NBS MONOGRAPH 25—SECTION 1

Standard X-ray Diffraction Powder Patterns

U.S. DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

THE NATIONAL BUREAU OF STANDARDS

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Standard X-ray Diffraction Powder Patterns

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

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*Not previously represented in the Powder Date File.

Errata (Circular 539)

Vol. 9. Page 56, *hkl* 357 should be 537.

Vol. 10. Page 7. *hkl* 231 should be 232.
Page 52, space group $P2_1/n$ should be $P2_1/c$.

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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:

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 1—Data for 46 Substances

Howard E. Swanson, Marlene Cook Morris,[1] Roger Stinchfield,[1] and Eloise H. Evans [1]

Forty-six standard X-ray diffraction powder patterns are presented. Fourteen are to replace twelve patterns already given in the X-ray Powder Data File, and thirty-four 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. The *d*-values were assigned Miller indices determined by comparison with calculated interplanar spacings and from space group considerations. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible.

Included are X-ray data for the following forty-six substances: $(NH_4)_2OsCl_6$, $Al_2SiO_4(F,OH)_2$, topaz, BiF_3, $CeCl_3$, $CeVO_4$, $CsClO_4$, $CsV(SO_4)_2 \cdot 12H_2O$, $Er_3Ga_2(GaO_4)_3$, $EuCl_3$, $EuOCl$, GdF_3, $GdOCl$, Gd_2O_3, $Ho[C_2H_5)SO_4]_3 \cdot 9H_2O$, $FeAs$, $LaBO_3$, $LaCl_3$, $La_2Mg_3(NO_3)_{12} \cdot 24H_2O$, Li_2MoO_4, Li_2O, Li_2WO_4, Lu_2O_3, $Mg_2Al_4Si_5O_{18}$ (low-cordierite), $Mg_2Al_4Si_5O_{18}$ (high-cordierite), $3Mg_2SiO_4 \cdot MgF_2$ (humite), $NdBO_3$, $NdCl_3$, $Nd_3Ga_2(GaO_4)_3$, NiAsS (gersdorffite), $NiCO_3$, NiS, millerite, KH_2AsO_4, $PrCl_3$, $SmCl_3$, SmF_3, $Sm_3Ga_2(GaO_4)_3$, SmOCl, Ag_2CO_3, Ag_2O, Na_2MoO_4, Na_2WO_4, Tl_2WO_4, $Yb_3Ga_2(GaO_4)_3$, $Y_3Ga_2(GaO_4)_3$, YOCl, $Zr(IO_3)_4$.

INTRODUCTION

The National Bureau of Standards in its program[2] for the revision and evaluation of published X-ray data for the X-ray Powder Data File presents data in this report for 46 compounds. This paper is the eleventh of a series of "Standard X-ray Diffraction Patterns." The designation "Circular 539" used in previous issues has been discontinued in favor of a new series, "Monograph 25." Included are patterns recommended to replace data on 12 cards now in the file. The patterns for 34 compounds not represented in the file have been added. These compounds are: ammonium chloroosmate, bismuth fluoride, cerium(III) vanadate, cesium perchlorate, cesium vanadium sulfate dodecahydrate, erbium gallium oxide 3:5, europium(III) chloride, europium oxychloride, gadolinium oxychloride, gadolinium oxide, holmium ethylsulfate nonahydrate, iron arsenide, lanthanum borate lanthanum(III) chloride, lanthanum magnesium nitrate 24-hydrate, lithium molybdate, lithium oxide, lithium tungstate, lutetium oxide, magnesium aluminum silicate (orthorhombic), neodymium borate, neodymium gallium oxide 3:5, nickel arsenic sulfide (gersdorffite), nickel(II) carbonate, potassium dihydrogen arsenate, praseodymium(III) chloride, samarium(III) chloride, samarium oxychloride, sodium molybdate, thallium(I) tungstate, ytterbium gallium oxide 3:5, yttrium gallium oxide 3:5, yttrium oxychloride, zirconium iodate.

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

ASTM cards. Each section of this Monograph contains a table listing the ASTM file card numbers, the three strongest lines, the radiations used, and the literature references for each card. Cards listed in the 1960 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 ASTM cards are listed.

NBS sample. Many of the samples used to make NBS patterns were special preparations (of exceptionall high purity) obtained or prepared only in small quantities. 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 provided by the X-ray pattern itself, since 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.

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[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 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; and Vol. 10, September 1960.

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

At least two patterns for intensity measurements were prepared to check reproducibility. Samples that gave satisfactory intensity patterns usually had an average particle-size well within the recommended range of 5 to 10 μ, as suggested by Alexander, Klug, and Kummer [2]. A special cell with one open end was used for making intensity measurements. 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. 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 intensity 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. These specimens were prepared by packing into a shallow holder a sample containing approximately 5-wt percent tungsten powder that served as an internal standard. The lattice constant used for tungsten at 25 °C is 3.1648 A, as determined by Jette and Foote [3]. All of the NBS patterns, unless otherwise noted, are made at 25 °C, using either filtered copper radiation ($K\alpha_1$) or cobalt radiation ($K\alpha_1$), having the wavelengths 1.5405 A, and 1.7889 A, respectively.

