar{1}23$	1.961	10	1.963	w	1.963	20
201	------	----	--------	----	1.935	3
$1\bar{3}1$	1.910	10	1.915	vw	1.918	3
$\bar{2}12$	------	----	1.902	w	1.9027	14
014	1.870	10	1.865	w	1.8663	16
$\bar{1}14$	------	----	--------	----	1.8158	4
$\bar{2}21$	------	----	--------	----	1.7980	4
040	------	----	1.731	vw	1.7326	11
$\bar{2}13$	1.719	30	1.717	w	1.7178	21
041	1.689	5	1.689	vw	1.6908	6
114	------	----	--------	----	1.6096	3
$\bar{1}41$	1.580	20	1.586	vw	1.5873	13
$\bar{2}23$	------	----	--------	----	1.5788	9
$\bar{2}04$	1.556	5	1.554	vw	1.5541	8
$\bar{1}05$	1.542	10	1.539	vw	1.5398	7
015	1.512	10	1.513	vw	1.5127	11
034	1.484	5	1.482	vw	1.4832	10
$2\bar{1}3$	1.475	5	1.469	vw	1.4704	9
$\bar{1}34$	1.455	20	1.458	vw	1.4590	14
--------	------	----	1.445	vw	------	----
223, 232 105	1.412	5	--------	----	1.3789	6
$\bar{3}12$	------	----	1.356	vw	1.3561	6
134	------	----	1.344	vw	1.3452	7
240	1.336	10	1.3311	vw	1.3329	10
$\bar{3}03$	------	----	1.3182	vw	1.3193	7
052	------	----	1.3050	vw	1.3048	7

		a	b	c	β
		A	A	A	
1943	Ramsdell [2]	4. 21	6. 93	7. 86	99.32°
1958	Djurle [1]	4. 227	6. 925	7. 862	99.55°
1958	Frueh [3]	4. 23	6. 91	7. 87	99.58°
1960	National Bureau of Standards	4. 229	6. 931	7. 862	99.61° at 25° C

monoclinic from X-ray analysis, it will continue to be known as argentite. The term acanthite is not needed for either phase since above 180° C Ag_2S would be high-temperature, or cubic argentite.

Card number	Index lines	Radiation	Source
9–422	2. 60 2. 45 2. 38	Copper	A. R. Graham, Univ. of Toronto, Ontario, Canada (1949).

Additional published patterns

Source	Radiation
Djurle [1] 1958	Copper

NBS sample. The sample of argentite was precipitated from the reaction of $AgNO_3$ and H_2S. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent of silicon and 0.0001 to 0.001 percent of copper.

The sample was a black opaque powder.

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

Pattern	1	2	3
Graham	$\bar{1}21$	112	$\bar{1}03$
Djurle	$\bar{1}21$	$\bar{1}11$	111
National Bureau of Standards	$\bar{1}21$	121	$\bar{1}03$

Structural data. Ramsdell [2] in 1943 determined that argentite is monoclinic, has the space group $P2_1/n$ (No. 14), and $8(Ag_2S)$ per unit cell. Frueh [3] in 1958 described a primitive orientation with $4(Ag_2S)$ per unit cell. The unit cell measurements of Ramsdell and Djurle have been converted to this primitive orientation and Ramsdell's values have been converted from kX to angstrom units for comparison with the NBS values.

The density of argentite calculated from the NBS lattice constants is 7.243 g/cm^3 at 25° C.

References

[1] S. Djurle, The system Ag_2S-Cu_2S, Acta Chem. Scand. **12,** 1427 (1958).
[2] L. S. Ramsdell, The crystallography of acanthite, Ag_2S, Am. Min. **28,** 401–425 (1943).
[3] A. J. Frueh Jr., The crystallography of silver sulfide, Ag_2S, Z. Krist. **110,** 136 (1958).

Alpha-Sodium Tetrametaphosphate Tetrahydrate, α-$Na_4P_4O_{12}\cdot 4H_2O$ (monoclinic)

ASTM cards. None.

