NBS MONOGRAPH 25—SECTION 2

Standard X-ray Diffraction Powder Patterns

U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

THE NATIONAL BUREAU OF STANDARDS

Functions and Activities

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

Publications

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

A complete listing of the Bureau's publications can be found in NBS Circular 460, Publications of the National Bureau of Standards, 1901 to June 1947 ($1.25), the Supplement to NBS Circular 460, July 1947 to June 1957 ($1.50), and Miscellaneous Publication 240, July 1957 to June 1960 (includes titles of papers published in outside journals 1950 to 1959) ($2.25); available from the Superintendent of Documents, Government Printing Office, Washington, D.C.

UNITED STATES DEPARTMENT OF COMMERCE • Luther H. Hodges, *Secretary*

NATIONAL BUREAU OF STANDARDS • A. V. Astin, *Director*

Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, M. C. Morris,
Roger P. Stinchfield, and Eloise H. Evans

National Bureau of Standards Monograph 25 — Section 2

Issued May 3, 1963

For sale by the Superintendent of Documents, U.S. Government Printing Office
Washington 25, D.C. - Price 35 cents

Library of Congress Catalog Card Number: 53–61386

Contents

*Not previously listed in the Powder Data File.

Standard X-ray Diffraction Powder Patterns

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

NBS Circular 539, Volume 1, Standard X-ray Diffraction Powder Patterns (Data for 54 inorganic substances) 45 cents
NBS Circular 539, Volume 2, Standard X-ray Diffraction Powder Patterns (Data for 30 inorganic substances) 45 cents
NBS Circular 539, Volume 3, Standard X-ray Diffraction Powder Patterns (Data for 34 inorganic substances) 45 cents
NBS Circular 539, Volume 4, Standard X-ray Diffraction Powder Patterns (Data for 42 inorganic substances) 45 cents
NBS Circular 539, Volume 5, Standard X-ray Diffraction Powder Patterns (Data for 45 inorganic substances) 45 cents
NBS Circular 539, Volume 6, Standard X-ray Diffraction Powder Patterns (Data for 44 inorganic substances) 40 cents
NBS Circular 539, Volume 7, Standard X-ray Diffraction Powder Patterns (Data for 53 substances) 40 cents
NBS Circular 539, Volume 8, Standard X-ray Diffraction Powder Patterns (Data for 61 substances)45 cents
NBS Circular 539, Volume 9, Standard X-ray Diffraction Powder Patterns (Data for 43 substances) 40 cents
NBS Circular 539, Volume 10, Standard X-ray Diffraction Powder Patterns (Data for 40 substances) 40 cents
NBS Monograph 25, Section 1, Standard X-ray Diffraction Powder Patterns (Data for 46 substances) 40 cents

Send orders with remittance to: Superintendent of Documents, U.S. Government Printing Office, Washington 25, D.C. Remittances from foreign countries should include an additional one-fourth of the purchase price for postage.

Errata

Circular 539
Vol. 8, Page 3, the *hkl* 314 should be 202.
Page 71, space group $R\bar{3}$ should be R3m (No. 160).
Vol. 10, Page 32, the *hkl* 186 should be deleted.
Page 51, the *hkl* 201 should be 004.
Page 52, space group $P2_1/n$ is correct as originally printed.

Monograph 25
Sec. 1, Page 17, the radiation indicated in the table heading should be Co not Cu.
Page 37, under *NBS sample,* chalcopurite should be chalcopyrite.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 2—Data for 37 Substances

Howard E. Swanson, Marlene Cook Morris, [1]

Roger P. Stinchfield, [1] **and Eloise H. Evans** [1]

Standard X-ray diffraction powder patterns are presented for the following thirty-seven substances: Al $(PO_3)_3$, SbF_3*, $Ba_3(AsO_4)_2$*, $Ba(ClO_4)_2 \cdot 3H_2O$, $Cd(CN)_2$*, $CdWO_4$, Cs_2OsBr_6*, Cs_2OsCl_6*, α-$CrPO_4$, $Co[Hg(CNS)_4]$*, β-$CoSO_4$, $Dy_3Ga_2(GaO_4)_3$*, $ErMnO_3$*, $Eu_3Ga_2(GaO_4)_3$*, $Gd_3Ga_2(GaO_4)_3$*, Li_3AsO_4*, $Li_3P_3O_9 \cdot 3H_2O$*, $Li_2WO_4 \cdot \frac{1}{2}H_2O$*, $Lu_3Ga_2(GaO_4)_3$*, $LuMnO_3$*, $MnWO_4$ (huebnerite), HgF_2*, $NiSO_4$, $NiWO_4$*, K_2ReCl_6, K_2RuCl_5NO*, $RbClO_4$*, $RbIO_4$*, Ag_2SeO_4*, NaCNO*, $Na_2WO_4 \cdot 2H_2O$, β-$Na_4P_4O_{12} \cdot 4H_2O$, $Sr_3(AsO_4)_2$*, Tl_3AsO_4*, $TlClO_4$*, $YAsO_4$, $ZnWO_4$*. Eleven are to replace patterns already given in the X-ray Powder Data File issued by the American Society for Testing and Materials, and twenty-six patterns indicated by asterisks are for substances not previously included. The X-ray Powder Data File is a compilation of diffraction patterns from many sources and is used for the identification of unknown crystalline materials by matching spacing and intensity measurements. The patterns were made with a Geiger counter X-ray diffractometer, using samples of high purity. When possible, the *d*-values were assigned Miller indices determined by comparison with calculated interplanar spacings and from space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible.

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 in this report for 37 compounds. This paper is the twelfth of a series of "Standard X-ray Diffraction Patterns." [3] The designation "Circular 539" used previously has been discontinued in favor of the new series, "Monograph 25." This is the second section of the new series Monograph 25. Included are patterns recommended to replace data on 11 cards now present in the file. The patterns for 26 compounds not included in the file have been added. These compounds are: antimony(III) fluoride, barium arsenate, cadmium cyanide, cesium bromoosmate(IV), cesium chloroosmate(IV), cobalt mercury thiocyanate, dysprosium gallium oxide 3:5, erbium manganite, europium gallium oxide 3:5, gadolinium gallium oxide 3:5, lithium arsenate, lithium trimetaphosphate trihydrate, lithium tungstate hemihydrate, lutetium gallium oxide 3:5, lutetium manganite, mercury(II) fluoride, nickel tungstate, potassium nitroso chlororhenate, rubidium perchlorate, rubidium periodate, silver selenate, sodium cyanate, strontium arsenate, thallium arsenate, thallium(II) perchlorate, and zinc tungstate.

The experimental procedure and general plan of these reports have not changed greatly from previous volumes of the NBS Circular (see ref. 3). However, the basic technique is discussed, in this section, with minor changes that affect this volume's data.

---

[1] Research Associate 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 and 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; Vol. 9, February 1960; Vol. 10, September 1960; and Monograph 25—Section 1, March 1962.

Powder Data cards. Each section of this Monograph contains a table listing the Powder Data File card numbers, the three strongest lines, the radiation used, and the literature references for each card. Cards listed through the 1961 index to the Powder Data File [1] [4] are included in the table.

Additional published patterns. Literature references for patterns that have not been published as Powder Data cards are listed.

NBS sample. Many of the samples used to make NBS patterns were special preparations of high purity obtained from a variety of sources or prepared in small quantities in our laboratory by J. de Groot. Unless otherwise noted, the spectrographic analyses were done at NBS after recrystallization or heat treatment of the sample. The limit of detection for the alkali elements was 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 usually provided by the X-ray pattern itself, when it was indexed by comparison with theoretical *d*-values. Treating the sample by appropriate annealing, recrystallization, or heating in hydrothermal bombs improved the quality of most of the patterns. The refractive index measurements were made by grain-immersion methods in white light using oils standardized in sodium light.

X-ray techniques. At least three patterns for intensity measurements were prepared to check reproducibility. Samples that gave satisfactory intensity patterns usually had an average particle-size smaller than 10μ, as discussed by Alexander, Klug, and Kummer [2]. A special cell with one open end was used for making intensity measurements. The sample was prepared by clamping a flat piece of glass temporarily over the surface of this holder, and while it was held in a vertical position, the sample was drifted in from the open end. The glass was then carefully removed so that the surface of the sample could be exposed to the X-ray beam. To powders 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 intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the intensity of the strongest line. Additional patterns were obtained for *d*-value measurements. Specimens for these patterns were prepared by packing into a shallow holder a sample containing approximately 5-wt percent tungsten powder that served as an internal standard. When tungsten lines were found to interfere, 25 percent silver was used in place of tungsten. The lattice constants used were 3.1648 A for tungsten and 4.0861 A for silver at 25 °C, as determined by Jette and Foote [3]. All of the NBS patterns, unless otherwise noted, are made at 25° C, using either filtered copper or cobalt radiation ($K_{\alpha 1}$), having the wavelengths 1.5405 A, and 1.7889 A, respectively.

Structural data. For cubic materials a value for the lattice constant was calculated for each *d*-value. However, 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 on the IBM 7090, using those *d*-values for which only one set of Miller indices could be assigned. The number of significant figures reported for *d*-values in the NBS pattern is limited by the quality of each sample as indicated by residuals obtained from least squares refinement.

Published unit cell data in kX units were converted to angstrom units as recommended in 1946 [4] using the factor 1.00202.

The space groups are listed with both the Schoenflies and short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography [5].

Orthorhombic cell dimensions are presented according to the Dana convention [6] $b>a>c$.

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 [7] in 1956 and the Avogadro number (6.0240×10^{23}) reported by Straumanis [8] in 1954.

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

References

[1] Index to the X-ray Powder Data File, American Society for Testing and Materials, Philadelphia, Pa. (1961).

[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] International Tables for X-ray Crystallography, **1,** 1952.

[6] Dana's System of Mineralogy, **1,** 6 (1944).

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

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

Aluminum Metaphosphate, $Al(PO_3)_3$ (cubic)

Powder Data cards

Card number	Index lines	Radiation	Source
2–0246	4. 38 3. 70 3. 41	Molyb-denum	Hendricks and Wyckoff [1] 1927.

Additional published patterns. None.

NBS sample. The sample of aluminum metaphosphate was made at NBS by adding fine γ-Al_2O_3 powder to hot HPO_3. The sample was then heated to fume off the excess acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of silicon and platinum; and 0.001 to 0.01 percent each of barium, iron, magnesium, nickel, lead, and antimony.

The sample is colorless. The index of refraction is 1.545.

The *d*-values of the three strongest lines are: 4.34, 3.43, and 3.67 A.

Structural data. Hendricks and Wyckoff [1] determined in 1927 that aluminum metaphosphate has the space group T_d^6—$I\bar{4}3d$ (No. 220) and 16[$Al(PO_3)_3$] per unit cell.

The lattice constant reported by Hendricks and Wyckoff has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1927	Hendricks and Wyckoff [1]----	13.66
1962	National Bureau of Standards-	13.729 at 25 °C

The density of aluminum metaphosphate calculated from the NBS lattice constant is 2.709 g/cm³ at 25 °C.

Reference

1] S. B. Hendricks and R. W. G. Wyckoff, The space group of aluminum metaphosphate, Am. J. Sci. **213** No. 13, 491–496 (1927).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		A
211	5. 61	25	13. 73
220	4. 85	17	13. 72
310	4. 34	100	13. 72
321	3. 67	57	13. 72
400	3. 432	62	13. 73
420	3. 070	30	13. 73
332	2. 927	46	13. 73
422	2. 801	5	13. 72
510	2. 692	28	13. 73
521	2. 507	13	13. 73
530	2. 354	22	13. 73
611	2. 227	17	13. 73
620	2. 171	11	13. 73
541	2. 118	5	13. 73
631	2. 024	2	13. 73
444	1. 981	9	13. 72
710	1. 941	7	13. 72
640	1. 903	6	13. 72
721	1. 869	18	13. 73
642	1. 835	2	13. 73
732	1. 743	13	13. 73
811	1. 6900	2	13. 73
820	1. 6648	14	13. 728
653	1. 6412	6	13. 730
822	1. 6179	12	13. 728
831	1. 5963	18	13. 732
752	1. 5549	2	13. 732
840	1. 5349	1	13. 729
842	1. 4986	11	13. 730
921	1. 4803	10	13. 728
930	1. 4473	11	13. 730
932	1. 4161	7	13. 730
844	1. 4013	3	13. 730
941	1. 3870	5	13. 731
10·0·0	1. 3730	1	13. 730
10·1·1	1. 3594	2	13. 729
10·2·0	1. 3462	5	13. 729
950	1. 3333	2	13. 727
10·3·1	1. 3092	7	13. 731
871	1. 2860	5	13. 731
10·4·0	1. 2748	2	13. 730
10·3·3	1. 2641	4	13. 732
10·4·2	1. 2532	1	13. 728
11·1·0	1. 2433	7	13. 733
11·2·1	1. 2231	8	13. 729
880	1. 2135	<1	13. 729
11·3·0	1. 2042	3	13. 730
11·3·2	1. 1862	6	13. 731
10·6·0	1. 1772	1	13. 728
11·4·1	1. 1688	3	13. 730

Aluminum Metaphosphate, $Al(PO_3)_3$ (cubic)—Continued

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		*A*
10· 6·2	1. 1605	5	13. 731
965	1. 1522	2	13. 730
12· 1·1	1. 1364	8	13. 731
12· 2·0	1. 1287	<1	13. 731
11· 5·2	1. 1212	2	13. 731
12· 2·2	1. 1137	2	13. 731
12· 3·1	1. 1064	1	13. 730
11· 6·1	1. 0924	1	13. 731
12· 4·2	1. 0722	1	13. 731
11· 6·3	1. 0657	1	13. 731
10· 8·2	1. 0594	2	13. 731
13· 1·0	1. 0529	<1	13. 729
13· 2·1	1. 0409	1	13. 730
12· 4·4	1. 0348	<1	13. 728
13· 3·0	1. 0291	<1	13. 730
13· 3·2	1. 0177	<1	13. 730
12· 6·2	1. 0121	1	13. 729
13· 4·1	1. 0067	6	13. 730
888	0. 9910	<1	13. 732
13· 5·0	. 9857	5	13. 729
14· 1·1	. 9759	1	13. 732
14· 2·0	. 9709	2	13. 731
12· 7·3	. 9661	1	13. 731
14· 3·1	. 9567	3	13. 731
12· 8·0	. 9521	<1	13. 731
13· 5·4	. 9475	3	13. 731
14· 3·3	. 9385	1	13. 729
14· 4·2	. 9343	1	13. 731
13· 7·0	. 9299	3	13. 730
14· 5·1	. 9215	3	13. 730

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		*A*
12· 8·4	. 9173	<1	13. 729
15· 2·1	. 9051	3	13. 727
15· 3·0	. 8975	2	13. 729
14· 6·2	. 8937	2	13. 729
15· 3·2	. 8900	<1	13. 730
15· 4·1	. 8826	3	13. 730
12·10·0	. 8789	2	13. 729
14· 7·1	. 8754	2	13. 730
14· 6·4	. 8718	1	13. 729
15· 5·0	. 8683	2	13. 729
15· 5·2	. 8615	3	13. 730
16· 1·1	. 8547	3	13. 729
16· 2·0	. 8513	3	13. 727
15· 6·1	. 8482	3	13. 729
16· 3·1	. 8418	5	13. 729
15· 6·3	. 8356	3	13. 730
16· 4·0	. 8325	1	13. 730
16· 3·3	. 8295	4	13. 731
15· 7·2	. 8235	4	13. 730
16· 5·1	. 8176	3	13. 730
15· 6·5	. 8118	2	13. 729
17· 1·0	. 8062	3	13. 729
17· 2·1	. 8007	1	13. 729
16· 6·2	. 7980	2	13. 729
17· 3·0	. 7953	1	13. 729
17· 3·2	. 7900	1	13. 729
17· 4·1	. 7849	5	13. 730
16· 6·4	. 7823	3	13. 729
Average value of last five lines			13. 729

Antimony(III) Fluoride, SbF_3 (orthorhombic)

Powder Data cards. None. Data on ASTM card 1–0523 probably represents oxyfluoride produced when antimony fluoride is exposed in air.