Structural data. Although the lattice constants obtained at NBS of cubic materials were calculated for each *d*-value, the constants 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 704, using those *d*-values for which only one *hkl* could be assigned. The number of significant figures reported for *d*-values in the NBS pattern is limited by the quality of each sample and by its structural symmetry.

Published unit-cell data were converted to angstrom units as internationally defined in 1946 [4] using the factor 1.00202. When cell values based upon more than one cell configuration have been taken from the literature, corrections that were made to make them comparable have been indicated. The limits of error generally published with unit-cell data have not been included in the table because the number of determinations and their accuracy and variations were such that a statistical evaluation would be unjustified.

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

Orthorhombic cell dimensions are presented according to the Dana Convention [5] $b>a>c$ rather than with a permutation as is occasionally given in the literature.

The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter and are based upon atomic weights reported by E. Wichers [6] in 1956 and the Avogadro number (6.0240×10^{23}) reported by Straumanis [7] in 1954. The refractive index measurements were made by grain-immersion methods in white light using oils standardized in sodium light.

References

[1] Index to the X-ray Powder Data File, American Society for Testing Materials, Philadelphia, Pa. (1959).

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

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

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

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

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

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

Conversion Factors for Comparison of Peak Height and Integrated Intensities

Occasionally someone wishes to compare integrated intensity values with the peak height to background measurements made at the NBS for the Powder Data File. Conversion factors, applicable when copper radiation is used, can be read from the chart in figure 1 as a function of 2θ. Factors from the right side of the chart, multiplied by peak height values, give the corresponding integrated intensities. Factors for converting peak-height intensities to integrated intensities are on the left side of the chart.

The ordinate values used in determining the curve in figure 1 are the ratios of the integrated intensity to the peak height intensity for each line in medium to sharp patterns obtained from $(NH_4)_2PtCl_6$, W, and $Ca_3Al_2(GeO_4)_3$. A curve based upon diffuse peaks or another radiation would be expected to vary from this one.

The patterns used for these measurements were scanned slowly (4 in. equal to one degree) to produce a broad peak. The area of the peak was recorded with a planimeter (G. Coradi, Zurich, Switzerland). Later, additional integrated intensity data were obtained by cutting out the peaks and weighing them. Since both integrating methods seemed to give equal precision, and a large number of points were needed to obtain the curve, all data from the three patterns were included.