Additional published patterns

Source	Radiation
Bell, Audrieth and Hill [1] Thilo and Rätz [2]	Copper

NBS sample. The sample of sodium tetrametaphosphate tetrahydrate was prepared by Helen Ondik of NBS by hydrolytic cleavage of the α form of phosphorus (V) oxide below 15° C and neutralized by sodium hydroxide. The sample was purified by salting out with sodium chloride and repeated recrystallizations with water and ethanol. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of barium, calcium, silicon, and strontium.

The sample was colorless. The indices of refraction are N_α=1.440, N_β=1.458, and N_γ=1.476.

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

Alpha-Sodium Tetrametaphosphate Tetrahydrate, α-$Na_4P_4O_{12}.4H_2O$ (monoclinic)

hkl	1949 Thilo and Rätz Cu, 1.5405 A		1952 Bell, Audrieth and Hill ----------		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
011	------	----	7. 73	s	7. 63	76
020, 100	------	----	6. 22	s	6. 17	92
021	------	----	------	----	5. 21	5
$11\bar{1}$, 002	------	----	4. 79	s	4. 844	63
111	------	----	------	----	4. 718	60
012	------	----	------	----	4. 509	3
120	4. 33	s	4. 32	w	4. 369	17
121	------	----	------	----	3. 933	20
031	3. 85	s	3. 83	vs	3. 790	97
102	------	----	------	----	3. 728	25
112	------	----	------	----	3. 571	8
130	------	----	------	----	3. 424	10
$12\bar{2}$	3. 24	d	3. 27	vvs	3. 295	100
$13\bar{1}$					3. 254	69
122	------	----	3. 17	w	3. 194	22
032	------	----	------	----	3. 133	19
013	------	----	------	----	3. 122	19
040, 200	3. 08	vvs	3. 09	w	3. 089	25
041	------	----	------	----	2. 938	9
211, $11\bar{3}$	2. 81	s	2. 81	vs	2. 827	69
140, 220	------	----	2. 74	w	2. 760	19
113					2. 739	20
$22\bar{1}$	------	----	------	----	2. 685	18
$14\bar{1}$	------	----	2. 67	w	2. 669	7
141	2. 62	vs	2. 62	vw	2. 638	14
221					2. 633	15
042	------	----	------	----	2. 602	7
123, 202	------	----	------	----	2. 554	14
033	2. 47	s	2. 54	s	2. 539	36
$14\bar{2}$, 004	------	----	2. 42	w	2. 417	18
051,	2. 38	vw	2. 38	vw	2. 392	8
231, $13\bar{3}$					2. 375	8
222	------	----	------	----	2 360	5
150	------	----	------	----	2. 293	5
024	------	----	2. 26	s	2. 253	40
$11\bar{4}$	------	----	------	----	2. 247	23
151, 104	2. 21	s	2. 19	w	2. 222	16
052					2. 199	11
114, 240	------	----	------	----	2. 186	16
232	------	----	------	----	2. 170	5
213	------	----	------	----	2. 148	5
$24\bar{1}$	------	----	------	----	2. 145	3
241	------	----	------	----	2. 120	4
$14\bar{3}$	------	----	------	----	2. 115	5
124	2. 10	vw	2. 09	vw	2. 087	4
$15\bar{2}$, 034						
152, 060	------	----	------	----	2. 060	2
310	------	----	------	----	2. 021	6
061	------	----	2. 01	w	2. 015	8

hkl	1949 Thilo and Rätz Cu, 1.5405 A		1952 Bell, Audrieth and Hill ----------		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
$31\bar{1}$	------	----	------	----	2.001	6
$13\bar{4}$	------	----	------	----	1.996	1
311, 242	------	----	1.96	w	1.968	8
053					1.961	10
134, 160	------	----	------	----	1.955	8
320	------	----	------	----	1.949	8
233, 250	------	----	------	----	1.928	10
$32\bar{1}$	------	----	------	----	1.924	7
$21\bar{4}$	------	----	1.91	w	1.913	6
015, 161	------	----	------	----	1.906	10
044	------	----	------	----	1.903	14
$31\bar{2}$	------	----	------	----	1.895	9
062	------	----	------	----	1.890	6
153	1.86	d	1.85	m	1.854	18
$22\bar{4}$					1.850	18
025, $11\bar{5}$	------	----	------	----	1.842	9
330	------	----	1.83	m	1.837	9
$33\bar{1}$	------	----	------	----	1.823	10
322, $12\bar{5}$	------	----	1.79	vw	1.7855	8
252	1.76	vvw	1.76	w	1.7762	8
$23\bar{4}$	------	----	------	----	1.7543	6
034, 125	------	----	------	----	1.7499	5
$31\bar{3}$	------	----	------	----	1.7458	6
063	------	----	------	----	1.7348	5
260, 340	------	----	------	----	1.7122	3
332	------	----	------	----	1.6989	6
261	1.68	s	1.68	m	1.6805	12
341	(a)		(b)		1.6760	16