Additional published patterns. None.

NBS sample. The sample of antimony fluoride was obtained from City Chemical Company, New York, N.Y. The material was sublimed at NBS and then mixed with silicone grease to protect it from oxidation in the atmosphere. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum iron, magnesium, and silicon.

The sample was colorless and optically negative with the indices of refraction N_α=1.587, N_β=1.615, and N_γ=1.629. 2V=~65°.

The *d*-values of the three strongest lines are: 3.621, 3.728, and 1.810 A.

Structural data. Byström and Westgren [1] in 1943 determined that antimony(III) fluoride is orthorhombic with the space group C_{2v}^{16}—Ama2 (No. 40) and 4(SbF_3) per unit cell. The lattice constants of Byström and Westgren have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1943	Byström and Westgren.	7. 26	7. 51	4. 96
1962	National Bureau of Standards.	7. 241	7. 456	4. 940 at 25 °C

The density of antimony(III) fluoride calculated from the NBS lattice constants is 4.451 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard tungsten, a=3.1648 A	
	d	*I*
	A	
020	3. 728	53
200	3. 621	100
111	3. 580	16
120	3. 317	3
211	2. 718	<1
220	2. 597	4
002	2. 472	<1
031	2. 221	6
131	2. 123	6
311	2. 083	5
022	2. 059	1
202	2. 040	1
320	2. 028	2
122	1. 981	1
231	1. 892	2
040	1. 864	8
400	1. 810	21
140	1. 805	13
222	1. 790	2
240, 411	1. 656	1
331	1. 633	2
420	1. 6284	2
113	1. 5697	<1
322	1. 5668	1
042	1. 4875	<1
340	1. 4756	1
402	1. 4605	<1
142	1. 4580	1
051	1. 4279	2
431	1. 4028	1
151	1. 4003	2
242	1. 3760	<1
511	1. 3661	3
422	1. 3594	<1
520	1. 3503	<1
133	1. 3486	<1
313	1. 3379	<1
251	1. 3282	2
440	1. 2986	<1
233	1. 2834	<1
342	1. 2667	<1
004	1. 2348	<1
351	1. 2286	<1
160	1. 2249	1
531	1. 2130	<1
600	1. 2069	4
333	1. 1930	<1
522	1. 1841	<1
024	1. 1724	<1
204	1. 1695	<1
611	1. 1584	<1
124	1. 1566	<1
620	1. 1484	3
540	1. 1433	<1
451	1. 1208	<1
224	1. 1155	<1
053, 360	1. 1049	<1
162	1. 0971	<1
602	1. 0844	<1
513	1. 0760	<1
631	1. 0605	<1
253	1. 0573	<1
071, 622	1. 0413	1
542	1. 0376	<1

Reference

[1] A. Byström and A. Westgren, X-ray analysis of antimony trifluoride, Arkiv. Kemi, Mineral. Geol. **17B,** No. 2, 1–8 (1943).

Barium Arsenate, $Ba_3(AsO_4)_2$ (trigonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of barium arsenate was prepared at NBS by reacting solutions of barium chloride and arsenic(V) acid. The precipitate was washed several times, dissolved in nitric acid, reprecipitated by addition of ammonia, and heated at 1,000 °C for 1 hr. 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, lead, megnesium, and silicon.

The sample was colorless and too fine-grained to allow determination of the indices of refraction.

The *d*-values of the three strongest lines are: 3.24, 2.888, and 2.1532 A.

Structural data. Durif [1] in 1959 determined that barium arsenate is isostructural with barium phosphate, with the space group D_{3d}^5—$R\bar{3}m$ (No. 166) and $1[Ba_3(AsO_4)_2]$ per rhombohedral unit cell or $3[Ba_3(AsO_4)_2]$ per hexagonal unit cell.

Lattice constants

		a	*c*
		A	*A*
1959	Durif [1]	5. 753	21. 18
1962	National Bureau of Standards.	5. 774	21. 204 at 25 °C

hkl (hex.)	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
003	7. 08	<1
101	4. 88	4
104	3. 64	7
015	3. 24	100
110	2. 888	89
021	2. 482	1
202	2. 433	6
009	2. 356	7
024	2. 260	7
116	2. 2360	1
205	2. 1532	43
1·0·10	1. 9521	26
211	1. 8819	2
119	1. 8246	8
214	1. 7797	2
125	1. 7262	30
300	1. 6667	16
0·2·10	1. 6168	11
2·0·11	1. 5258	<1
0·1·14	1. 4491	4
220	1. 4433	13
2·1·10	1. 4108	18
309	1. 3606	2
134	1. 3421	<1
315	1. 3180	12
2·0·14	1. 2957	2
1·1·15	1. 2696	11
229	1. 2306	3
404	1. 2166	<1
045	1. 1990	5
1·2·14	1. 1816	3
0·2·16	1. 1705	<1
1·3·10	1. 1605	9
235	1. 1073	6
410	1. 0911	6

hkl (hex.)	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
3·0·15,413	1. 0780	10
4·0·10	1. 0767	5
0·1·20	1. 0370	2
3·1·14	1. 0228	1
2·2·15,0·0·21	1. 0096	6
3·2·10	1. 0090	7
419	. 9901	2
2·0·20	. 9761	1
505	. 9736	2
0·4·14	. 9638	2
330,3·0·18	. 9621	3
2·1·19	. 9611	4
422	. 9410	<1
244	. 9305	1
1·2·20	. 9246	4
425	. 9224	7
2·3·14	. 9144	3
0·5·10	. 9045	2
339	. 8909	1
0·0·24	. 8836	<1
155	. 8786	4
1·3·19	. 8695	3
4·1·15,3·0·21	. 8636	10
3·3·12,1·1·24	. 8449	3
3·1·20	. 8424	3
1·0·25	. 8362	1
5·0·14	. 8344	2
600	. 8334	2
5·1·10	. 8269	4
0·4·20	. 8086	1
345	. 8070	4
0·1·26	. 8050	3
0·2·25	. 8032	1
520	. 8007	6
3·2·19	. 8000	3
523,3·3·15	. 7955	4
609	. 7857	1
3·0·24	. 7807	3

The density of barium arsenate calculated from the NBS lattice constants is 5.612 g/cm³ at 25 °C.

Reference

[1] A. Durif, Structure cristalline des orthovanadates et orthoarseniates de baryum et de strontium, Acta Cryst. **12,** 420–421 (1959).

Barium Perchlorate Trihydrate, $Ba(ClO_4)_2 \cdot 3H_2O$ (hexagonal)

Powder Data cards

Card number	Index lines	Radiation	Source
1–0931	2. 90 3. 65 2. 14	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of barium perchlorate trihydrate was prepared at NBS by the reaction of solutions of barium carbonate and perchloric acid. The sample was purified by recrystallization. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, chromium, iron, magnesium, and sodium.

The sample was colorless and optically negative with the refractive indices N_0=1.533 and Ne= 1.532.

The *d*-values of the three strongest lines are: 3.646, 2.912, and 4.84 A.

Structural data. West [2] in 1934 determined that barium perchlorate trihydrate is hexagonal with the space group C_6^6—$P6_3$ (No. 173) or C_{6h}^2—$P6_3/m$ (No. 176) and $2[Ba(ClO_4)_2 \cdot 3H_2O]$ per unit cell. The unit cell measurements of West [2] have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1934	West [2]	7. 295	9. 659
1960	Mani and Ramaseshan [3].	7. 278	9. 64
1962	National Bureau of Standards.	7. 294	9. 674 at 25 °C.

The density of barium perchlorate trihydrate calculated from the NBS lattice constants is 2.907 g/cm³ at 25 °C.

References

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

[2] C. D. West, Crystal structures of some hydrated compounds, Z. Krist. **88A,** 198–204 (1934).

[3] N. V. Mani and S. Ramaseshan, The crystal structure of barium perchlorate trihydrate $Ba(ClO_4)_2 \cdot 3H_2O$ and the crystal coordination of Ba^{++} ion, Z. Krist. **114,** 200–214 (1960).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, *a*=3.1648 A	
	d	*I*
	A	
100	6. 32	34
002	4. 84	36
102	3. 839	15
110	3. 646	100
200	3. 158	3
112	2. 912	73
103	2. 872	14
202	2. 644	13
004	2. 422	8
210	2. 389	14
211	2. 317	6
104, 203	2. 257	21
212	2. 142	25
300	2. 106	18
301	2. 057	2
114	2. 015	9
302	1. 9309	19
204, 213	1. 9197	6
220	1. 8250	5
310	1. 7524	8
222	1. 7069	5
214	1. 6995	2
205	1. 6485	4
312	1. 6472	2
304, 223	1. 5880	7
400	1. 5790	5
106	1. 5618	2
401	1. 5582	1
313	1. 5388	<1
402	1. 5009	6
116	1. 4744	9
224	1. 4564	3
320	1. 4493	2
206	1. 4363	5
314	1. 4196	3
322	1. 3875	5
410	1. 3780	9
216	1. 3364	5
412	1. 3253	7
404, 323	1. 3222	5
306	1. 2801	2
500	1. 2629	<1
324	1. 2432	2
502	1. 2221	3
330	1. 2157	1
226	1. 2080	1
414	1. 1975	2
316	1. 1866	2
332	1. 1787	3

Cadmium Cyanide, $Cd(CN)_2$ (cubic)

Powder Data cards. None.

Additional published pattern. Shugam and Zhdanov [1] 1945.

NBS sample. The sample of cadmium cyanide was prepared at NBS from solutions of cadmium chloride and sodium cyanide. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent sodium; 0.01 to 0.1 percent silicon; and 0.001 to 0.01 percent each of aluminum, barium, calcium, iron, nickel, and titanium.

The color of the sample was white. The index of refraction is 1.443.

The *d*-values of the three strongest lines are: 4.458, 2.575, and 2.229 A.

Structural data. Shugam and Zhdanov [1] in 1945 determined that cadmium cyanide has the cuprous oxide structure, the space group T_d^1—$P\bar{4}3m$ (No. 215), and 2[$Cd(CN)_2$] per unit cell. The lattice constant reported by Shugam and Zhdanov has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1945	Shugam and Zhdanov [1]	6.33
1962	National Bureau of Standards	6.3050 at 25 °C

The density of cadmium cyanide calculated from the NBS lattice constant is 2.178 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		*A*
110	4.458	100	6.305
111	3.640	7	6.304
200	3.153	6	6.306
211	2.575	32	6.307
220	2.229	13	6.305
310	1.9935	8	6.304
222	1.8198	2	6.304
321	1.6851	6	6.3050
411	1.4860	3	6.3046
420	1.4099	<1	6.3052
332	1.3442	<1	6.3049
510	1.2366	1	6.3054
Average value of last five lines			6.3050

Reference

[1] E. A. Shugam and G. S. Zhdanov, The crystal structure of cadmium cyanide, Acta Physicochim. U.R.S.S. **20,** 247–252 (1945).

Cadmium Tungstate, $CdWO_4$ (monoclinic)

Powder Data cards

Card number	Index lines	Radiation	Source
1–0488	3.80 3.05 2.53	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. Coing-Boyat [2] 1961.

NBS sample. The sample of cadmium tungstate was prepared at NBS from solutions of cadmium chloride and sodium tungstate. The precipitate was washed several times and then heated to 800 °C for 10 min. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent sodium; and 0.001 to 0.01 percent silicon.

The color of the sample was pale yellow. The indices of refraction could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are: 3.077, 3.020, and 2.536 A.

Structural data. Coing-Boyat [2] in 1961 determined that cadmium tungstate is monoclinic with the most probable space group C_{2h}^5—$P2_1/c$ (No. 14) and 2 ($CdWO_4$) per unit cell and is probably isostructural with $MgWO_4$. Sharp [3] in 1960 reported that the most probable space group for cadmium tungstate was C_{2h}^5—$P2_1/b$ (No. 14); however, this space group did not completely satisfy our data.

Cadmium Tungstate, $CdWO_4$ (monoclinic)—Continued

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, silver, a=4.0861 A	
	d	*I*
	A	
010	5. 87	7
100	5. 04	12
$1\bar{1}0$	3. 818	43
$\bar{1}11$	3. 077	100
111	3. 020	87
020	2. 928	26
021, 002	2. 536	54
200	2. 514	23
$2\bar{1}0$	2. 311	2
$\bar{1}02$	2. 287	3
121	2. 253	7
$\bar{1}12$	2. 131	5
112	2. 092	8
030	1. 953	2
022	1. 916	18
220	1. 907	17
$1\bar{3}0$	1. 820	23
$\bar{2}02$	1. 809	17
$\bar{2}21$	1. 797	16
221	1. 774	21
202	1. 762	13
$\bar{1}31$	1. 718	4
131	1. 708	2
212	1. 688	<1
310	1. 611	3
$\bar{1}13$	1. 557	15
$\bar{3}11$	1. 546	14
$2\bar{3}0$	1. 543	12
$\bar{2}22$	1. 539	10
113	1. 535	13
311	1. 524	12
222	1. 510	6
$\bar{1}32$	1. 485	10
132	1. 472	11
040, 023	1. 465	9

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal Standard, silver, a=4.0861 A	
	d	*I*
	A	
$\bar{1}23$	1. 414	1
$0\bar{4}1$	1. 407	11
$\bar{2}13$	1. 379	2
$\bar{3}12$	1. 375	2
$\bar{1}41$	1. 357	1
141	1. 353	<1
213	1. 350	<1
312	1. 345	1
$\bar{2}32$	1. 327	1
232	1. 308	<1
033, $\bar{2}23$	1. 278	3
330	1. 272	6
042	1. 268	5
400	1. 257	5
223	1. 254	4
$\bar{3}31$	1. 238	<1
$\bar{2}41$	1. 2319	7
241	1. 2242	6
$\bar{1}14$	1. 2105	<1
$\bar{3}13$	1. 1814	3
024	1. 1638	2
420	1. 1549	3
313	1. 1522	5
$\bar{3}32$	1. 1458	6
$\bar{2}04$	1. 1435	1
051	1. 1415	6
$\bar{4}21$	1. 1321	3
332, 124	1. 1285	4
204	1. 1206	3
$\bar{3}23$	1. 1149	4
043	1. 1072	3

Lattice constants

		a	b	c	β
		A	*A*	*A*	
1960	Sharp [3]	5. 028	5. 868	5. 076	91. 45°
1961	Coing-Boyat [2]	5. 026	5. 854	5. 074	91. 48°
1962	National Bureau of Standards	5. 029	5. 859	5. 074	91. 47 at 25 °C

The density of cadmium tungstate calculated from the NBS lattice constants is 8.003 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,** 457–512 (1938).