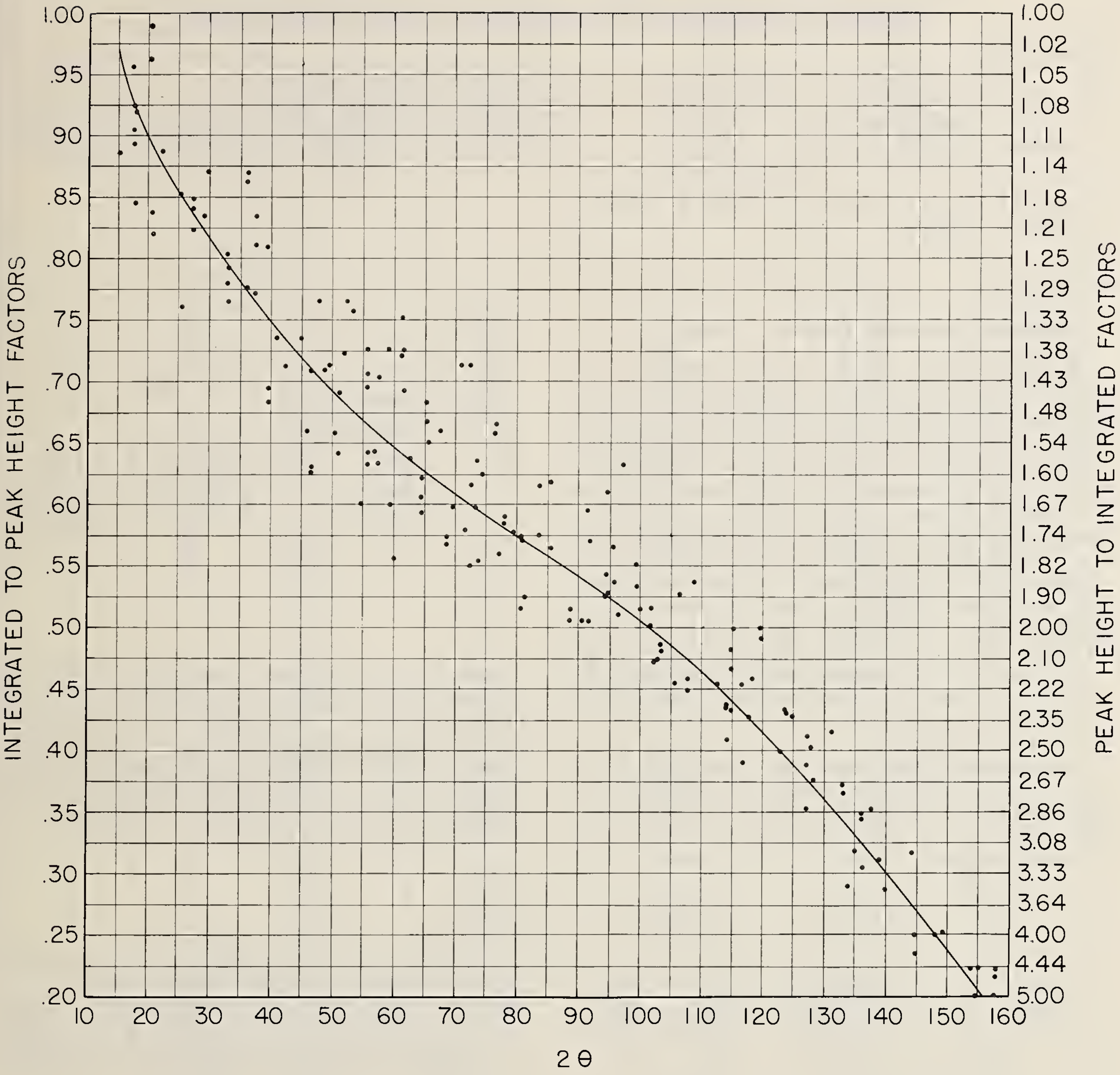

Figure 1. *Conversion factors for comparison of peak height and integrated intensities for copper radiation with medium to sharp peaks.*

Aluminum Fluosilicate, topaz, $Al_2SiO_4(F,OH)_2$ (orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
[a] 2–0704 2–0705	2. 96 1. 40 1. 38	Copper	British Museum

[a] From Scotland.

Additional published patterns. None.

NBS samples. Samples of topaz from three different sources were used. Spectrographic analysis of each sample showed the following impurities: (Minas Gerais, Brazil) 0.01 to 0.1 percent of germanium; 0.001 to 0.01 percent each of gallium, iron, sodium, titanium, and zinc; and 0.0001 to 0.001 percent each of boron, calcium, copper, lead, magnesium, and tin. (Durango, Mexico) 0.01 to 0.1 percent of iron; 0.001 to 0.01 percent each of boron, gallium, germanium, sodium, titanium, and zinc; and 0.0001 to 0.001 percent each of calcium, lead, magnesium, manganese, and tin. (Thomas Mountain, Utah) 0.01 to 0.1 percent of iron; 0.001 to 0.01 percent each of gallium, germanium, sodium, titanium, and zinc; and 0.0001 to 0.001 percent each of boron, calcium, lead, magnesium, and tin.

The samples from Brazil and Utah were colorless. The sample from Mexico was slightly discolored brown. Topaz is optically positive with $2V \cong 55°$ and the following indices of refraction for each sample:

Source	N_α	N_β	N_γ
Brazil	1. 613	1. 615	1. 622
Mexico	1. 608	1. 611	1. 618
Utah	1. 608	1. 611	1. 618
Average	1. 610	1. 612	1. 619

The average *d*-values of the three strongest lines are: 2.937, 3.195, and 3.693 A.

Structural data. Leonhardt [1] in 1924 determined that topaz has the space group D_{2h}^{16}– Pmnb (No. 62) and $4[Al_2SiO_4(F,OH)_2]$ per unit cell.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1924	Leonhardt [1]	8. 39	8. 80	4. 65
1928	Alston and West [2]	8. 39	8. 80	4. 65
1961	National Bureau of Standards:			
	Brazil	8. 392	8. 797	4. 649
	Mexico	8. 395	8. 789	4. 649
	Utah	8. 394	8. 791	4. 648
	NBS average	8. 394	8. 792	4. 649 at 26 °C

According to Pardee, Glass, and Stevens [3] the beta refractive index varies with the amount of fluorine present. The average value of the NBS beta refractive index indicates an approximate formula $Al_2SiO_4F_{1.9}(OH)_{0.1}$, corresponding to 19.6 percent fluorine. This formula, together with the average values of the NBS lattice constants, gives an average density of 3.558 g/cm³ at 26 °C.

References

[1] J. Leonhardt, Röntgenographische Untersuchungen am Topas, Z. Krist. **59,** 216–229 (1924).

[2] N. A. Alston and J. West, The structure of topaz $[Al_2(F, OH)_2SiO_4]$, Z. Krist. **69,** 149–167 (1928).

[3] J. T. Pardee, Jewell J. Glass, and R. E. Stevens, Massive low-fluorine topaz from the Brewer Mine, South Carolina, Am. Mineralogist **22,** 1058–1064 (1937).