[a] Thirteen additional lines are omitted.
[b] Twenty-six additional lines are omitted.

Pattern	1	2	3
Bell, Audrieth, and Hill	$12\bar{2}$, $13\bar{1}$	031	211, $11\bar{3}$
Thilo and Rätz	040, 200	141, 221	120
National Bureau of Standards	$12\bar{2}$	031	020, 100

Structural data. Ondik, MacGillavry, and Block [3] in 1959 determined the structure of the low temperature form of sodium tetrametaphosphate tetrahydrate which has the space group $P2_1/c$ (No. 14) with $2(Na_4P_4O_{12} \cdot 4H_2O)$ per unit cell. A high temperature form of sodium tetrametaphosphate tetrahydrate is also reported in the literature by Thilo and Rätz [2] and by Bonneman [4].

The following unit-cell measurements are compared with the NBS values.

The density of sodium tetrametaphosphate tetrahydrate calculated from the NBS lattice constants is 2.163 g/cm^3 at 25° C.

		a	b	c	β
		A	A	A	
1949	Andress, Gehring, and Fischer [5]	6. 17	12. 33	9. 61	92°35′
1955	Barney and Gryder [6]	6. 16	12. 32	9. 65	92°30′
1960	National Bureau of Standards	6. 170	12. 358	9. 667	92°16′ at 25° C

References

[1] R. N. Bell, L. F. Audrieth, and O. F. Hill, Preparation of sodium tetrametaphosphate, Ind. Eng. Chem. **44,** No. 3, 568–572 (1952).

[2] E. Thilo and R. Rätz, Über die Kinstituten des Natriumtetraphosphates und Eigenschaften der Tetraphosphate, Z. anorg. u. allgem. Chem. **260,** 255–266 (1949).

[3] H. M. Ondik, C. H. MacGillavry, and S. Block, The structure of the monoclinic form of sodium tetrametaphosphate tetrahydrate. To be published in Acta Cryst.

[4] P. Bonneman, Sur les tétramétaphosphates, Compt. rend. **204,** 865 (1937).

[5] K. R. Andress, W. Gehring, and K. Fischer, Das Naturiumtetrametaphosphat $Na_4[(PO_3)_4]\cdot 4H_2O$, Z. anorg. u. allgem. Chem. **260,** 331–336 (1949).

[6] D. L. Barney and J. W. Gryder, Ion-exchange purification of sodium tetrametaphosphate, J. Am. Chem. Soc. **77,** 3195–3198 (1955).

Tellurium(IV) Oxide, paratellurite, TeO_2 (tetragonal)

ASTM cards. Synthetic TeO_2 (tetragonal) is given on card 8–484 [1]. A second pattern is presented because it has now been found as a mineral.

NBS sample. The form commonly found in nature is the orthorhombic mineral tellurite. Since all our attempts to produce the orthorhombic form in the laboratory have yielded only the tetragonal TeO_2, it is strange that a tetragonal mineral has not been noted previously.