[2] J. Coing-Boyat, Groupe d'espace du tungstate de cadmium, $CdWO_4$, Acta Cryst. **14,** 1100 (1961).

[3] W. E. Sharp, Lattice constants of $CdWO_4$, Z. Krist. **114,** 151–153 (1960).

Cesium Bromoosmate (IV), Cs_2OsBr_6 (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium bromoosmate was prepared at NBS by R. Johannesen from solutions of cesium bromide and bromoosmic acid. Spectrographic analysis showed the only major impurity to be 0.001 to 0.01 percent of sodium.

The color of the sample was very dark brown. The refractive index could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are: 2.665, 3.077, and 6.154 A.

Structural data. The structure of cesium bromoosmate has not been reported. However, because of the similarity of patterns, it is thought to be isostructural with ammonium bromoosmate having the space group O_h^5—Fm3m (No. 225) with $4(Cs_2OsBr_6)$ per unit cell.

Lattice constant

		a
		A
1962	National Bureau of Standards	10.659 at 25 °C.

The density of cesium bromoosmate calculated from the NBS lattice constant is 5.130 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal Standard, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		*A*
111	6. 154	79	10. 659
200	5. 239	7	10. 658
220	3. 770	63	10. 663
311	3. 214	26	10. 660
222	3. 077	91	10. 659
400	2. 665	100	10. 660
331	2. 4466	5	10. 664
420	2. 3844	4	10. 663
422	2. 1765	21	10. 663
511	2. 0517	18	10. 661
440	1. 8844	61	10. 660
531	1. 8017	16	10. 659
600	1. 7762	3	10. 657
620	1. 6851	9	10. 658
533	1. 6252	5	10. 657
622	1. 6067	18	10. 658
444	1. 5382	16	10. 657
711	1. 4923	8	10. 657
640	1. 4780	3	10. 658
642	1. 4242	8	10. 658
731	1. 3875	4	10. 658
800	1. 3321	5	10. 657
822	1. 2560	3	10. 658
751	1. 2307	3	10. 658
622	1, 2225	5	10. 658
840	1. 1920	12	10. 662
911	1. 1700	3	10. 659
664	1. 1361	3	10. 658
931	1. 1172	4	10. 657
844	1. 0879	7	10. 659
933	1. 0714	3	10. 660
10·2·0	1. 0451	5	10. 658
951	1. 0303	5	10. 658
10·2·2	1. 0257	3	10. 659
953	0. 9939	3	10. 658
10·4·2	. 9730	1	10. 659
880	. 9422	2	10. 660
11·3·1	. 9312	2	10. 658
10·6·0	. 9139	3	10. 658
11·3·3	. 9041	2	10. 659
10·6·2	. 9009	3	10. 660
12·0·0	. 8884	5	10. 661
11·5·1	. 8792	1	10. 660
12·2·2	. 8645	1	10. 658
11·5·3	. 8562	1	10. 660
12·4·0	. 8428	4	10. 661
991	. 8349	2	10. 759
10·8·2	. 8223	2	10. 658
13·1·1	. 8151	3	10. 659
12·4·4	. 8035	3	10. 660
13·3·1	. 7967	2	10. 659
Average value of last five lines			10. 659

Cesium Chloroosmate (IV), Cs_2OsCl_6 (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium chloroosmate was prepared at NBS by R. Johannesen from solutions of cesium chloride and chloroosmic acid. Spectrographic analysis showed the following major impurities: 0.01 to 1.0 percent sodium and 0.001 to 0.01 percent each of aluminum and silicon.

The color of the sample was deep orange. The refractive index could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are: 3.616, 5.905, and 2.557 A.

Structural data. The structure of cesium chloroosmate has not been reported. However, because of the similarity of patterns, it is thought to be isostructural with ammonium chloroosmate having the space group O_h^5—Fm3m (No. 225) with $4(Cs_2OsCl_6)$ per unit cell.

Lattice constant

		a
		A
1962	National Bureau of Standards	10.230 at 25 °C.

The density of cesium chloroosmate calculated from the NBS lattice constant is 4.148 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		A
111	5. 905	68	10. 228
220	3. 616	100	10. 228
311	3. 085	27	10. 232
222	2. 953	27	10. 228
400	2. 557	55	10. 228
331	2. 347	9	10. 230
422	2. 089	37	10. 230
511	1. 969	14	10. 231
440	1. 8090	32	10. 233
531	1. 7293	12	10. 231
620	1. 6174	14	10. 229
533	1. 5603	3	10. 232
622	1. 5426	3	10. 232
444	1. 4763	8	10. 228
711	1. 4324	7	10. 229
642	1. 3668	13	10. 228
731	1. 3320	3	10. 231
800	1. 2790	3	10. 232
822	1. 2057	5	10. 231
751	1. 1814	2	10. 231
662	1. 1735	2	10. 230
840	1. 1437	4	10. 230
911	1. 1229	2	10. 230
664	1. 0905	3	10. 230
931	1. 0723	2	10. 229
844	1. 0442	3	10. 231
933	1. 0283	1	10. 231
10·2·0	1. 0032	4	10. 231
951	0. 9890	3	10. 230
10·2·2	. 9843	1	10. 229
953	. 9539	1	10. 229
10·4·2	. 9340	3	10. 231
11·1·1	. 9225	<1	10. 231
880	. 9042	3	10. 230
11·3·1	. 8939	2	10. 231
10·6·0	. 8773	3	10. 231
11·3·3	. 8678	3	10. 231
12·0·0	. 8525	3	10. 230
12·2·2	. 8298	3	10. 230
11·5·3	. 8218	2	10. 231
12·4·0	. 8088	2	10. 231
991	. 8013	2	10. 230
10·8·2	. 7893	2	10. 230
13·1·1	. 7823	1	10. 230
Average value of last five lines			10. 230

Chromium Orthophosphate, alpha, $CrPO_4$ (orthorhombic)

Powder Data cards

Card number	Index lines	Radiation	Source
*5–0233	5. 40 2. 74 5. 20	Copper---	National Bureau of Standards [1] 1951, [2] 1952.

*This ASTM card was reported without indices.

Additional published patterns. None.

NBS sample. The sample of alpha-chromium orthophosphate was prepared at NBS by grinding the hexahydrate and heating it to 1,500 °C. The ground hexahydrate actually inverts to the alpha form at 972 °C while the unground hexahydrate changes to beta and then to alpha-orthophosphate. Spectrographic analysis showed no impurities greater than 0.001 percent.

The color of the sample was deep blue. The refractive indices are $N_\alpha=1.761$ and $N_\gamma=1.844$. 2V is very large. The α form is strongly pleochroic.

The *d*-values of the three strongest lines are: 5.390, 2.741, and 5.203 A.

Structural data. Villadsen [3] in 1960 determined that alpha-chromium orthophosphate has an orthorhombic body-centered lattice having the lattice symbol I . . . . Therefore, the possible orthorhombic space groups are D_2^8—I222 (No. 23), D_2^9—$I2_12_12_1$ (No. 24), C_{2v}^{20}—Imm2 (No. 44), and D_{2h}^{25}—Immm (No. 71). According to Villadsen, there are either 8($CrPO_4$) per unit cell or 16($CrPO_4$) per unit cell.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1960	Villadsen [3]---	10. 41	12. 90	6.297
1962	National Bureau of Standards.	10. 405	12. 898	6.297 at 25 °C

The density of alpha-chromium orthophosphate calculated from the NBS lattice constants using $Z=16$ is 4.620 g/cm^3 at 25 °C. The density based on $Z=8$ appeared to be rather low for this compound.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
020	6. 444	17
011	5. 661	45
101	5. 390	100
200	5. 203	48
121	4. 139	4
211	3. 834	3
031	3. 548	7
002	3. 149	9
301	3. 039	22
022	2. 826	2
141	2. 766	13
240	2. 741	51
202	2. 693	40
400	2. 604	26
222	2. 479	7
251	2. 169	18
013	2. 071	5
440	2. 025	13
213	1. 927	5
303	1. 795	3
451	1. 7590	8
323	1. 7296	3
442	1. 7025	13
547	1. 6851	3
370	1. 6276	4
080	1. 6124	5
004	1. 5754	6
253	1. 5537	3
433	1. 5269	8
602	1. 5188	6
204	1. 5071	3
372	1. 4457	2
651	1. 4031	4
453	1. 3801	8
244	1. 3649	3
291	1. 3493	3

References

[1] Joint Committee Fellowship Report, National Bureau of Standards, Oct., 1951.

[2] B. M. Sullivan and H. F. McMurdie, Crystal forms of chromium orthophosphate, J. Research N.B.S. 48, No. 2, 159–162 (1952) RP2300.

[3] J. Villadsen, Halder Topsoe Res. Lab., Hellerup, Denmark (private communication).

Cobalt Mercury Thiocyanate, $Co[Hg(CNS)_4]$ (tetragonal)

Powder Data cards. None.

NBS sample. The sample of cobalt mercury thiocyanate was prepared at NBS by R. S. Johannesen from solutions of cobaltous nitrate and ammonium mercury thiocyanate. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of nickel and silicon.

The color of the sample was a brilliant blue and it is optically positive. The indices of refraction are $N_o=1.875$ and $N_e=1.905$.

The d-values of the three strongest lines are: 5.552, 3.284, and 7.85 A.

Structural data. Straumanis and Stahl [1] in 1944 determined that cobalt mercury thiocyanate has the space group $S_4^2-I\bar{4}$ (No. 82) and $2\{Co[Hg(CNS)_4]\}$ per unit cell.

Unit cell measurements reported by Straumanis and Stahl have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
		A	A
1944	Straumanis and Stahl [1].	11. 1092	4. 3740
1947	Jeffrey [2]	11. 09	4. 37
1962	National Bureau of Standards.	11. 105	4. 3819 at 25 °C

Straumanis and Stahl [1] reported that the thermal expansion coefficients for cobalt mercury thiocyanate were: $\alpha\perp c=-10.85\times10^{-6}$; $\alpha\|c=149.3\times10^{-6}$.

The density of cobalt mercury thiocyanate calculated from the NBS lattice constants is 3.022 g/cm³ at 25 °C.

References

[1] I. M. Straumanis and W. Stahl, Die gegenseitige Löslichkeit im ternären System Cadmium-, Kobalt-, Zinkquecksilberrhodanid, Z. physik. Chem. **193**, 97–111 (1944)

[2] J. W. Jeffrey, Crystal structure of $Co[Hg(CNS)_4]$, Nature **159**, 610 (1947).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A	
	d	I
	A	
110	7. 85	100
200	5. 552	100
101	4. 075	44
220	3. 992	41
310	3. 513	18
211	3. 284	70
301	2. 828	44
400	2. 776	6
330	2. 617	19
321	2. 520	39
420	2. 484	32
411	2. 295	25
510	2. 177	5
501	1. 980	19
440	1. 962	11
530	1. 903	7
521	1. 865	23
600	1. 850	14
620	1. 755	10
402	1. 721	4
611	1. 683	11
541	1. 6122	5
710	1. 5700	5
631	1. 5482	12
512	1. 5442	11
640	1. 5396	5
701	1. 4916	2
721	1. 4403	7
800	1. 3880	2
651	1. 3523	4
820	1. 3466	3
811	1. 3143	5
660	1. 3090	3
831	1. 2464	2
840	1. 2414	2
910	1. 2267	2
921	1. 1616	3
851	1. 1369	1
10·0·0	1. 1104	2
941	1. 0921	2
10·2·0	1. 0890	2
950	1. 0784	2
10·1·1	1. 0719	3
10·4·0	1. 0315	2

663956—63——3

Cobalt Sulfate, beta, $CoSO_4$ (orthorhombic)

Powder Data Cards

Card number	Index lines	Radiation	Source
3–0843	2. 58 3. 60 4. 30	Molybde-num	The Dow Chemical Company.

Additional published patterns. Hammel [1] 1938, Rentzeperis [2] 1958, and Pistorius [3] 1961. The reference for the comprehensive work reported by Pistorius was not available at the time this work was started. The *d*-values reported by Pistorius agree favorably with the NBS data.

NBS sample. The sample of cobalt sulfate was made from cobalt chloride and sulfuric acid. The precipitated sulfate was heated to 160 °C to drive off excess sulfuric acid. A second pattern was prepared after the sample was reheated to 400 °C with no observable change in spacing. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of nickel and silicon; and 0.01 to 0.1 percent each of aluminum, calcium, iron, and sodium.

The color of the sample was reddish-purple. The indices of refraction could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are: 2.605, 3.610, and 3.368 A.

Structural data. Rentzeperis [2] in 1958 determined that beta cobalt sulfate has the magnesium sulfate structure, the space group D_{2h}^{17}—Amam (No. 63) and 4($CoSO_4$) per unit cell. Hammel [1] and Hocart and Serres [4] both had previously reported lattice constants for what was later found to be the high-temperature α-$CoSO_4$ reported by Rentzeperis [2] to exist after heating above 700 °C.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1958	Rentzeperis [2]	6. 531	7. 876	5. 200
1961	Pistorius [3]	6. 516	7. 864	5. 191 at 25 °C
1962	National Bureau of Standards.	6. 522	7. 871	5. 198 at 25 °C

The density of beta-cobalt sulfate calculated from the NBS lattice constants is 3.857 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Co, 1.7889 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
011	4. 336	28
020	3. 936	21
111	3. 610	67
120	3. 368	45
211	2. 605	100
031	2. 342	38
202	2. 032	19
040	1. 967	12
320, 231	1. 902	10
222	1. 805	21
240	1. 684	13
113	1. 6379	18
400	1. 6305	12
331	1. 5938	7
411	1. 5261	10
420, 051	1. 5066	12
213	1. 5023	5
033	1. 4460	10
242	1. 4140	22
251	1. 3680	10
431	1. 3383	10

References

[1] F. Hammel, Contribution à l'étude des sulfates de la série magnésienne, Ann. chim. (Paris) **11,** 24–358 (1938).

[2] P. J. Rentzeperis, Die Kristallstruktur der beiden Modifikationen von wasserfreiem $CoSO_4$, Neues. Jahrb. Mineral. Monatsh. 210–215 (1958).

[3] C. W. F. T. Pistorius, Lattice constants and space groups of the low and high temperature polymorphic forms of anhydrous cobaltous sulfate, Acta Cryst. **14,** 543–544 (1961).

[4] R. Hocart and A. Serres, Magnetic properties and crystalline structure in the different varieties of anhydrous cobalt sulfate, Compt. rend. **193,** 1180–1182 (1931).

Dysprosium Gallium Oxide 3:5, $Dy_3Ga_2(GaO_4)_3$ (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of dysprosium oxide and gallium oxide. The mixture was pressed into pellets and heated at 1,350 °C for 6 hr; then ground, remixed, and again pressed into pellets and heated at 1,450 °C for 6 hr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent holmium; 0.001 to 0.01 percent each of erbium, thulium, and yttrium; and 0.0001 to 0.001 percent each of copper and silicon.