Aluminum Fluosilicate, topaz, Al_2SiO_4 (F, OH)$_2$ (orthorhombic)—Continued

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 26 °C Minas Gerais, Brazil		1961 National Bureau of Standards Cu, 1.5405 A at 26 °C Durango, Mexico		1961 National Bureau of Standards Cu, 1.5405 A at 26 °C Thomas Mountain, Utah		1961 National Bureau of Standards Cu, 1.5405 A at 26 °C Average	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
020	4. 396	4	4. 396	5	4. 394	5	4. 395	5
200	4. 191	4	4. 193	6	4. 199	3	4. 194	4
011	4. 109	12	4. 111	9	4. 114	11	4. 111	11
120	3. 894	6	3. 895	6	3. 898	7	3. 896	6
111	3. 690	54	3. 697	62	3. 693	65	3. 693	60
021	3. 194	58	3. 196	72	3. 195	69	3. 195	66
220	3. 035	32	3. 036	43	3. 037	37	3. 037	37
121	2. 986	21	2. 988	24	2. 985	25	2. 986	23
211	2. 934	100	2. 938	100	2. 939	100	2. 937	100
031	2. 4806	20	2. 4806	22	2. 4800	23	2. 4804	22
301	2. 3962	10	2. 3968	10	2. 3969	11	2. 3966	10
131	2. 3785	22	2. 3779	30	2. 3785	27	2. 3783	26
320	2. 3605	44	2. 3605	34	2. 3617	58	2. 3609	45
002	2. 3241	6	2. 3247	12	2. 3253	5	2. 3247	8
311	2. 3126	7	2. 3126	9	2. 3138	11	2. 3130	9
012	2. 2472	5	2. 2467	6	2. 2472	6	2. 2470	6
040	2. 1994	11	2. 1989	10	2. 1984	10	2. 1989	10
112	2. 1706	14	2. 1716	11	2. 1711	12	2. 1711	12
140	2. 1266	5	2. 1266	13	2. 1276	7	2. 1269	8
321	2. 1049	38	2. 1058	46	2. 1040	47	2. 1049	44
022	2. 0553	21	2. 0553	21	2. 0558	30	2. 0555	24
041	1. 9881	5	1. 9872	8	1. 9864	8	1. 9872	7
212	1. 9823	6	1. 9815	16	1. 9811	4	1. 9816	9
240	1. 9477	2	1. 9481	5	1. 9453	4	1. 9470	4
141	1. 9344	4	1. 9340	5	1. 9336	6	1. 9340	5
411	1. 8688	25	1. 8700	21	1. 8685	25	1. 8691	24
331	1. 8553	19	1. 8553	32	1. 8553	25	1. 8553	26
032	1. 8219	9	1. 8209	12	1. 8209	15	1. 8212	12
241	1. 7967	9	1. 7957	7	1. 7954	7	1. 7969	8
132	1. 7797	4	1. 7791	5	1. 7800	6	1. 7796	5
232	1. 6709	31	1. 6706	26	1. 6703	24	1. 6706	27
322	1. 6559	11	1. 6559	6	1. 6565	8	1. 6561	8
341	1. 6205	13	1. 6205	7	1. 6198	13	1. 6203	11
431	1. 6016	<1	1. 6021	5	1. 6006	1	1. 6014	2
042	1. 5975	2	1. 5968	5	1. 5978	2	1. 5974	3
501	1. 5788	2	1. 5790	1	1. 5795	1	1. 5791	1
142, 520	1. 5690	1	1. 5683	5	1. 5678	2	1. 5684	3
402	1. 5570	1	1. 5575	<1	1. 5575	<1	1. 5573	<1
511	1. 5534	<1	1. 5546	4	1. 5551	<1	1. 5544	1
003	1. 5496	<1	1. 5499	6	1. 5477	6	1. 5491	4
412	1. 5333	13	1. 5340	14	1. 5331	10	1. 5335	12
013, 332	1. 5264	16	1. 5267	11	1. 5262	20	1. 5264	16
440	1. 5181	4	1. 5181	10	1. 5179	4	1. 5180	6
113	1. 5018	<1	1. 4994	<1	1. 5007	<1	1. 5006	<1
242	1. 4929	1	1. 4925	2	1. 4925	2	1. 4926	2
521	1. 4858	2	1. 4862	6	1. 4860	2	1. 4860	3
060	1. 4648	3	1. 4642	9	1. 4650	4	1. 4647	5
023	1. 4615	6	1. 4609	11	1. 4617	10	1. 4614	9
160, 441	1. 4439	9	1. 4431	6	1. 4429	8	1. 4433	8
123	1. 4401	5	1. 4395	3	1. 4397	4	1. 4398	4
213	1. 4341	3	1. 4351	5	1. 4341	3	1. 4344	4
351	1. 4186	24	1. 4175	24	1. 4179	29	1. 4180	26
052	1. 4028	18	1. 4026	32	1. 4015	24	1. 4023	25

Ammonium Chloroosmate, $(NH_4)_2OsCl_6$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium chloroosmate was prepared at NBS by R. B. Johannesen from chloroosmic acid and ammonium chloride. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, beryllium, magnesium, and silicon.