We were surprised to see the tetragonal TeO_2 occurring with tellurite on a sample which we

hkl	1957 Synthetic National Bureau of Standards Cu, 1.5405 at 25° C		1960 N.M. #C5995 Cananea, Mexico NBS Cu, 1.5405 at 25° C	
	d	*I*	*d*	*I*
	A		A	
101	4. 07	9	4. 068	12*
110	3. 40	88	3. 404	86
111	3. 10	13	3. 107	13
102	2. 98	100	2. 988	100
112	2. 536	1	2. 536	1
200	2. 407	20	2. 407	20
201	2. 293	2	2. 296	3
210	2. 151	2	2. 151	3
211	2. 071	6	2. 071	5
113, 202	2. 034	1	2. 033	1
004	1. 903	8	1. 904	10
212	1. 872	65	1. 873	55
203	1. 745	<1	1. 746	2
220	1. 700	12	1. 701	12
114, 221	1. 660	22	1. 661	22
213	1. 6401	4	1. 641	4
301	1. 5684	3	1. 569	2
310	1. 5210	12	1. 5212	9
204	1. 4923	15	1. 4925	12
302	1. 4775	9	1. 4777	8
223, 312	1. 4127	2	1. 4129	2
303	1. 3554	1	1. 3554	<1
321	1. 3139	2	1. 3142	2
313	1. 3048	<1	1. 3048	2
224	1. 2681	4	1. 2682	5
322	1. 2590	4	1. 2590	7
215	1. 2433	1	1. 2431	2
106, 304	1. 2270	5	1. 2269	5
400	1. 2020	<1	1. 2026	2
116, 314	1. 1881	6	1. 1882	6
323	1. 1806	<1	1. 1812	4
411	1. 1531	<1	1. 1530	3
225	1. 1341	<1	1. 1339	<1
331	1. 1212	<1	1. 1214	1
412	1. 1158	2	1. 1159	2
216, 324	1. 0928	4	1. 0929	3
403, 332	1. 0866	<1	1. 0867	1
315, 240	1. 0753	<1	1. 0760	<1
421	1. 0647	<1	1. 0646	<1
107, 413	1. 0601	<1	1. 0599	<1
226, 404	1. 0164	1	1. 0167	2

*Intensity values for the synthetic material are probably more reliable because a larger sample was available.

obtained from George Switzer at the National Museum. Both oxides were found together as fine crystals on a large piece of native tellurium. It was possible to separate the two types of crystals and run diffraction patterns of each. The tellurium ores (U.S.N.M. #R8861 and #C5995) are from Cananea, Sonora, Mexico.

The tetragonal TeO_2 is being reported in the Am. Mineralogist as a new mineral with the name paratellurite.

Spectrographic analysis made at the Geological Survey showed the following impurities: 0.06 percent iron; 0.05 percent calcium; 0.04 percent each of tin and magnesium; 0.02 percent manganese; 0.01 percent each of zirconium and barium; and 0.004 percent lead. The limit of detection of selenium was 10 percent, but an effort is being made to determine selenium by another method.

The color of the crystals was greyish to colorless.

The indices of refraction were 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 each pattern are as follows:

Pattern	1	2	3
National Bureau of Standards (synthetic)	102	110	212
National Bureau of Standards (natural)	102	110	212

Structural data. Stehlik and Balak [2] in 1948 determined that tetragonal TeO_2 has either the space group $P4_12_12$ (No. 92) or $P4_32_12$ (No. 96), and $4(TeO_2)$ per unit cell.

Lattice constants

		a	*c*
		A	*A*
1957	National Bureau of Standards synthetic (paratellurite)	4. 809	7. 614
1960	National Bureau of Standards, paratellurite	4. 810	7.613 at 25° C.

The density of paratellurite calculated from the NBS lattice constants is 6.017 g/cm³ at 25° C.

References

[1] Standard X-ray diffraction patterns, NBS Circ. 539 **7,** 56 (1957).

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

Zinc Germanate, Zn_2GeO_4 (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
3–0689	2. 89 2. 69 1. 87	Copper	Schütz [1] 1936.

Additional published patterns. None.

NBS sample. The sample of zinc germanate was prepared at the NBS by reaction of zinc oxide and germanium oxide, in a sealed platinum tube at 1,200° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, cobalt, and silicon; 0.001 to 0.01 percent each of calcium, chromium, copper, iron, magnesium, manganese, and nickel.