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

The *d*-values of the three strongest lines are 2.752, 2.512, and 1.645 A.

Structural data. S. Schneider and R. Roth [1] showed that dysprosium gallium oxide 3:5 has the garnet structure, having the space group O_h^{10}—Ia3d (No. 230), and 8[$Dy_3Ga_2(GaO_4)_3$] per unit cell.

Lattice constants

		A
1956	Bertaut and Forrat [2]	12.32
1962	National Bureau of Standards	12.307 at 25 °C

The density of dysprosium gallium oxide 3:5 calculated from the NBS lattice constant is 7.325 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, silver, a=4.0861 A		
	d	*I*	*a*
	A		A
211	5.023	14	12.304
220	4.350	6	12.304
321	3.290	10	12.310
400	3.076	30	12.304
420	2.752	100	12.307
422	2.512	44	12.306
431	2.413	5	12.304
521	2.247	10	12.307
440	2.176	2	12.309
611	1.997	9	12.310
444	1.777	14	12.311
640	1.707	32	12.309
721	1.675	6	12.308
642	1.645	36	12.308
732	1.564	4	12.311
800	1.5382	14	12.306
822	1.4503	5	12.306
840	1.3760	9	12.307
842	1.3430	20	12.310
921	1.3271	1	12.307
664	1.3120	7	12.308
932	1.2695	3	12.308
10·2·0	1.2068	4	12.307
10·3·1	1.1737	2	12.310
10·4·0	1.1426	17	12.306
10·3·3	1.1330	<1	12.308
10·4·2	1.1235	9	12.307
11·2·1	1.0967	3	12.310
880	1.0880	7	12.309
12·0·0	1.0256	6	12.307
12·2·0	1.0117	5	12.308
12·2·2	0.9983	9	12.308
12·4·4	.9278	3	12.309
13·3·0	.9228	2	12.312
12·6·0	.9173	11	12.307
12·6·2	.9073	5	12.307
888	.8881	4	12.306
14·3·1	.8576	3	12.309
12·8·0	.8534	2	12.308
14·4·0	.8452	10	12.306
14·4·2	.8373	9	12.307

References

[1] S. Schneider and R. Roth, Solid state reactions involving oxides of trivalent cations (to be published in J. Research NBS).

[2] F. Bertaut and F. Forrat, Étude des combinaisons des oxides des terres rares avec l'alumine et la galline, Compt. rend. **243,** 1219–1222 (1956).

Erbium Manganite, $ErMnO_3$ (hexagonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of erbium manganite was prepared at NBS by S. Schneider from stoichiometric mixtures of erbium oxide and manganous carbonate. The mixture was pressed into pellets and heated at 1,000 °C for 41 hr; then ground, remixed, again pressed into pellets and heated at 1,150 °C for 21 hr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum and magnesium; and 0.001 to 0.01 percent each of calcium, chromium, copper, iron, and silicon.

The sample was a black opaque powder. The *d*-values of the three strongest lines are: 2.695, 3.059, and 1.7659 A.

Structural data. Yakel, Koehler, Bertaut, and Forrat [1] in 1960 determined that erbium manganite has the space group C_{6v}^3—$P6_3cm$ (No. 185), and 6($ErMnO_3$) per unit cell. Erbium manganite is isostructural with lutetium manganite.

Lattice constants

		a	*c*
		A	*A*
1960	Yakel, Koehler, Bertaut, and Forrat [1].	6.1150	11.411
1962	National Bureau of Standards.	6.1166	11.435 at 25 °C.

The density of erbium manganite calculated from the NBS lattice constants is 7.264 g/cm³ at 25 °C.

Reference

[1] H. L. Yakel, W. C. Koehler, E. F. Bertaut, and E. F. Forrat, Erbium Manganite—a new ABO_3 structure, Acta Cryst. **13,** 1015 (1960).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
002	5.717	30
102	3.885	9
110	3.059	50
111	2.955	33
004	2.858	35
112	2.695	100
104	2.516	7
202	2.403	6
113	2.385	3
114	2.088	38
204	1.944	6
212	1.8900	4
115	1.8312	6
106	1.7931	10
300	1.7659	40
302	1.6874	9
214	1.6396	5
116	1.6170	19
206	1.5470	5
220	1.5290	7
221	1.5156	4
304	1.5023	25
222	1.4769	16
117	1.4409	3
008	1.4298	2
108	1.3801	9
224	1.3481	7
314	1.3067	2
225	1.2714	2
208	1.2576	2
226	1.1926	5
218,316	1.1636	5
410	1.1558	4
411	1.1506	1
412	1.1330	9
324	1.1184	5
1·0·10	1.1178	4
308	1.1109	3
406	1.0876	<1
414	1.0715	8
2·0·10	1.0499	1
228	1.0444	<1
415	1.0315	1
318, 326	1.0245	5
330	1.0193	4
332	1.0037	2
2·1·10	0.9930	3
416	.9883	4
408	.9715	1
334	.9602	3
417	.9433	<1
335	.9314	2
3·1·10	.9023	2

Europium Gallium Oxide 3:5, $Eu_3Ga_2(GaO_4)_3$ (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of europium oxide and gallium oxide. The mixture was pressed into pellets and heated at 1,350 °C for 6 hr; then ground, remixed, again pressed into pellets and heated at 1,450 °C for 6 hr. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent silicon; and 0.0001 to 0.001 percent each of barium, calcium, and erbium.

The color of the sample was white. The index of refraction was above 2.0 as determined by the available refractive index liquids.

The *d*-values of the three strongest lines are: 2.773, 2.531, and 1.6573 A.

Structural data. Schneider, Roth, and Waring [1] in 1961 showed that europium gallium oxide 3:5 has the garnet structure, having the space group O_h^{10}—Ia3d (No. 230), and $8[Eu_3Ga_2(GaO_4)_3]$ per unit cell.

Lattice constant

		A
1962	National Bureau of Standards	12.401 at 25 °C

The density of europium gallium oxide 3:5 calculated from the NBS lattice constant is 6.940 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal Standard, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		A
211	5. 063	14	12. 402
220	4. 384	5	12. 400
321	3. 314	8	12. 400
400	3. 099	32	12. 396
420	2. 773	100	12. 401
422	2. 531	45	12. 399
431	2. 432	3	12. 401
521	2. 264	10	12. 400
440	2. 192	4	12. 400
611	2. 012	11	12. 403
631	1. 829	1	12. 405
444	1. 790	14	12. 402
640	1. 7196	30	12. 400
721	1. 6874	4	12. 400
642	1. 6573	35	12. 402
732	1. 5749	5	12. 401
800	1. 5504	13	12. 403
840	1. 3866	9	12. 402
842	1. 3534	17	12. 404
921	1. 3374	3	12. 403
664	1. 3224	7	12. 405
932	1. 2796	2	12. 406
941	1. 2531	1	12. 405
10·2·0	1. 2162	1	12. 405
10·3·1	1. 1827	2	12. 404
10·4·0	1. 1517	17	12. 404
10·4·2	1. 1323	8	12. 403
11·2·1	1. 1049	3	12. 403
880	1. 0962	6	12. 402
11·3·2	1. 0713	2	12. 401
12·0·0	1. 0336	3	12. 403
12·2·0	1. 0196	5	12. 404
11·5·2	1. 0128	3	12. 404
12·2·2	1. 0060	7	12. 403
11·6·1	0. 9867	3	12. 403
11·6·3	. 9627	<1	12. 403
12·4·4	. 9349	5	12. 403
12·6·0	. 9244	10	12. 402
13·3·2	. 9194	<1	12. 403
12·6·2	. 9142	5	12. 401
888	. 8951	5	12. 403
14·3·1	. 8640	3	12. 401
12·8·0	. 8599	5	12. 402
14·4·0	. 8517	8	12. 401
14·4·2	. 8438	16	12. 401
14·5·1	. 8323	1	12. 401
Average value of last five lines			12. 401

Reference

[1] S. J. Schneider, R. S. Roth, and J. L. Waring, Solid state reactions involving oxides of trivalent cations, J. Research NBS **65A** (Phys. and Chem.) No. 4, 345–374 (1961).

Gadolinium Gallium Oxide 3:5, $Gd_3Ga_2(GaO_4)_3$ (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of gadolinium oxide and gallium oxide. The mixture was pressed into pellets and heated at 1,350 °C for 6 hrs; then ground, remixed, and again pressed into pellets and heated at 1,450 °C for 6 hrs. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of europium and terbium; and 0.001 to 0.01 percent of silicon.

The color of the sample was white. The index of refraction is greater than 2.00.

The *d*-values of the three strongest lines are: 2.768, 2.526, and 1.6540 A.

Structural data. S. Schneider and R. Roth [1] showed that gadolinium gallium oxide 3:5 has the garnet structure, having the space group O_h^{10}—Ia3d (No. 230), and $8[Gd_3Ga_2(GaO_4)_3]$ per unit cell.

Lattice constants

		A
1956	Bertaut and Forrat [2]	12.39
1962	National Bureau of Standards	12.376 at 25 °C

The density of gadolinium gallium oxide 3:5 calculated from the NBS lattice constant is 7.093 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal Standard, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		A
211	5. 052	15	12. 375
220	4. 375	8	12. 374
321	3. 307	10	12. 374
400	3. 094	32	12. 376
420	2. 768	100	12. 379
422	2. 526	42	12. 375
431	2. 428	5	12. 380
521	2. 259	21	12. 373
440	2. 188	6	12. 377
611	2. 0077	10	12. 376
444	1. 7865	14	12. 377
640	1. 7160	32	12. 374
721	1. 6842	7	12. 376
642	1. 6540	36	12. 377
732	1. 5720	3	12. 378
800	1. 5468	13	12. 374
840	1. 3837	10	12. 376
842	1. 3503	20	12. 376
921	1. 3348	3	12. 378
664	1. 3193	6	12. 376
10·2·0	1. 2138	5	12. 378
10·3·1	1. 1800	5	12. 376
10·4·0	1. 1491	15	12. 376
10·3·3	1. 1392	2	12. 375
10·4·2	1. 1297	10	12. 375
11·2·1	1. 1025	5	12. 376
880	1. 0938	6	12. 375
12·0·0	1. 0315	7	12. 378
12·2·0	1. 0173	8	12. 376
12·2·2	1. 0038	10	12. 376
11·6·3	0. 9603	3	12. 373
12·4·4	. 9328	5	12. 375
12·6·0	. 9224	9	12. 375
12·6·2	. 9123	6	12. 375
888	. 8931	7	12. 375
14·3·1	. 8623	3	12. 376
12·8·0	. 8581	3	12. 376
14·4·0	. 8500	8	12. 376
14·4·2	. 8422	8	12. 378
Average value of last five lines			12. 376

References

[1] S. Schneider and R. Roth, Solid state reactions involving oxides of trivalent cations (to be published in J. Research NBS).

[2] F. Bertaut and F. Forrat, Étude des combinaisions des oxides des terres rares avec l'alumine et la galline, Compt. rend. **243,** 1219–1222 (1956).

Lithium Arsenate, Li_3AsO_4 (orthorhombic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of lithium arsenate was prepared at NBS by reaction of solutions of lithium carbonate and arsenic (V) acid. The precipitate was washed and then heated to 1,000 °C for 10 min. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of antimony and lead; 0.01 to 0.1 percent each of aluminum, bismuth, calcium, magnesium, and silicon.

The sample was colorless. The refractive indices were not determined because the particle size of the sample was too small.

The *d*-values of the three strongest lines are: 3.89, 4.09, and 3.643 A.

Structural data. Zemann [1] in 1960 determined that lithium arsenate is probably isotypic with lithium phosphate, with the olivine structure, the space group D_{2h}^{16}—Pmnb (No. 62), and $4(Li_3AsO_4)$ per unit cell.

Lattice constant

		a	*b*	*c*
		A	*A*	*A*
1962	National Bureau of Standards.	6. 279	10. 768	4.955 at 25 °C

The density of lithium arsenate calculated from the NBS lattice constants is 3.166 g/cm³ at 25 °C.

Reference

[1] J. Zemann, Die Kristallstruktur von Lithiumphosphat, Li_3PO_4, Acta Cryst. **13,** 863–867 (1960).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
020	5. 39	36
120	4. 09	99
101	3. 89	100
021	3. 643	69
121	3. 151	45
200	3. 141	46
220	2. 712	52
040	2. 692	31
140, 002	2. 476	48
221	2. 377	227
041	2. 366	16
022	2. 249	4
141	2. 213	11
122	2. 118	19
240	2. 043	2
320	1. 950	12
202	1. 945	12
301	1. 927	9
241	1. 889	16
222	1. 828	15
042	1. 824	13
321	1. 8151	10
060	1. 7944	5
142	1. 7502	7
160	1. 7256	2
061	1. 6871	<1
340	1. 6521	7
161	1. 6294	12
103	1. 5975	7
023	1. 5788	6
242	1. 5761	7
400	1. 5695	14
260	1. 5582	22
322	1. 5322	7
420	1. 5071	2
062	1. 4539	3
421	1. 4419	6
223	1. 4104	16
342	1. 3746	6
440	1. 3561	3
080	1. 3462	<1
402	1. 3261	6
262	1. 3190	12
180, 412	1. 3158	12
361	1. 3139	10
081	1. 2986	3
303	1. 2968	3

Lithium Trimetaphosphate Trihydrate, $Li_3P_3O_9 \cdot 3H_2O$ (trigonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of lithium trimetaphosphate trihydrate was prepared at NBS by E. D. Eanes by adding an excess amount of $AgNO_3$ to a solution of $Na_3P_3O_9 \cdot 1\frac{1}{2}H_2O$. A slurry of the silver salt was metathesized with LiCl. After filtering to remove AgCl, the product was precipitated from solution with ethanol. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, barium, and sodium; and 0.001 to 0.01 percent each of aluminum, lead, magnesium, and silicon.

The sample is colorless and optically positive. The indices of refraction are $N_o = 1.468$, and $N_e = 1.472$.

The *d*-values of the three strongest lines are: 4.965, 3.128, and 6.24 A.

Structural data. The structure of lithium trimetaphosphate trihydrate was determined by E. D. Eanes [1] in 1961 at NBS. The space group is C_{3v}^5—R3m (No. 160) and $3(Li_3P_3O_9 \cdot 3H_2O)$ per hexagonal unit cell or $1(Li_3P_3O_9 \cdot 3H_2O)$ per rhombohedral unit cell.

Lattice constant

		a	*c*
		A	*A*
1962	National Bureau of Standards.	12. 513	5. 5900 at 25 °C

The density of lithium trimetaphosphate trihydrate calculated from the NBS lattice constants is 2.048 g/cm³ at 25 °C.