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

The *d*-values of the three strongest lines are: 5.71, 4.94, and 2.978 A.

Structural data. The structure of ammonium chloroosmate has not been published but, because of the similarity of patterns, it is thought to be isostructural with ammonium chloroplatinate. The NBS pattern was indexed assuming the space group O_h^5 Fm3m (No. 225) and $4(NH_4)_2OsCl_6$ per unit cell.

Lattice constants

1961	National Bureau of Standards--	*A* 9. 881 at 25 °C

The density of ammonium chloroosmate calculated from the NBS lattice constant is 3.022 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 *A* at 25 °C		
	d	*I*	*a*
	A		*A*
111	5. 71	100	9. 89
200	4. 94	64	9. 88
220	3. 491	26	9. 874
311	2. 978	45	9. 877
222	2. 851	4	9. 876
400	2. 469	36	9. 876
331	2. 267	16	9. 881
420	2. 209	29	9. 879
422	2. 016	10	9. 876
511	1. 902	19	9. 883
440	1. 747	19	9. 882
531	1. 670	17	9. 880
600	1. 647	13	9. 882
620	1. 562	4	9. 879
533	1. 507	6	9. 882
444	1. 426	6	9. 880
711	1. 3835	8	9. 880
640	1. 3701	5	9. 880
642	1. 3204	4	9. 881
731	1. 2864	6	9. 881
800	1. 2349	3	9. 879
733	1. 2072	3	9. 881
820	1. 1983	6	9. 881
822	1. 1645	2	9. 881
751	1. 1411	4	9. 882
840	1. 1047	4	9. 881
911	1. 0845	4	9. 880
842	1. 0780	4	9. 880
664	1. 0531	1	9. 879
931	1. 0357	3	9. 880
844	1. 0083	4	9. 879
933	0. 9929	4	9. 879
10·0·0	. 9878	1	9. 878
10·2·0	. 9687	2	9. 879
951	. 9550	2	9. 879
953	. 9212	1	9. 879
10·4·0	. 9173	2	9. 880
10·4·2	. 9019	1	9. 880
11·1·1	. 8908	<1	9. 879
880	. 8733	<1	9. 880
11·3·1	. 8632	2	9. 880
10·4·4	. 8600	1	9. 881
10·6·0	. 8473	1	9. 881
11·3·3	. 8381	<1	9. 881
12·0·0	. 8234	2	9. 881
11·5·1	. 8149	<1	9. 880
12·2·0	. 8121	<1	9. 880
12·2·2	. 8015	<1	9. 882
11·5·3	. 7936	1	9. 880
Average value of last five lines--------			9. 881

Bismuth Fluoride, BiF_3 (orthorhombic)

ASTM cards. None. Data on card number 2–1235 is for bismuth oxygen fluoride, Bi_2OF_4, instead of bismuth fluoride, BiF_3.

Additional published patterns. None.

NBS sample. The sample of bismuth fluoride was prepared by Olen Kraus of NBS by reacting bismuth oxide with a large excess of hydrofluoric acid at 80 °C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium, and 0.001 to 0.01 percent each of aluminum, barium, calcium, iron, magnesium, and silicon.

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

The *d*-values of the three strongest lines are: 3.406, 2.970, and 3.508 A.

Structural data. Zachariasen and Plettinger [1] in 1950 determined that bismuth fluoride has yttrium fluoride-type structure, the space group D_{2h}^{16}-Pnma (No. 62), and 4(BiF_3) per unit cell.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1955	Aurivillius and Lundqvist [2]	6. 56	7. 04	4. 83
1949	Zachariasen and Plettinger [1]	6. 56	7. 03	4. 86
1961	National Bureau of Standards	6. 563	7. 021	4.845 at 25 °C

The density of bismuth fluoride calculated from the NBS lattice constants is 7.912 g/cm³ at 25 °C.

References

[1] W. H. Zachariasen and H. Anne Plettinger, Mass Spectroscopy and Crystal Structure Division Quarterly Report, Argonne National Laboratory Report 4400, 12–16 (September 1, 1949–November 30, 1949). Quoted in Zalkin and Templeton [3].

[2] B. Aurivillius and T. Lundqvist, X-ray studies on the system $BiF_3-Bi_2O_3$. I. Preliminary phase analysis and a note on the structure of BiF_3, Acta Chem. Scand. **9**, 1206–1208 (1955).

[3] A. Zalkin and D. H. Templeton, The crystal structures of YF_3 and related compounds, J. Am. Chem. Soc. **75**, 2453–2458 (1953).