The sample was 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 Schütz were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Schütz	113	410	333
National Bureau of Standards	410	113	220

Structural data. Goldschmidt [2] in 1931 determined that zinc germanate is isomorphous with willemite (Zn_2SiO_4), has the space group $R\bar{3}$ (No. 148), and $18(Zn_2GeO_4)$ per unit hexagonal cell, or $6(Zn_2GeO_4)$ per unit rhombohedral cell. The unit-cell measurements of Goldschmidt have been converted to the hexagonal form for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1931	Goldschmidt [2]	14. 11	9.49
1936	Schütz [1]	14. 19	9.46
1960	National Bureau of Standards.	14. 231	9.530 at 25° C

Zinc Germanate, Zn_2GeO_4 (trigonal)

hkl (hex.)	1936 Schütz Cu, 1.5418 A		1960 National Bureau of Standards Cu, 1.5405 A at 25° C	
	d	*I*	*d*	*I*
	A		A	
110	----	-----	7. 12	22
012	----	-----	4. 440	<1
211	----	-----	4. 181	2
300	4. 10	60	4. 111	36
220	3. 55	80	3. 559	72
113	2. 88	100	2. 900	89
410	2. 68	100	2. 689	100
223	2. 37	80	2. 369	66
600	2. 05	40	2. 0540	12
520	1. 97	40	1. 9737	11
333	1. 88	100	1. 9008	49
603	1. 73	40	1. 7244	10
523	1. 66	40	1. 6763	15
710	1. 63	60	1. 6326	16
006	1. 58	60	1. 5881	17
630	1. 55	60	1. 5530	15
306	1. 50	10	1. 4813	3
713	1. 44	100	1. 4519	44
550	1. 42	20	1. 4232	6
633	1. 38	80	1. 3954	23
416	1. 36	80	1. 3675	25
820	----	-----	1. 3446	2
336	----	-----	1. 3201	<1
553	----	-----	1. 2989	1
740	1. 28	20	1. 2783	2
606	1. 25	20	1. 2564	3
823, 526	1. 22	40	1. 2378	7
660, 018 743	1. 19	40	1. 1857	6
10·1·0, 208	1. 17	20	1. 1698	3
716	1. 14	40	1. 1382	6
636	1. 11	40	1. 1100	6
238, 10·1·3	----	-----	1. 0978	1
850	1. 08	10	1. 0849	1
508, 933	1. 07	20	1. 0723	1
556	----	-----	1. 0598	3
119, 844	1. 05	10	1. 0469	2
906	1. 03	60	1. 0370	6
12·0·0, 348 853	----	-----	1. 0268	6
11·2·0	1. 01	20	1. 0164	1
229	----	-----	1. 0147	3
746	1. 00	20	0. 9958	2
10·4·0, 078	0. 986	10	. 9869	2
268, 12·0·3	----	-----	. 9773	3
11·2·3	. 963	40	. 9682	2
339	----	-----	. 9668	3
960, 808 10·4·3	. 940	80	. 9423	5
529	----	-----	. 9328	1
936	----	-----	. 9260	<1
13·1·0, 648	----	-----	. 9112	2
378, 963	----	-----	. 9036	<1
12·3·0, 856	. 893	40	. 8962	2
719	. 887	20	. 8881	4
639	----	-----	. 8746	2
4·3·10	----	-----	. 8624	1
11·2·6	----	-----	. 8558	1
758, 11·5·3 10·4·6, 7·0·10	----	-----	. 8381	3
829, 794	----	-----	. 8317	1
5·4·10	----	-----	. 8162	2
749	----	-----	. 8154	2
966, 0·8·10	----	-----	. 8104	4
678, 10·7·3	----	-----	. 8056	2
0·0·12	----	-----	. 7939	1
990, 4·6·10	----	-----	. 7905	3

The density of zinc germanate calculated from the NBS lattice constants is 4.780 g/cm³ at 25° C.

References

[1] W. Schütz, Die Kristallchemische Verwandtschaft Zwischen Germanium und Silicium, Z. Physik. Chem. B **31,** 299 (1936).

[2] V. M. Goldschmidt, Zur Kristallchemie der Germanium, Nachr. Ges. Wiss. Gottingen Math-physik Kl **1931,** 184–190 (1931).

CUMULATIVE INDEX TO VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, AND 10 [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.

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