Reference

[1] E. D. Eanes and H. Ondik, The structure of lithium dipotassium trimetaphosphate monohydrate, Acta Cryst. **15**, 1280–1285 (1962).

hkl (hex)	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a = 3.1648$ A	
	d	*I*
	A	
110	6. 24	51
101	4. 965	100
021	3. 889	37
300	3. 610	13
211	3. 302	38
220	3. 128	66
012	2. 706	23
131	2. 647	29
202	2. 483	3
401	2. 437	8
410	2. 365	11
122	2. 309	7
321	2. 272	9
330	2. 085	10
312	2. 047	2
051	2. 021	2
042	1. 947	<1
241	1. 924	7
003, 232	1. 858	8
511	1. 838	3
600	1. 805	2
113	1. 786	6
520	1. 736	5
502	1. 712	1
431	1. 698	2
303	1. 657	1
422	1. 652	4
223	1. 601	3
152	1. 598	3
161	1. 585	5
440	1. 564	1
342	1. 502	2
701	1. 491	3
413	1. 4635	5
621	1. 4513	3
710	1. 4355	4
612	1. 4227	2
333	1. 3895	2
104	1. 3857	3
630	1. 3652	2
072	1. 3544	2
541	1. 3469	2

Lithium Tungstate Hemihydrate, $Li_2WO_4 \cdot \frac{1}{2}H_2O$ (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of lithium tungstate hemihydrate was obtained from the City Chemical Company, New York, N.Y. Upon fusion this substance loses 3.18 percent water and converts to the anhydrous trigonal form. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, copper, iron, lead, molybdenum, and silicon.

The sample was colorless. The refractive index was not determined because the particle size was too small.

The *d*-values of the three strongest lines are: 4.81, 2.774, and 3.398 A.

Lithium Tungstate Hemihydrate, $Li_2WO_4 \cdot \frac{1}{2}H_2O$ (cubic)—Continued

Structural data. No reference was found for the structure of this compound. The lattice is apparently primitive cubic and the unit cell probably contains $6(Li_2WO_4 \cdot \frac{1}{2}H_2O)$.

The density of lithium tungstate hemihydrate calculated from the NBS lattice constant is 4.682 g/cm³ at 25 °C. The average pycnometric density was approximately 4.3 g/cm³ at 25 °C.

Lattice constant

		a
		A
1962	National Bureau of Standards	8.3203 at 25 °C

hkl	1962 National Bureau of Standards Cu,1.5405 A at 25 °C Internal standard, tungsten, *a*=3.1648 A		
	d	*I*	*a*
	A		*A*
100	8. 32	47	8. 32
110	5. 89	8	8. 33
111	4. 81	100	8. 33
200	4. 16	15	8. 32
210	3. 723	30	8. 325
211	3. 398	81	8. 323
220	2. 942	30	8. 321
300	2. 774	82	8. 322
310	2. 631	38	8. 320
311	2. 509	9	8. 321
222	2. 402	13	8. 321
321	2. 224	11	8. 321
400	2. 080	11	8. 320
410	2. 018	33	8. 320
411	1. 9612	16	8. 3207
331	1. 9091	37	8. 3216
420	1. 8606	21	8. 3209
421	1. 8155	6	8. 3197
332	1. 7739	4	8. 3209
422	1. 6984	12	8. 3204
500	1. 6642	10	8. 3210
510	1. 6316	5	8. 3196
511	1. 6014	10	8. 3211
520	1. 5449	7	8. 3195
521	1. 5190	20	8. 3199
440	1. 4708	24	8. 3201
522	1. 4485	14	8. 3210
530	1. 4269	10	8. 3202
531	1. 4065	13	8. 3210
600	1. 3868	7	8. 3208
611	1. 3498	8	8. 3207
620	1. 3157	3	8. 3212
621	1. 2994	13	8. 3202
541	1. 2837	2	8. 3193
533	1. 2689	2	8. 3207

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C. Internal standard, tungsten, *a*=3.1648 A		
	d	*I*	*a*
	A		*A*
622	1. 2544	5	8. 3207
630	1. 2403	7	8. 3202
631	1. 2268	5	8. 3206
444	1. 2010	<1	8. 3208
700	1. 1887	2	8. 3209
710	1. 1766	3	8. 3198
711	1. 1651	9	8. 3205
720	1. 1428	4	8. 3197
721	1. 1323	7	8. 3207
642	1. 1118	6	8. 3199
722	1. 1022	2	8. 3214
730	1. 0924	5	8. 3195
731	1. 0832	2	8. 3202
650	1. 0653	2	8. 3203
732	1. 0567	4	8. 3205
800	1. 0401	3	8. 3208
810	1. 0320	10	8. 3203
811	1. 0242	6	8. 3206
733	1. 0166	7	8. 3212
820	1. 0090	6	8. 3204
821	1. 0017	3	8. 3207
653	0. 9946	2	8. 3214
822	. 9805	6	8. 3198
830	. 9738	2	8. 3202
831	. 9673	4	8. 3210
751	. 9608	3	8. 3208
662	. 9545	2	8. 3211
832	. 9481	2	8. 3195
900	. 9245	4	8. 3205
911	. 9133	6	8. 3206
842	. 9078	4	8. 3201
920	. 9024	1	8. 3197
921	. 8973	6	8. 3212
664	. 8869	1	8. 3199
922	. 8820	4	8. 3208
930	. 8771	2	8. 3209
931	. 8722	3	8. 3203
852	. 8628	3	8. 3205
932	. 8582	5	8. 3206
844	. 8492	6	8. 3204
940	. 8448	3	8. 3203
941	. 8405	2	8. 3205
933	. 8362	6	8. 3201
10·0·0	. 8320	2	8. 3200
10·1·0	. 8279	7	8. 3203
10·1·1	. 8239	1	8. 3206
Average value of last five lines			8. 3203

663956—63——4

Lutetium Gallium Oxide 3:5, $Lu_3Ga_2(GaO_4)_3$ (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of gallium oxide and lutetium oxide. The mixture was pressed into pellets and heated at 1,350 °C for 6 hr; then ground, remixed, and again pressed into pellets and heated at 1,450 °C for 6 hr. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of erbium and silicon; and 0.0001 to 0.001 percent each of dysprosium, yttrium, and ytterbium.

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

The *d*-values of the three strongest lines are: 2.724, 2.487, and 1.628 A.

Structural data. S. Schneider and R. Roth [1] showed that lutetium gallium oxide has the garnet structure, having the space group O_h^{10}—Ia3d (No. 230), and 8[$La_3Ga_2(GaO_4)_3$] per unit cell.

Lattice constant

1962	National Bureau of Standards.	A 12.183 at 26 °C

The density of lutetium gallium oxide 3:5 calculated from the NBS lattice constant is 7.826 g/cm³ at 26 °C.

Reference

[1] S. Schneider and R. Roth, Solid state reactions involving oxides of trivalent cations (to be published in J. Research NBS).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		A
211	4.973	19	12.181
220	4.308	6	12.185
321	3.256	12	12.183
400	3.046	31	12.184
420	2.724	100	12.182
422	2.487	44	12.184
510	2.389	3	12.182
521	2.224	13	12.181
440	2.154	3	12.185
611	1.976	12	12.181
631	1.796	2	12.181
444	1.758	17	12.180
640	1.689	32	12.180
721	1.658	6	12.184
642	1.628	34	12.181
732	1.547	3	12.181
800	1.523	14	12.184
653	1.456	2	12.182
822	1.436	2	12.185
752	1.3797	1	12.185
840	1.3620	8	12.182
842	1.3291	21	12.181
921	1.3138	2	12.184
664	1.2986	7	12.182
932	1.2566	2	12.183
10·1·1	1.2063	1	12.183
10·2·0	1.1947	2	12.184
10·3·1	1.1617	3	12.184
10·4·0	1.1311	20	12.182
10·3·3	1.1215	2	12.183
10·4·2	1.1120	7	12.181
11·2·1	1.0853	3	12.182
880	1.0768	8	12.183
11·3·2	1.0523	2	12.181
10·6·0	1.0447	2	12.183
12·0·0	1.0151	5	12.181
12·2·0	1.0014	5	12.183
11·5·2	0.9947	1	12.183
12·2·2	.9881	8	12.182
11·6·1	.9691	1	12.181
11·6·3	.9455	<1	12.182
13·2·1	.9235	1	12.181
12·4·4	.9183	6	12.183
12·6·0	.9080	12	12.182
13·3·2	.9031	1	12.183
12·6·2	.8981	5	12.182
888	.8792	5	12.183
14·1·1	.8657	1	12.181
14·2·0	.8615	1	12.184
14·3·1	.8488	2	12.183
12·8·0	.8447	4	12.182
14·4·0	.8368	12	12.184
14·4·2	.8289	10	12.182
Average value of last five lines			12.183

Lutetium Manganite, $LuMnO_3$ (hexagonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of lutetium manganite was prepared at NBS by S. Schneider from stoichiometric mixtures of lutetium oxide and manganous carbonate. The mixture was pressed into pellets and heated at 1,000 °C for 41 hr then reheated at 1,150 °C for 21 hr. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium and magnesium; and 0.001 to 0.01 percent each of aluminum and silicon.

The sample was a black opaque powder.

The *d*-values of the three strongest lines are: 2.668, 3.022 and 1.7449A.

Structural data. Yakel, Koehler, Bertaut, and Forrat [1] in 1960 determined that lutetium manganite has the space group C_{6v}^3—$P6_3cm$ (No. 185), and 6[$LuMnO_3$][5] per unit cell.

Lattice constants

		a	*c*
		A	*A*
1960	Yakel, Koehler, Bertaut, and Forrat. [1]	6. 0428	11. 369
1962	National Bureau of Standards.	6. 0455	11. 394 at 25 °C.

[5] The density based on pyenometer measurements of a pressed pellet is 7.5 g/cm³. indicating the number of molecules per unit cell as 6.

The density of lutetium manganite calculated from the NBS lattice constants is 7.676 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
02	5. 694	34
002	3. 851	11
110	3. 022	53
111	2. 922	26
004	2. 848	29
112	2. 668	100
104	2. 501	9
202	2. 378	5
114	2. 073	36
204	1. 927	6
212	1. 869	5
115	1. 820	7
106	1. 785	11
300	1. 7449	39
302	1. 6684	10
214	1. 6252	7
116	1. 6075	19
206	1. 5370	6
220	1. 5112	9
221	1. 4979	5
304	1. 4877	27
222	1. 4609	15
117	1. 4334	3
008	1. 4246	3
312	1. 4071	1
108	1. 3741	8
216	1. 3701	3
224	1. 3351	8
314	1. 2940	3
118	1. 2882	4
225	1. 2595	4
208	1. 2511	2
404	1. 1895	2
226	1. 1826	5
322	1. 1752	2

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal Standard, tungsten, a=3.1648 A	
	d	*I*
	A	
218	1. 1561	5
316	1. 1534	5
410	1. 1425	5
411	1. 1370	2
412	1. 1203	1
1·0·10	1. 1131	4
227	1. 1072	6
308	1. 1034	2
406	1. 0777	1
1·1·10	1. 0661	1
414	1. 0603	7
2·0·10	1. 0447	3
228	1. 0364	3
502	1. 0297	2
415	1. 0213	1
318	1. 0166	4
1·0·11	1. 0158	1
330	1. 0077	4
332	0. 9923	2
2·1·10	. 9874	2
416	. 9791	4
408	. 9638	1
417	. 9351	2
1·0·12	. 9344	1
328	. 9181	3
3·1·10	. 8964	3
2·0·12	. 8928	2

Reference

[1] H. L. Yakel, W. C. Koehler, E. F. Bertaut, and E. F. Forrat, Erbium manganite—a new ABO_3 structure, Acta Cryst. **13,** 1015 (1960).

Manganese(II) Tungstate (huebnerite), $MnWO_4$ (monoclinic)

Powder Data cards

Card number	Index lines	Radiation	Source
10–477	3. 00 2. 96 3. 78	Iron	Berry [1].

Additional published patterns. None.

NBS sample. The sample of manganese tungstate was prepared at NBS by reacting solutions of manganese(II) chloride and sodium tungstate. The precipitate was washed, dried, and heated to 1,000 °C for 10 min. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of silicon, and 0.001 to 0.01 percent of calcium.

The color of the sample was yellow brown. The refractive indices were not determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are: 2.996, 2.954, and 4.84 A.

Structural data. Broch [2] in 1929 determined that manganese tungstate has magnesium tungstate structure, the space group C_{2h}^4—P2/c (No. 13), and 2($MnWO_4$) per unit cell. The lattice constants of Broch have been converted from kX to angstrom units for comparison with the NBS values.

The density of manganese tungstate calculated from the NBS lattice constants is 7.234 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
010	5. 76	22
100	4. 84	63
011	3. 78	59
110	3. 70	56
$\bar{1}11$	2. 996	100
111	2. 954	95
020	2. 880	29
002, 021	2. 497	54
120	2. 474	9
200	2. 416	19
$\bar{1}02$	2. 237	16
121	2. 209	26
$\bar{1}12$	2. 087	7
112	2. 057	11
$\bar{2}11$	2. 051	12
211	2. 021	10
030	1. 9205	5
022	1. 8871	16
220	1. 8507	16
130	1. 7843	26
$\bar{1}22$	1. 7666	6
$\bar{2}02$	1. 7539	19
$\bar{2}21$	1. 7440	19
221	1. 7266	28
202	1. 7196	20
$\bar{1}31$	1. 6839	4
$\bar{2}12$	1. 6777	5
131	1. 6762	5
212	1. 6472	3
300	1. 6096	3
013	1. 5996	6
310	1. 5501	2
$\bar{1}13$	1. 5273	16
032	1. 5221	12
113	1. 5100	12
230	1. 5023	8
$\bar{2}22$	1. 4981	8
$\bar{3}11$	1. 4886	16
222	1. 4754	11
311	1. 4723	16
$\bar{1}32$	1. 4568	12
132	1. 4467	12
023	1. 4423	15
320	1. 4048	2
$\bar{1}23$	1. 3879	4
041	1. 3834	11
123	1. 3751	3
$\bar{3}02$	1. 3654	2
$\bar{3}21$	1. 3587	6
321, $\bar{2}13$	1. 3458	4
302	1. 3408	4
$\bar{1}41$	1. 3316	4
141, $\bar{3}12$	1. 3284	8
213	1. 3216	3
312	1. 3056	2
$\bar{2}32$	1. 2949	4
232	1. 2804	4

References

[1] L. G. Berry, Queen's University, Kingston, Ontario, Canada.

[2] E. K. Broch, Untersuchungen über Kristallstrukturen des Wolframittypus und des Scheelittypus, Skrifter Norsk. Videns.-Akad. Oslo I. Mat.-Naturv. Kl **1929**, No. 8.

Manganese (II) Tungstate (huebnerite), $MnWO_4$ (monoclinic)—Continued

Lattice constants

		a	*b*	*c*	*β*
		A	*A*	*A*	
1930	Broch [2]	4. 85	5. 77	4. 98	90.88°
1962	National Bureau of Standards	4. 829	5. 759	4. 998	91.16° at 25 °C

Mercury (II) Fluoride, HgF_2 (cubic)

Powder Data cards. None

Additional published patterns. None.

NBS sample. The sample of mercury (II) fluoride was obtained from the A. D. Mackay Company, Inc., New York, N.Y. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of silicon, and 0.001 to 0.01 percent of tin.

The color of the sample was orange. The refractive index was not determined because of the small particle size.

The *d*-values of the three strongest lines are: 3.196, 1.9576, and 2.768 A.