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
011	3. 985	7
101	3. 897	47
020	3. 508	48
111	3. 406	100
200	3. 278	4
210	2. 970	49
121	2. 607	23
211	2. 533	2
002	2. 420	12
102	2. 272	2
112	2. 161	8
221	2. 148	7
131	2. 006	37
301, 022	1. 993	39
202	1. 949	1
311	1 918	10
230, 122	1. 905	26
212	1. 877	27
040	1. 755	9
321	1. 734	20
222	1. 704	2
400	1. 640	5
132	1. 630	2
141	1. 600	6
410	1. 597	5
312	1. 582	3
013	1. 574	4
113	1. 530	6
331, 411	1. 517	5
232	1. 497	10
420	1. 486	4
241, 322	1. 474	1
203	1. 4489	2
123	1. 4318	4
042, 421	1. 4215	6
142	1. 3890	2
402	1. 3587	4
051	1. 3483	2
430	1. 3436	5
223	1. 3399	7
332, 412	1. 3341	4
033	1. 3293	2
151	1. 3214	8
341	1. 3180	11
242, 133	1. 3028	4
303	1. 2995	4
431	1. 2955	2
250	1. 2913	3
313	1. 2777	1
501, 422	1. 2670	6
251, 511	1. 2471	6
233	1. 2326	1
323	1. 2187	4
004	1. 2112	2
440	1. 1987	4

Cerium(III) Chloride, $CeCl_3$ (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
9–68	2.56 2.11 3.56	Copper	Zachariasen [1] 1955

Additional published patterns

Source	Radiation
Kojima, Inoue, and Ishiyama [2]	Copper

NBS sample. The sample of cerium chloride was received as a hydrate from Lindsay Chemical Co., West Chicago, Ill. It was dried in a hydrogen chloride atmosphere at 30 mm total pressure and 450 °C for one and one-half hours. It was then transferred in a dry box to a dry atmosphere sample holder used to prepare the patterns. An analysis from Lindsay Chemical Co. showed the following impurities: less than 0.1 percent combined of lanthanum, praseodymium, and neodymium.

The sample was colorless. The indices of refraction could not be determined because the sample was too hygroscopic.

The *d*-values of the three strongest lines are: 2.586, 6.47, and 3.590A.

Structural data. Zachariasen [3] in 1948 determined that cerium chloride has the uranium chloride-type structure, the space group C_{6h}^2-$P6_3/m$ (No. 176) and $2(CeCl_3)$ per unit cell.

Lattice constants

		a	c
		A	A
1948	Zachariasen [3]	7.451	4.313
1951	Kojima, Inoue, and Ishiyama [2].	7.451	4.313
1961	National Bureau of Standards.	7.454	4.312 at 25 °C.

The density of cerium chloride calculated from the NBS lattice constants is 3.944 g/cm^3 at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
100	6.47	84
110	3.729	48
101	3.590	78
200	3.229	19
111	2.824	51
201	2.586	100
210	2.438	16
002, 300	2.153	47
211	2.125	71
102	2.048	16
112, 220	1.864	19
202	1.792	11
311	1.654	12
212	1.615	13
302	1.523	17
320	1.482	17
410	1.408	23
321	1.401	23
312	1.3776	6
203	1.3126	9
402	1.2923	6
500	1.2912	<1
213	1.2382	11
412	1.1790	9
511	1.1192	8
323	1.0313	11

References

[1] W. Zachariasen, The crystal structure of trichlorides, tribromides and trihydroxides of uranium and of rare earth elements, U.S. Atomic Energy Comm. TID **5212,** 157–164 (1955).

[2] T. Kojima, T. Inoue, and T. Ishiyama, Crystal structure of cerium compounds II, studies on cerium compounds by X-Ray analysis of crystal structure (Report 2), J. Electrochem. Soc. Japan **19,** 383–386 (1951).

[3] W. Zachariasen, Crystal chemical studies of the 5-f series of elements, Acta Cryst. **1,** 265–268 (1948).

Cerium(III) Vanadate, $CeVO_4$ (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cerium(III) vanadate was prepared at NBS by reacting stoichiometric solutions of cerium(III) chloride heptahydrate and ammonium metavanadate. It was then heated at 750 °C for 15 min to improve the crystallinity. The cerium(III) chloride heptahydrate was obtained from the Lindsay Chemical Co., West Chicago, Ill. Their analysis showed a total maximum impurity of rare earth oxides of 0.1 percent, largely lanthanum, praseodymium, and neodymium. Spectrographic analysis at NBS showed the following additional impurities for $CeVO_4$: 0.01 to 0.1 percent of silicon, and 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, and nickel.

The color of the sample was an opaque yellow brown.

The *d*-values of the three strongest lines are: 3.70, 2.761, and 1.898 A.

Structural data. Milligan and Vernon [1] in 1952 determined that cerium(III) vanadate has zircon-type structure, and the space group D_{4h}^{19}-I4/amd (No. 141) with $4(CeVO_4)$ per unit cell.