Structural data. Ebert and Woitnek [1] in 1933 determined that mercury (II) fluoride has the fluorite structure, the space group O_h^5—Fm3m (No. 225), and 4(HgF_2) per unit cell. The lattice constant of Ebert and Woitnek has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1933	Ebert and Woitnek [1]	5. 55
1962	National Bureau of Standards	5. 5373 at 25 °C

The density of mercury (II) fluoride calculated from the NBS lattice constant is 9.332 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standards, tungsten, a=3.1648 A		
	d	*I*	*a*
	A		*A*
111	3. 196	100	5. 536
200	2. 768	43	5. 537
220	1. 9576	46	5. 5369
311	1. 6695	40	5. 5371
222	1. 5983	8	5. 5367
400	1. 3844	7	5. 5376
331	1. 2705	12	5. 5380
420	1. 2383	9	5. 5378
422	1. 1302	9	5. 5368
511	1. 0657	7	5. 5375
440	0. 9789	4	5. 5377
531	. 9361	10	5. 5379
600	. 9229	7	5. 5373
620	. 8756	8	5. 5377
533	. 8444	8	5. 5368
622	. 8348	4	5. 5372
444	. 7993	2	5. 5374
Average value of last five lines			5. 5373

Reference

[1] F. Ebert and H. Woitnek, Kristallstrukturen von Fluoriden. II. HgF, HgF_2, CuF und CuF_2, Z. anorg. u. allgem. Chem. **210,** 269–272 (1933).

Nickel Sulfate, $NiSO_4$ (orthorhombic)

Powder Data cards.

Card number	Index lines	Radiation	Source
1–1102	2. 55 4. 30 3. 58	Molybdenum	Dow Chemical Company, Midland, Michigan.

Additional published pattern. Hammel [1] 1939.

NBS sample. The sample of nickel sulfate was prepared by heating nickel sulfate hexahydrate, obtained from Baker and Adamson Chemical Co., with H_2SO_4 at 160 °C. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, iron, magnesium, and silicon; and 0.0001 to 0.001 percent each of barium and copper.

The color of the sample was greenish-yellow.

The optical sign and the N_β could not be determined because the sample was too fine-grained. The other refractive indices were $N_\alpha = 1.695$ and $N_\gamma = 1.723$.

The *d*-values of the three strongest lines are: 2.553, 3.564, and 3.334 A.

Structural data. Dimaras [2] in 1957 determined the structure of nickel sulfate; it has the space group D_{2h}^{17}—Cmcm (No. 63) and 4($NiSO_4$) per unit cell. Hammel [1] had previously reported lattice constants for nickel sulfate as $a = 4.63$, $b = 6.52$, and $c = 8.51$ A.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1957	Dimaras [2]	5. 155	7. 842	6. 338
1962	National Bureau of Standards.	5. 1596	7. 8362	6. 3378 25 °C.

The density of nickel sulfate calculated from the NBS lattice constants is 4.011 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a = 3.1648$ A	
	d	*I*
	A	
110	4. 314	41
020	3. 921	28
111	3. 564	80
021	3. 334	50
200	2. 579	47
112	2. 553	100
130	2. 331	48
220	2. 156	3
221	2. 037	5
202	2. 001	27
040	1. 959	16
132	1. 879	7
023	1. 860	8
222	1. 781	25
310	1. 679	7
042	1. 667	15
311	1. 629	8
004	1. 5845	10
133	1. 5652	7
241	1. 5147	7
150	1. 4999	6
312	1. 4839	12
024	1. 4691	7
151	1. 4592	3
330	1. 4363	13
242	1. 3996	26
152	1. 3552	6
134	1. 3104	5
400	1. 2894	20
243	1. 2545	3
153	1. 2229	3
115	1. 2161	4
421	1. 2027	3

References

[1] F. Hammel, Contribution á l'étude des sulfates de la série magnésienne, Ann. chim. **11,** 247–358 (1939).

[2] P. I. Dimaras, Morphology and structure of anhydrous nickel sulfate, Acta Cryst. **10,** 313–315 (1957).

Nickel Tungstate, $NiWO_4$ (monoclinic) [6]

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of nickel tungstate was prepared at NBS by the reaction of solutions of nickel chloride and sodium tungstate. The precipitate was washed, dried, and heated to 1,100 °C for 15 min. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of silicon; and 0.001 to 0.01 percent each of aluminum, calcium, lead, and magnesium.

The color of the sample was light brown. The refractive indices were not determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are: 2.889, 1.6788, and 2.455 A.

Structural data. Broch [1] in 1929 determined that nickel tungstate has the magnesium tungstate structure, the space group C_{2h}^4—P2/c (No. 13), and 2 ($NiWO_4$) per unit cell. The lattice constants of Broch have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*	*β*
		A	*A*	*A*	
1930	Broch [1]	4. 69	5. 67	4. 94	89. 67°
1957	Keeling [2].	4. 60	5. 66	4. 91	90. 08°
1962	National Bureau of Standards.	4. 600	5. 665	4. 912	≈90. at 25 °C

The density of nickel tungstate calculated from the NBS lattice constants is 7.952 g/cm³ at 25 °C.

hkl (ortho.) [6]	1962 National Bureau of Standards Cu, 1 5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
010	5. 67	7
100	4. 60	32
011	3. 71	34
110	3. 57	34
111	2. 889	100
020	2. 834	15
002, 021	2. 455	39
120	2. 412	7
200	2. 301	12
102, 121	2. 166	25
210	2. 131	2
112	2. 024	11
211	1. 955	11
030	1. 888	3
022	1. 856	10
220	1. 786	7
130	1. 7471	19
122	1. 7208	6
202, 221	1. 6788	40
131	1. 6452	1
212	1. 6091	2
013	1. 5729	3
300	1. 5337	2
032	1. 4973	4
113	1. 4882	17
310	1. 4801	2
230	1. 4596	3
222	1. 4441	7
132	1. 4234	16
311, 023	1. 4173	23
041	1. 3609	7
123	1. 3546	3
320	1. 3485	1
141	1. 3047	5
302, 321	1. 3008	7
312	1. 2676	3
232	1. 2549	3
004, 042	1. 2276	3
223, 240	1. 2068	3
330	1. 1905	5
322	1. 1824	2
241	1. 1712	7
114	1. 1610	1
400	1. 1498	2
050	1. 1331	1
410, 024	1. 1266	1
150	1. 0998	4
411, 313	1. 0980	7

References

[1] E. K. Broch, Untersuchungen über Kristallstrukturen des Wolframittypus und des Scheelittypus, Skrifter Norsk. Videns.-Akad. Oslo I. Mat.-Naturv. Kl. **1929** No. 8.

[2] R. O. Keeling, Jr., The structure of $NiWO_4$, Acta Cryst. **10**, 209–213 (1957).

[6] (Separation of monoclinic doublets was not detected in the NBS pattern, so it was indexed as orthorhombic.)

Potassium Chlororhenate, K_2ReCl_6 (cubic)

Powder Data cards

Card number	Index lines	Radiation	Source
3-0085	5. 7 2. 47 2. 98	Copper---	Aminoff [1] 1936.

Additional published patterns. None.

NBS sample. The sample of potassium chlororhenate was prepared at NBS by R. Johannesen from chlororhenic acid. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent silicon, sodium, and rubidium; and 0.0001 to 0.001 percent of calcium.

The color of the sample was yellow. The refractive index could not be determined because the color was too intense.

The *d*-values of the three strongest lines are: 5.68, 3.48, and 2.967 A.

Structural data. Aminoff [1] in 1936 determined that potassium chlororhenate has the potassium chloroplatinate structure,t he space group O_h^5—Fm3m (No. 225) and $4(K_2ReCl_6)$ per unit cell. The unit cell measurement reported by Aminoff has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1936	Aminoff [1]----------	9. 881
1962	National Bureau of Standards.	9. 840 at 25 °C.

The density of potassium chlororhenate calculated from the NBS lattice constant is 3.325 g/cm³ at 25 °C.

Reference

[1] Brita Aminoff, Über die Kristallstruktur von K_2ReCl_6, Z. Krist. (A) **94,** 246–248 (1936).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, silver, a=4.0861 A		
	d	*I*	*a*
	A		A
111	5. 68	100	9. 84
200	4. 92	39	9. 85
220	3. 48	42	9. 84
311	2. 967	42	9. 842
222	2. 840	8	9. 839
400	2. 460	40	9. 841
331	2. 257	15	9. 838
420	2. 201	15	9. 843
422	2. 008	15	9. 840
511	1. 894	15	9. 842
440	1. 739	19	9. 840
531	1. 663	13	9. 839
600	1. 640	6	9. 839
620	1. 556	4	9. 838
533	1. 500	3	9. 839
444	1. 420	5	9. 840
711	1. 3781	6	9. 842
640	1. 3647	2	9. 841
642	1. 3152	4	9. 842
731	1. 2813	3	9. 842
800	1. 2300	<1	9. 840
733	1. 2022	<1	9. 840
820	1. 1933	2	9. 840
822	1. 1598	2	9. 841
751	1. 1364	2	9. 842
840	1. 1003	3	9. 841
911	1. 0803	2	9. 842
842	1. 0740	2	9. 843
664	1. 0491	<1	9. 841
931	1. 0315	<1	9. 840
844	1. 0046	2	9. 843
933	0. 9890	1	9. 840
10·0·0	. 9843	<1	9. 843
10·2·0	. 9650	1	9. 841
951	. 9514	<1	9. 841
953	. 9175	1	9. 839
10·4·0	. 9135	2	9. 839
10·4·2	. 8984	<1	9. 841
11·1·1	. 8874	<1	9. 842
880	. 8699	<1	9. 842
11·3·1	. 8598	3	9. 841
10·4·4	. 8567	<1	9. 843
10·6·0	. 8439	<1	9. 841
11·3·3	. 8347	<1	9. 841
12·0·0	. 8201	1	9. 841
11·5·1	. 8115	<1	9. 839
12·2·2	. 7981	<1	9. 840
11·5·3	. 7904	<1	9. 840
Average value of last five lines-------			9. 840

Potassium Nitroso Chlororuthenate, K_2RuCl_5NO

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium nitroso chlororuthenate was prepared at NBS by R. Johannesen by heating together on a steam bath a soluble ruthenium salt, potassium chloride, and concentrated nitric acid.

The color of the sample was very dark red. The refractive indices are $N_\alpha=1.750$, $N_\beta=1.762$, and $N_\gamma=1.777$. 2V is approximately 90°.

The *d*-values of the three strongest lines are: 5.75, 5.62, and 2.594 A.

Structural data. The structure of potassium nitroso chlororuthenate has not been reported.

1962 National Bureau of Standards
Cu, 1.5405 A at 25 °C
Internal standard, tungsten, $a=3.1648$ A

d	*I*
A	
6.50	<4
6.39	<4
6.13	8
5.75	100
5.62	93
5.28	17
5.20	27
4.79	29
4.36	<4
4.08	6
3.96	10
3.73	4
3.52	23
3.45	27
3.328	16
3.176	<4
3.091	12
3.059	11
3.027	15
2.996	14
2.934	7
2.873	13
2.805	36
2.720	36
2.632	8
2.594	48
2.481	<4
2.409	7
2.393	10
2.277	15
2.262	10
2.211	10
2.167	<4
2.137	<4
2.105	7
2.071	14
2.063	16
2.037	7
1.999	4
1.980	10

Rubidium Perchlorate, $RbClO_4$ (orthorhombic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium perchlorate was prepared at NBS by the reaction of a solution of rubidium nitrate with perchloric acid. The precipitate was recrystallized several times to improve the purity. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of cesium, potassium, and sodium; and 0.001 to 0.01 percent of silicon.

The sample is colorless and optically negative with the indices of refraction $N_\alpha=1.465$, $N_\beta=1.470$, and $N_\gamma=1.472$. $2V=60°$.

The **d**-values of the three strongest lines are: 3.63, 3.26, and 2.228 A.

Structural data. Büssem and Herrmann [1] in 1928 determined that rubidium perchlorate has the potassium sulfate structure, the space group D_{2h}^{16}-Pbnm (No. 62), and 4($RbClO_4$) per unit cell. At 279 °C the orthorhombic form transforms to face-centered cubic. The lattice constants of Büssem and Herrmann have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1928	Büssem and Herrmann [1].	7. 55	9. 29	5. 82
1962	National Bureau of Standards.	7. 490	9. 269	5. 814 at 25 °C

The density of rubidium perchlorate calculated from the NBS lattice constants is 3.042 g/cm³ at 25 °C.

Reference

[1] W. Büssem and K. Herrmann, Röntgenographische Untersuchung der einwertigen Perchlorate, Z. Krist **67,** 405–408 (1928).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A	
	d	*I*
	A	
111	4. 12	23
200	3. 74	41
021	3. 63	100
210	3. 47	50
121	3. 26	89
211	2. 982	51
002	2. 907	37
130	2. 858	7
221	2. 605	22
022	2. 464	8
310	2. 410	3
230	2. 384	4
122	2. 339	16
040	2. 318	<1
311	2. 228	60
140	2. 214	38
231	2. 206	38
041	2. 153	8
321	2. 057	<1
132	2. 038	4
330	1. 9418	10
103	1. 8765	3
400	1. 8725	3
331	1. 8416	5
410	1. 8356	4
150	1. 7997	1
023	1. 7875	5
142	1. 7609	10
411	1. 7505	4
123	1. 7387	6
420	1. 7357	4
340	1. 6984	4
213	1. 6928	8
421	1. 6633	1
250	1. 6609	2
332	1. 6145	13
251	1. 5970	3
402	1. 5741	2
412	1. 5518	5
431	1. 5438	2
303	1. 5303	1

Rubidium Periodate, $RbIO_4$ (tetragonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium periodate was prepared at NBS by the reaction of solutions of sodium periodate and rubidium nitrate. The precipitate obtained was recrystallized several times to improve the purity. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of sodium; 0.01 to 0.1 percent of potassium; and 0.001 to 0.01 percent each of cesium and silicon.

The sample was colorless and optically positive with the refractive indices N_o=1.603 and N_e=1.621.

The *d*-values of the three strongest lines are: 3.52, 2.193, and 2.961 A.

Structural data. Beintema [1] in 1937 determined that rubidium periodate has the scheelite structure, the space group C_{4h}^6—$I4_1/a$ (No. 88), and 4($RbIO_4$) per unit cell. The unit cell measurements reported by Beintema have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1937	Beintema [1]	5. 89	12. 96
1962	National Bureau of of Standards.	5. 921	13. 052 at 25 °C.

The density of rubidium periodate calculated from the NBS lattice constants is 4.011 g/cm³ at 25 °C.