Lattice constants

		a	*c*
		A	*A*
1952	Milligan and Vernon [1]	7. 34	6.47
1961	National Bureau of Standards.	7. 399	6.496 at 25 °C

The density of cerium(III) vanadate calculated from the NBS lattice constants is 4.763 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
101	4. 89	30
200	3. 70	100
211	2. 948	9
112	2. 761	67
220	2. 615	19
202	2. 441	5
301	2. 306	16
103	2. 078	10
321	1. 955	9
312	1. 899	50
400	1. 849	16
213	1. 811	4
411	1. 729	2
420	1. 653	10
303	1. 627	4
004	1. 624	4
402	1. 606	2
332	1. 5361	12
204	1. 4875	10
501	1. 4429	4
224	1. 3799	10
512	1. 3248	10
440	1. 3079	3
600	1. 2332	4
503, 404	1. 2208	6
215	1. 2096	2
611	1. 1955	2
532	1. 1819	8
620	1. 1697	3
523, 424	1. 1595	9
325	1. 0979	1
631	1. 0875	1
116, 613	1. 0603	6
415	1. 0524	1
701	1. 0432	2
640	1. 0262	2
543	1. 0192	2
444	1. 0184	2

Reference

[1] W. O. Millegan and L. W. Vernon, Crystal structure of heavy metal orthovanadates, J. Phys. Chem. **56,** 145–148 (1952).

Cesium Perchlorate, $CsClO_4$ (orthorhombic)

ASTM cards. None

Additional published patterns. None.

NBS sample. The sample of cesium perchlorate was prepared at NBS by reacting solutions of ammonium perchlorate and cesium bromide. It was recrystallized several times to insure purity. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of rubidium; 0.01 to 0.1 percent of sodium; and 0.001 to 0.01 percent of aluminum.

The sample is colorless and optically negative with the indices of refraction $N\alpha=1.473$, $N\beta=1.477$, and $N\gamma=1.479$. $2V\cong 50°$.

The *d*-values of the three strongest lines are: 3.427, 2.322, and 3.814 A.

Structural data. Büssem and Herrmann [1] in 1928 determined that cesium perchlorate has potassium sulfate-type structure, the space group D_{2h}^{16}—Pbnm (No. 62), and $4(CsClO_4)$ per unit cell. In addition, they recognized a cubic form at temperatures above 220 °C.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1928	Büssem and Herrmann [1].	9. 84	6. 01	7. 81
1930	Herrmann and Ilge [2].	9. 870	6. 038	7. 777
1961	National Bureau of Standards.	9. 848	6.029	7. 813 at 25 °C

The density of cesium perchlorate calculated from the NBS lattice constants is 3.326 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 *A* at 25 °C	
	d	*I*
	A	
020	4. 92	12
101	4. 77	17
111	4. 30	42
120	4. 17	6
200	3. 909	40
021	3. 814	76
210	3. 632	51
121	3. 427	100
211	3. 111	38
002	3. 015	45
221	2. 728	16
131,112	2. 705	7
022	2. 572	14
230	2. 514	12
122	2. 442	16
202	2. 386	7
140	2. 347	42
311, 212, 231	2. 322	86
041	2. 280	12
222	2. 147	2
132	2. 135	9
330	2. 040	14
400	1. 952	4
103	1. 946	6
312, 331	1. 932	8
232	1. 930	7
410	1. 916	8
113, 150	1. 911	6
023	1. 861	10
142	1. 852	14
411	1. 826	5
420	1. 816	8
123	1. 810	8
340	1. 788	<1
213, 250	1. 758	6
421	1. 738	<1
242	1. 7128	<1
332,251	1. 6885	20
133	1. 6749	2
402	1. 6388	2
412, 431	1. 6171	13
152	1. 6132	10
061	1. 5830	4

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 Modifikationen der Perchlorate, Z. Krist. **A75,** 4–166 (1930).

Cesium Vanadium Sulfate Dodecahydrate, $CsV(SO_4)_2\cdot 12H_2O$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium vanadium sulfate dodecahydrate was prepared at NBS by R. B. Johannesen from solutions of cesium sulfate and vanadium sulfate. Spectrograhic analysis showed the following impurities: 0.1 to 1.0 percent aluminum; 0.01 to 0.1 percent each of silver, calcium, chromium, iron, lithium, magnesium, manganese, nickel, and titanium.

The sample was purple. The index of refraction is 1.483.

The *d*-values of the three strongest lines are: 4.3986, 2.8535, and 2.7817A.

Structural data. The structure of cesium vanadium sulfate dodecahydrate has not been published. Cesium vanadium sulfate dodecahydrate appears to be a beta alum since the intensities of the NBS pattern agree closely with those of other beta alums. Lipson [1] in 1935 determined the structure of the beta alums as having the space group T_h^6—Pa3 (No. 205) and $4[CsV(SO_4)_2 . 12H_2O]$ per unit cell.