Reference

[1] J. Beintema, Die Kristallstruktur der Alkaliperrhenate und—jodate, Z. Krist **97A,** 300–332 (1937).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
101	5. 39	14
112	3. 52	100
004	3. 26	17
200	2. 961	20
202	2. 694	<1
211	2. 594	3
114	2. 573	2
213	2. 262	1
204	2. 193	22
220	2. 093	10
222	1. 9939	<1
116	1. 9301	11
215	1. 8585	2
312	1. 7994	17
224	1. 7618	10
321, 008	1. 6300	2
305	1. 5739	<1
323	1. 5356	<1
217	1. 5237	<1
400	1. 4796	2
208	1. 4283	6
316	1. 4186	9
332	1. 3642	4
404	1. 3476	3
420	1. 3237	3
228	1. 2864	2
1·1·10	1. 2454	1
424	1. 2262	3
501	1. 1788	<1
336	1. 1750	1
512	1. 1438	3
408	1. 0964	1
0·9·12	1. 0880	<1
3·1·10	1. 0711	1
440	1. 0468	<1
428	1. 0283	1
516	1. 0248	2
2·0·12	1. 0212	1
532	1. 0034	1
444	0. 9969	1
600	. 9869	<1
2·2·12	. 9650	1
3·3·10	. 9532	<1
604	. 9447	<1
620	. 9363	<1
536	. 9200	1
1·1·14	. 9100	<1
624	. 8997	1
448	. 8808	3

Silver Selenate, Ag_2SeO_4 (orthorhombic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of silver selenate was obtained from City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent sodium; and 0.001 to 0.01 percent each of calcium, magnesium, and silicon.

The color of the sample was grey-white. The indices of refraction could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are: 2.930, 2.742, and 3.246 A.

Structural data. Herrman and Ilge [1] in 1931 determined that silver selenate has the silver sulfate structure, the space group D_{2h}^{24}—Fddd (No. 70), and 8(Ag_2SeO_4) per unit cell. The unit cell measurements reported by Herrman and Ilge have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1931	Herrman and Ilge [1].	10. 232	12. 841	6. 081
1962	National Bureau of Standards.	10. 388	12. 981	6. 0499 at 25 °C

The density of silver selenate calculated from the NBS lattice constants is 5.839 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
220	4. 061	6
040	3. 246	73
311	2. 930	100
022	2. 742	81
202	2. 615	4
331	2. 469	37
222	2. 425	4
151	2. 325	3
242	2. 036	4
260	1. 997	4
351	1. 965	37
511	1. 945	6
531	1. 791	2
062	1. 7599	23
313	1. 7278	15
620	1. 6740	7
080	1. 6226	6
333	1. 6170	14
371	1. 5786	12
004	1. 5127	7
602	1. 5038	7
353	1. 4473	6
224	1. 4173	<1
044	1. 3707	8
642	1. 3638	10
660	1. 3523	7
391	1. 3001	5
373	1. 2698	4
751	1. 2610	1
0·10·2	1. 1926	5
315	1. 1380	3
911	1. 1303	2
624	1. 1222	3
393	1. 1110	2
084	1. 1064	3
682	1. 1033	3
3·11·1	1. 0985	2
0·12·0	1. 0817	2
355,862	1. 0456	2
6·10·0	1. 0391	3
664	1. 0083	2
026	0. 9966	1
3·11·3	. 9771	1

Reference

[1] K. Herrman and W. Ilge, Die Struktur des Silbersulfats, Z. Krist. **80,** 402–415 (1931).

Sodium Cyanate, NaCNO (trigonal)

Powder Data cards. None.

Additional published pattern. None.

NBS sample. The sample of sodium cyanate was obtained from the City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, iron, magnesium, and silicon; and 0.001 to 0.01 percent each of barium, nickel, and strontium.

The color of the sample was white and it is optically positive. The indices of refraction are $N_e = 1.629$, and $N_0 \approx 1.390$

The *d*-values of the three strongest lines are: 2.872, 1.794, and 2.167 A.

Structural data. Bassière [1] in 1938 determined that sodium cyanate has the sodium hydrofluoride structure, the space group C_{3v}^5—R3m (No. 160) with 3(NaCNO) per unit cell. The unit cell measurements reported by Bassière have been coverted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1938	Bassière [1]_____	3. 583	15. 13
1962	National Bureau of Standards.	3. 5851	15.110 at 25 °C.

The density of sodium cyanate calculated from the NBS lattice constants is 1.949 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a = 3.1648$ A	
	d	*I*
	A	
003	5. 038	7
101	3. 044	11
012	2. 872	100
006	2. 517	1
104	2. 400	10
015	2. 167	18
110	1. 794	21
107	1. 774	9
113	1. 689	2
009	1. 6788	2
018	1. 6134	2
021	1. 5442	<1
202	1. 5210	6
116	1. 4605	<1
024	1. 4357	1
205	1. 3810	2
1·0·10	1. 3589	3
027	1. 2600	3
119	1. 2253	1
208	1. 1989	<1
122	1. 1595	2
214	1. 1206	1
125	1. 0937	<1
0·2·10	1. 0827	<1
300	1. 0348	1
217	1. 0307	2
0·1·14	1. 0194	<1
2·1·10	0. 9270	1
1·0·16	. 9035	1
220	. 8964	1
2·0·14	. 8863	<1

Reference

[1] M. Bassière, Sur la structure de l'isocyanate de sodium, Compt. rend. **206,** 1309–1311 (1938)

Sodium Orthotungstate (VI) Dihydrate, $Na_2WO_4 \cdot 2H_2O$ (orthorhombic)

Powder Data cards

Card number	Index lines	Radiation	Source
1–0107	6. 9 4. 22 3. 17	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of sodium orthotungstate dihydrate was obtained from the Allied Chemical and Dye Corp., New York, N.Y. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of calcium and lead.

The sample is colorless and optically positive. The indices of refraction are $N_\alpha = 1.554$, $N_\beta = 1.556$, and $N_\gamma = 1.568$.

The *d*-values of the three strongest lines are: 6.91, 3.17, and 4.23 A.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1960	Pistorius [3]___	10. 601	13. 842	8. 456
1962	National Bureau of Standards.	10. 604	13. 844	8. 455 at 25 °C.

The density of sodium orthotungstate dihydrate calculated from the NBS lattice constants is 3.523 g/cm³ at 25 °C.

Structural data. Poljak and Becka [2] in 1958 determined that sodium orthotungstate dihydrate is isomorphous with sodium orthomolybdate dihydrate, having the space group D_{2h}^{15}—Pbca (No. 61) and $8(Na_2WO_4 \cdot 2H_2O)$ per unit cell.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, silver, a=4.0861 A	
	d	*I*
	A	
020	6. 91	100
111	5. 98	22
200	5. 29	21
121	4. 78	15
002	4. 23	63
220	4. 21	2
131	3. 79	15
022	3. 61	60
040	3. 46	17
122	3. 42	6
202	3. 309	47
231	3. 221	14
311	3. 173	80
141	3. 069	36
132	2. 988	54
240	2. 898	22
241	2. 745	6
232	2. 684	43
331, 312	2. 664	38
410	2. 601	6
151	2. 556	1
420	2. 475	2
250	2. 457	6
242	2. 394	11
251	2. 359	8
133	2. 347	8
060	2. 309	6
430	2. 302	6
043, 161	2. 181	30
143	2. 145	8
252	2. 121	15
004, 351	2. 112	12
440	2. 106	4
511	2. 034	30
062	2. 028	20
162	1. 993	18
521	1. 970	6
450	1. 915	3
171	1. 894	22
442	1. 886	12
531	1. 879	15
270	1. 855	4
271	1. 809	6
063	1. 789	6
433	1. 784	5
600	1. 766	8
172	1. 764	9
452	1. 746	8
080	1. 732	2
353	1. 728	11
620	1. 712	9
272	1. 699	5
513	1. 684	19
621, 181	1. 676	19
551	1. 652	7
523	1. 646	5
462	1. 610	3
344	1. 605	6
372	1. 596	9
363	1. 592	9
182	1. 583	5
640	1. 576	4
552	1. 563	4
064	1. 559	3
632	1. 538	1
561	1. 535	1
282	1. 531	3
235	1. 521	7
145	1. 508	2
191	1. 500	2
650	1. 489	3
472	1. 486	10
711	1. 483	8
642	1. 476	2
623	1. 464	7
291, 480, 335	1. 452	2
553	1. 445	3
174, 155	1. 431	1
364, 702	1. 426	2
534, 283	1. 422	5
415	1. 418	5
652	1. 405	2
660	1. 402	2
345	1. 396	3
0·10·0	1. 386	2
643, 544	1. 373	2
563	1. 365	2
604	1. 356	10

References

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

[2] R. J. Poljak and L. N. Becka, Estudio cristalográfico del molbdato de sodio dihidrato, Anales asoc. quím. argentina, **46**, 199–203 (1958).

[3] C. W. F. T. Pistorius, Unit cell and space group of sodium molybdate dihydrate, Z. Krist. **114**, 154–155 (1960).

Sodium Tetrametaphosphate Tetrahydrate, high form $Na_4P_4O_{12}\cdot 4H_2O$ (triclinic)

Powder Data cards

Card number	Index lines	Radiation	Source
*11–389	9. 4 5. 2 3. 10	Copper	Corbridge and Tromans (1) 1958.

*This card refers to the high form and identifies it as alpha-sodium tetrametaphosphate tetrahydrate.

Additional published patterns. Thilo and Rätz [2] 1949, Bell, Audrieth, and Hill [3] 1952, and Bonneman [4] 1937.

NBS sample. The sample of sodium tetrametaphosphate tetrahydrate was prepared at NBS by H. Ondik according to the Warschauer [5] process and purified by the method used by Barney and Gryder [6]. The triclinic form was obtained by precipitating very slowly from solutions with alcohol above approximately 30 °C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, chromium, and tungsten; and 0.001 to 0.01 percent each of iron, magnesium, manganese, nickel, silver, tin, titanium, and zirconium.

The sample is colorless.

The *d*-values of the three strongest lines are: 5.17, 9.25, and 3.075 A.

Structural data. Ondik [7] in 1961 determined the structure of the high temperature form of sodium tetrametaphosphate tetrahydrate which has the space group C_i^1—$P\bar{1}$ (No. 2) with 1 ($Na_4P_4O_{12}\cdot 4H_2O$) per unit cell. The low temperature form of sodium tetrametaphosphate tetrahydrate is reported on Powder Data cards numbered 11–15 and 11–15a.

The density of sodium tetrametaphosphate tetrahydrate calculated from the NBS lattice constants is 2.146 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal Standard, Tungsten, a=3.1648 A	
	d	*I*
	A	
010	9. 25	95
100	6. 31	31
001	5. 83	30
$0\bar{1}1$	5. 64	54
$\bar{1}10$	5. 56	9
$\bar{1}01$	5. 17	100
110	4. 90	65
$1\bar{1}1$	4. 756	30
020	4. 616	8
011	4. 438	25
$\bar{1}11$	4. 300	34
$\bar{1}20$	3. 988	13
$1\bar{1}1$	3. 803	46
120	3. 505	30
$1\bar{2}1$	3. 332	39
021	3. 234	67
$\bar{2}01$	3. 227	37
200	3. 153	24
$\bar{2}10$	3. 115	91
$1\bar{1}2$, 030, $0\bar{3}1$	3. 075	93
$\bar{2}11$	3. 046	32
$\bar{1}02$	3. 037	32
$\bar{1}30$, 002	2. 920	12
210	2. 867	3
$0\bar{2}2$	2. 819	28
$\bar{1}31$	2. 795	35
$\bar{2}20$	2. 785	11
$\bar{1}12$	2. 724	5
$\bar{2}21$	2. 656	23
$\bar{2}21$	2. 637	24
130	2. 631	30
121	2. 609	41
012	2. 598	38
$\bar{1}31$	2. 514	8
031	2. 471	21
$0\bar{3}2$	2. 461	42
220	2. 454	34
$\bar{1}32$	2. 428	1
$1\bar{2}2$	2. 385	8
102	2. 378	18
$\bar{2}30$	2. 367	14
$\bar{1}22$	2. 326	7
040	2. 309	5
$\bar{1}40$	2. 268	8
$\bar{2}31$	2. 235	7
$1\bar{4}1$, $\bar{2}31$	2. 220	13
$\bar{1}41$	2. 209	21
$1\bar{3}2$	2. 180	7
$\bar{3}11$	2. 172	7
$\bar{2}22$	2. 148	1
$\bar{3}10$	2. 112	13
$\bar{1}13$	2. 106	15
300	2. 102	11
$\bar{2}30$	2. 067	5
$\bar{1}42$, $\bar{1}23$	2. 054	7

References

[1] D. E. C. Corbridge and F. R. Tromans, Identification of sodium phosphates with an x-ray focusing camera, Anal. Chem. **30,** 1101–1110 (1958).

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

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

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

[5] F. Warschauer, Z. anorg. allgem. Chem. **36,** 137 (1903).

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

[7] Helen M. Ondik and Stanley Block, The structure of the monoclinic form of sodium tetrametaphosphate tetrahydrate, Acta Cryst. **14,** 555–561 (1961).

Sodium Tetrametaphosphate Tetrahydrate, high form $Na_4P_4O_{13}\cdot 4H_2O$ (triclinic)—Con.

Lattice constants

		a	*b*	*c*	α	β	γ
		A	*A*	*A*			
1962	National Bureau of Standards.	6. 653	9. 577	6. 321	103. 40°	106. 98°	93. 29° at 25 °C

Strontium Arsenate, $Sr_3(AsO_4)_2$ (trigonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of strontium arsenate was prepared at NBS by reacting solutions of strontium chloride and arsenic(V) acid. The precipitate was washed several times, dissolved in nitric acid, repreeipitated by addition of ammonia, and heated to 1,110 °C for 1 hour. Speetrographic analysis showed the following impurities: 0.01 to 0.1 pereent each of aluminum, antimony, lead, and silieon; and 0.001 to 0.1 pereent eaeh of barium, calcium, eopper, iron, magnesium, and tin.

The sample was eolorless and too fine-grained to allow determination of the indices of refraction.

The *d*-values of the three strongest lines are: 3.08, 2.796, and 2.071 A.

Structural data. Durif [1] in 1959 determined that strontium arsenate is isostructural with strontium phosphate, with the spaee group D_{3d}^5—$R\bar{3}m$ (No. 166) and $1[Sr_3(AsO_4)_2]$ per rhombohedral unit cell or $3[Sr_3(AsO_4)_2]$ per hexagonal unit cell.

Lattice constants

		a	*c*
		A	*A*
1959	Durif [1]	5. 581	19.98
1962	National Bureau of Standards.	5. 587	20.004 at 25 °C

The density of strontium arsenate ealeulated from the NBS lattiee eonstants is 4.980 g/em³ at 25 °C.

hkl (hex.)	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
006	3. 33	3
015	3. 08	100
110	2. 796	96
202	2. 352	8
009	2. 223	9
024	2. 178	6
205	2. 071	50
1·0·10	1. 8489	33
119, 208	1. 7394	2
125	1. 6639	34
300	1. 6129	19
0·2·10	1. 5421	13
2·0·11	1. 4537	2
220	1. 3970	17
2·1·10	1. 3502	18
0·0·15	1. 3338	2
315	1. 2725	13
1·1·15	1. 2036	12
229, 318	1. 1826	2
045	1. 1579	6
1·2·14	1. 1259	<1
1·3·10	1. 1148	10
235	1. 0695	8
410	1. 0558	8
4·0·10, 327	1. 0351	4
3·0·15	1. 0278	9
1·3·13	1. 0116	<1
0·1·20	0. 9795	3
3·2·10	. 9706	6
2·2·15	. 9646	5
419	. 9538	<1
505	. 9405	3
330	. 9312	3
2·0·20	. 9244	2
2·1·19	. 9125	2
425	. 8913	6
1·2·20	. 8775	5
0·5·10, 247	. 8711	3
155	. 8492	5
2·4·10, 517	. 8315	5
4·1·15	. 8278	12
4·2·11	. 8169	<1
600	. 8063	4
3·1·20	. 8019	4
1·1·24	. 7987	2
5·1·10	. 7969	5
1·0·25	. 7894	2
345	. 7801	5

Reference

[1] A. Durif, Structure cristalline des orthovanadates et orthoarseniates de baryum et de strontium, Acta Cryst. **12**, 420–421 (1959).

Thallium (I) Arsenate, Tl_3AsO_4 (hexagonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of thallous arsenate was prepared at NBS by reaction of a solution of thallous sulfate with a solution of arsenic oxide in concentrated nitric acid. The sparingly soluble precipitate was recrystallized from a boiling aqueous solution. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, silicon, and sodium; and 0.001 to 0.01 percent each of copper, iron, lead, and magnesium.

The sample was pale yellow. The indices of refraction were not determined because they were greater than 2.00.

The *d*-values of the three strongest lines are: 3.015, 3.303, and 2.786 A.

Structural data. No reference was found for the structure of thallous arsenate; however, it is thought to be isostructural with thallous phosphate, with the space group $C_6^6-P6_3$ (No. 173) and $2(Tl_3AsO_4)$ per unit cell.

Lattice constant

		a	*c*
		A	*A*
1962	National Bureau of Standards.	8. 516	5.234 at 25° C.

The density of thallous arsenate calculated from the NBS lattice constants is 7.596 g/cm³ at 25 °C. The average density obtained with the Berman balance was 7.51 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A	
	d	*I*
	A	
100	7. 39	8
110	4. 26	30
200	3. 687	26
111	3. 303	97
201	3. 015	100
210	2. 786	58
002	2. 617	25
300	2. 458	19
112	2. 230	11
301	2. 226	11
202	2. 135	11
220	2. 130	9
310	2. 0451	24
221	1. 9721	6
212	1. 9076	46
311	1. 9053	49
400	1. 8437	3
302	1. 7924	7
320	1. 6920	5
222	1. 6518	3
312	1. 6113	40
203	1. 5778	16
411	1. 5384	4
402	1. 5074	1
213	1. 4788	<1
500	1. 4752	3
322, 501	1. 4202	12
420	1. 3937	5
331	1. 3702	2
223	1. 3500	1
421	1. 3471	1
313	1. 3276	7
004	1. 3091	4
502	1. 2851	6
114	1. 2511	1
422	1. 2303	5
323	1. 2147	2
601	1. 1965	<1
431, 520	1. 1811	9
304	1. 1551	6
503	1. 1264	6
314	1. 1023	3
333	1. 1010	4
423	1. 0893	1
522	1. 0764	5

Thallium(I) Perchlorate, $TlClO_4$ (orthorhombic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of thallium perchlorate was prepared at NBS by reaction of solutions of thallium(I) sulfate and barium perchlorate. The product was purified by recrystallization. Spectrographic analysis showed the following to be the chief impurity: 0.001 to 0.01 percent of iron.

The sample was colorless and optically negative with the refractive indices $N_\alpha=1.640$, $N_\beta=1.644$, $N_\gamma=1.647$, and $2V \cong 70°$.

The d-values of the three strongest lines are: 3.64, 2.234, and 3.278 A.

Structural data. Büssem and Herrmann [1] in 1928 determined that thallium(I) perchlorate has the $BaSO_4$ structure, the space group D_{2h}^{16}—Pbnm (No. 62), and 4($TlClO_4$) per unit cell. According to Herrmann and Ilge [2] and Braekken and Harang [3], at temperatures above 266 °C, there exists a cubic form with the $KClO_4$ structure.

Lattice constants

		a	b	c
		A	A	A
1928	Büssem and Herrmann [1].	7. 52	9. 44	5. 89
1962	National Bureau of Standards.	7. 510	9. 304	5. 845 at 25 °C

The lattice constants of Büssem and Herrmann were converted from kX to angstrom units for comparison with the NBS values.

The density of thallium perchlorate calculated from the NBS lattice constants is 4.940 g/cm^3 at 25 °C.

References

[1] W. Büssem and K. Herrmann, Röntgenographische Untersuchung der einwertigen Perchlorate, Z. Krist. **67,** 405–408 (1928).

[2] K. Herrmann and W. Ilge, Röntgenographische Strukturerforschung der kubischen Modifikation der Perchlorate, Z. Krist. **75,** 41–66 (1930).

[3] H. Braekken and L. Harang, Die kubische Hochtemperaturstruktur einiger Perchlorate, Z. Krist. **75,** 538–549 (1930).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	I
	A	
110	5. 84	4
020	4. 65	30
101	4. 61	54
111	4. 14	39
120	3. 96	19
200	3. 76	40
021	3. 64	100
210	3. 485	59
121	3. 278	75
211	2. 992	36
002, 220	2. 922	40
130	2. 867	11
112, 221	2. 614	21
022	2. 475	9
310	2. 417	6
230	2. 391	3
122	2. 350	24
040	2. 326	4
202	2. 306	6
311	2. 234	78
140	2. 222	47
231	2. 213	42
041	2. 161	13
222	2. 066	5
132	2. 047	5
330	1. 9485	14
103	1. 8860	5
400	1. 8783	3
113, 331	1. 8479	8
410	1. 8409	6
023	1. 7970	6
142	1. 7688	14
411	1. 7552	5
123	1. 7480	5
213	1. 7001	4
421	1. 6681	1
223, 332	1. 6212	14
251	1. 6036	3
402	1. 5793	<1
412	1. 5572	8
060	1. 5501	10
431	1. 5485	12
303	1. 5374	4
313	1. 5167	8
233	1. 5107	6
061	1. 4981	9
043, 350	1. 4938	9
510	1. 4826	<1
161	1. 4696	9
004, 440	1. 4613	6
501	1. 4545	4

Yttrium Arsenate, $YAsO_4$ (tetragonal)

Powder Data cards

Card number	Index lines	Radiation	Source
2–0440	3. 39 1. 79 2. 60	Chromium	Strada and Schwendimann [1] 1934.

Additional published patterns. None.

NBS samples. The sample of yttrium arsenate was prepared at NBS by mixing solutions of yttrium chloride and sodium hydrogen arsenate. The precipitate was filtered, washed, and then heated to 750 °C. The yttrium chloride was obtained from the Lindsay Chemical Company, West Chicago, Ill. Their spectrographic analysis showed the presence of the following impurities in the chloride: a combined maximum as oxides of 0.1 percent of dysprosium and gadolinium and traces of terbium. Spectrographic analysis at NBS showed the following additional impurities in the arsenate: 0.1 to 1.0 percent of silicon; 0.01 to 0.1 percent of calcium and sodium; and 0.001 to 0.01 percent aluminum, boron, copper, iron, lead and magnesium.

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

The *d*-values of the three strongest lines are: 3.52, 2.661, and 1.8171 A.

Structural data. Strada and Schwendimann [1] in 1934 determined that yttrium arsenate has the zircon structure, the space group D_{4h}^{19}—$I4_1/amd$ (No. 141) and 4 ($YAsO_4$) per unit cell.

Lattice constants

		a	*c*
		A	*A*
1934	Strada and Schwendimann [1].	6. 914	6. 293
1957	Durif and Forrat [2]	7. 06	6. 30
1962	National Bureau of Standards.	7. 039	6. 292 at 25 °C

The density of yttrium arsenate calculated from the NBS lattice constants is 4.853 g/cm^3 at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
200	3. 52	100
112	2. 661	73
220	2. 490	18
202	2. 347	5
301	2. 199	6
103	2. 010	3
321	1. 866	4
312	1. 817	65
400	1. 760	16
420	1. 574	14
332	1. 468	16
204	1. 4359	11
501	1. 3737	<1
224	1. 3293	14
512	1. 2644	14
440	1. 2446	4
404, 600	1. 1731	11
532	1. 1272	15
424, 620	1. 1128	15
116	1. 0258	6
444, 640	0. 9760	7
316, 712	. 9488	14
604	. 9404	5
624	. 9085	8
732	. 8867	10
800	. 8799	3
820	. 8538	3
516	. 8349	10
644, 660	. 8295	7

References

[1] M. Strada and G. Schwendimann, La structura cristallina di alcuni fosfati dei metalli trivalenti. II. Arseniato e fosfato di ittrio, Gazz. chim. ital **64,** 662–674 (1934).

[2] A. Durif and F. Forrat, Sur quelques arséniates des terres rares à structure zircon, Compte rend. **245,** 1636–1638 (1957).

Zinc Tungstate, $ZnWO_4$ (monoclinic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of zinc tungstate was prepared at NBS by the reaction of solutions of zinc chloride and sodium tungstate. The precipitate was washed, dried, and heated to 1,000 °C for 10 min. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium and 0.001 to 0.01 percent of silicon.

The color of the sample was gray. The indices of refraction were not determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are: 2.931, 2.908, and 3.73 A.

Structural data. Broch [1] in 1929 determined that zinc tungstate has the magnesium tungstate structure, the space group C_{2h}^4—P2/c (No. 13), and $2(ZnWO_4)$ per unit cell. The lattice constants of Broch have been converted from kX to angstrom units.

The density of zinc tungstate calculated from the NBS lattice constants is 7.870 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	*I*
	A	
010	5. 72	10
100	4. 69	35
011	3. 73	38
110	3. 62	37
111	2. 931	100
$\bar{1}11$	2. 908	90
020	2. 859	23
021	2. 472	37
002	2. 464	34
120	2. 442	7
200	2. 346	16
121	2. 192	16
$\bar{1}02$	2. 191	16
$\bar{1}21$	2. 183	18
112	2. 046	7
$\bar{1}12$	2. 029	7
211	1. 994	5
$\bar{2}11$	1. 978	5
030	1. 906	2
022	1. 866	14
220	1. 813	13
130	1. 766	21
$\bar{1}22$	1. 740	<1
$\bar{1}22$	1. 7290	<1
202, 221	1. 7074	26
$\bar{2}21$	1. 6969	20
$\bar{2}02$	1. 6891	16
$\bar{1}31$	1. 6650	3
$\bar{1}31$	1. 6609	3
212	1. 6366	1
013	1. 5778	5
300	1. 5634	1
032	1. 5076	6
$\bar{1}13$	1. 5007	12
$\bar{1}13$	1. 4903	11
230	1. 4792	3
$\bar{2}22$	1. 4662	5
$\bar{2}22$	1. 4541	6
$\bar{3}11$	1. 4465	10
$\bar{3}11$, 132	1. 4379	19
$\bar{1}32$	1. 4326	17
023	1. 4236	11
041	1. 3732	10
$\bar{1}23$	1. 3663	<1
$\bar{1}23$	1. 3589	1

Lattice constants

		a	*b*	*c*	*β*
		A	*A*	*A*	
1930	Broch [1]	4. 69	5. 74	4. 96	89. 50°
1962	National Bureau of Standards	4. 691	5. 720	4. 925	89. 36 at 25 °C

Reference

[1] E. K. Broch, Untersuchungen über Kristallstrukturen des Wolframittypus und des Scheelittypus, Skrifter Norsk. Videns.-Akad. Oslo I. Mat.-Naturv. Kl. No. 8 (1929).

CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONOGRAPH 25, SECTION 1 AND SECTION 2 [5]

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

m—Monograph 25.

m—Monograph 25.

m—Monograph 25.

m—Monograph 25.

MINERAL INDEX

U.S. DEPARTMENT OF COMMERCE
Luther H. Hodges, *Secretary*

NATIONAL BUREAU OF STANDARDS
A. V. Astin, *Director*

THE NATIONAL BUREAU OF STANDARDS

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

WASHINGTON, D.C.

Electricity. Resistance and Reactance. Electrochemistry. Electrical Instruments. Magnetic Measurements. Dielectrics. High Voltage.

Metrology. Photometry and Colorimetry. Refractometry. Photographic Research. Length. Engineering Metrology. Mass and Scale. Volumetry and Densimetry.

Heat. Temperature Physics. Heat Measurements. Cryogenic Physics. Equation of State. Statistical Physics.

Radiation Physics. X-ray. Radioactivity. Radiation Theory. High Energy Radiation. Radiological Equipment. Nucleonic Instrumentation. Neutron Physics.

Analytical and Inorganic Chemistry. Pure Substances. Spectrochemistry. Solution Chemistry. Standard Reference Materials. Applied Analytical Research. Crystal Chemistry.

Mechanics. Sound. Pressure and Vacuum. Fluid Mechanics. Engineering Mechanics. Rheology. Combustion Controls.

Polymers. Macromolecules: Synthesis and Structure. Polymer Chemistry. Polymer Physics. Polymer Characterization. Polymer Evaluation and Testing. Applied Polymer Standards and Research. Dental Research.

Metallurgy. Engineering Metallurgy. Microscopy and Diffraction. Metal Reactions. Metal Physics. Electrolysis and Metal Deposition.

Inorganic Solids. Engineering Ceramics. Glass. Solid State Chemistry. Crystal Growth. Physical Properties. Crystallography.

Building Research. Structural Engineering. Fire Research. Mechanical Systems. Organic Building Materials. Codes and Safety Standards. Heat Transfer. Inorganic Building Materials. Metallic Building Materials.

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

Data Processing Systems. Components and Techniques. Computer Technology. Measurements Automation. Engineering Applications. Systems Analysis.

Atomic Physics. Spectroscopy. Infrared Spectroscopy. Far Ultraviolet Physics. Solid State Physics. Electron Physics. Atomic Physics. Plasma Spectroscopy.

Instrumentation. Engineering Electronics. Electron Devices. Electronic Instrumentation. Mechanical Instruments. Basic Instrumentation.

Physical Chemistry. Thermochemistry. Surface Chemistry. Organic Chemistry. Molecular Spectroscopy. Elementary Processes. Mass Spectrometry. Photochemistry and Radiation Chemistry.

Office of Weights and Measures.

BOULDER, COLO.

Cryogenic Engineering Laboratory. Cryogenic Equipment. Cryogenic Processes. Properties of Materials. Cryogenic Technical Services.

CENTRAL RADIO PROPAGATION LABORATORY

Ionosphere Research and Propagation. Low Frequency and Very Low Frequency Research. Ionosphere Research. Prediction Services. Sun-Earth Relationships. Field Engineering. Radio Warning Services. Vertical Soundings Research.

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

Radio Systems. Applied Electromagnetic Theory. High Frequency and Very High Frequency Research. Frequency Utilization. Modulation Research. Antenna Research. Radiodetermination.

Upper Atmosphere and Space Physics. Upper Atmosphere and Plasma Physics. High Latitude Ionosphere Physics. Ionosphere and Exosphere Scatter. Airglow and Aurora. Ionospheric Radio Astronomy.

RADIO STANDARDS LABORATORY

Radio Physics. Radio Broadcast Service. Radio and Microwave Materials. Atomic Frequency and Time-Interval Standards. Radio Plasma. Millimeter-Wave Research.

Circuit Standards. High Frequency Electrical Standards. High Frequency Calibration Services. High Frequency Impedance Standards. Microwave Calibration Services. Microwave Circuit Standards. Low Frequency Calibration Services.