Lattice constants

1961	National Bureau of Standards__	A 12.439 at 25 °C

The density of cesium vanadium sulfate dodecahydrate calculated from the NBS lattice constant is 2.043 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		*A*
111	7. 18	13	12. 44
200	6. 23	36	12. 46
210	5. 56	31	12. 44
211	5. 08	11	12. 44
220	4. 3986	100	12. 441
221	4. 1467	23	12. 440
311	3. 7509	6	12. 440
222	3. 5913	28	12. 440
302	3. 4502	8	12. 440
321	3. 3249	19	12. 441
400	3. 1099	37	12. 440
410	3. 0163	13	12. 437
331	2. 8535	59	12. 438
420	2. 7817	54	12. 440
421	2. 7152	8	12. 443
332	2. 6511	2	12. 435
422	2. 5397	34	12. 442
431	2. 4389	3	12. 436
511	2. 3938	17	12. 439
432	2. 3103	7	12. 441
521	2. 2711	4	12. 439
440	2. 1994	19	12. 442
522	2. 1656	4	12. 440
531	2. 1035	4	12. 444
600	2. 0737	19	12. 442
611	2. 0183	6	12. 442
620	1. 9664	30	12. 437
621	1. 9426	4	12. 439
533	1. 8974	10	12. 442
622	1. 8750	9	12. 437
630	1. 8542	3	12. 438
444	1. 7947	5	12. 434
711	1. 7412	12	12. 435
640	1. 7247	2	12. 437
641	1. 7083	2	12. 437
721	1. 6926	2	12. 438
642	1. 6620	25	12. 437
722	1. 6469	5	12. 434
731	1. 6189	7	12. 435
732	1. 5795	1	12. 437
800	1. 5554	2	12. 443
810	1. 5430	2	12. 440
733	1. 5201	5	12. 442
820	1. 5089	15	12. 443
821	1. 4975	3	12. 439
822	1. 4658	12	12. 438
751	1. 4365	1	12. 440
662	1. 4271	12	12. 441
832	1. 4175	1	12. 439
840	1. 3906	7	12. 438
911	1. 3651	4	12. 437
842	1. 3571	4	12. 438
664	1. 3260	2	12. 439
851	1. 3117	2	12. 444
931	1. 3039	4	12. 438
844	1. 2693	3	12. 437
10·0·0	1. 2437	2	12. 437
10·1·0	1. 2379	2	12. 441
10·2·0	1. 2194	12	12. 435
10·2·2	1. 1968	2	12. 438
953	1. 1599	4	12. 439
10·4·0	1. 1547	5	12. 437
10·4·2	1. 1357	4	12. 441
945	1. 1263	2	12. 440
11·2·1	1. 1079	2	12. 436
880	1. 0993	1	12. 437
11·3·1	1. 0869	1	12. 440
10·4·4	1. 0826	1	12. 438
10·6·0	1. 0666	2	12. 439
11·3·3	1. 0551	1	12. 439
10·6·2	1. 0513	1	12. 439
Average value of last five lines_______			12. 439

References

[1] H. Lipson, Existence of three alum structures, Nature **135,** 1912 (1935).

Erbium Gallium Oxide 35, $Er_3Ga_2(GaO_4)_3$ (cubic)

ASTM cards. None.

Additional published pattenns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of erbium oxide and gallium oxide. The sample 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: 0.0001 to 0.001 percent each of manganese and silicon.

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

The *d*-values of the three strongest lines are: 2.741, 2.501, and 1.6377A.

Structural data. S. Schneider, R. Roth, and J. L. Waring [1] showed that erbium gallium oxide has the garnet-type structure, having the space group O_h^{10}—Ia3d (No. 230) and $8[Er_3Ga_2(GaO_4)_3]$ per unit cell.

Lattice constants

		A
1956	Bertaut and Forrat [2]	12.25
1961	National Bureau of Standards	12.255 at 25 °C

The density calculated from NBS lattice constant is 7.521 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		A
211	5. 003	16	12. 25
220	4. 333	5	12. 25
321	3. 274	9	12. 25
400	3. 064	32	12. 26
420	2. 741	100	12. 26
422	2. 501	46	12. 25
431	2. 404	3	12. 26
521	2. 2370	11	12. 253
440	2. 1661	4	12. 253
611	1. 9881	10	12. 255
631	1. 8070	1	12. 256
444	1. 7688	15	12. 255
640	1. 6992	33	12. 253
721	1. 6676	5	12. 254
642	1. 6377	35	12. 255
732	1. 5560	3	12. 252
800	1. 5324	14	12. 259
653	1. 4646	2	12. 254
822	1. 4447	2	12. 258
752	1. 3877	1	12. 256
840	1. 3701	10	12. 254
842	1. 3372	18	12. 256
921	1. 3212	1	12. 252
664	1. 3061	5	12. 252
851	1. 2915	2	12. 252
932	1. 2641	3	12. 256
941	1. 2379	2	12. 255
10·1·1	1. 2133	1	12. 254
10·2·0	1. 2015	2	12. 252
10·3·1	1. 1682	3	12. 252
10·4·0	1. 1379	12	12. 256
10·3·3	1. 1282	3	12. 255
10·4·2	1. 1188	6	12. 256
11·2·1	1. 0918	2	12. 255
880	1. 0832	6	12. 255
11·3·2	1. 0585	2	12. 253
10·6·0	1. 0506	2	12. 252
12·0·0	1. 0212	3	12. 254
12·2·0	1. 0074	4	12. 256
11·5·2	1. 0005	1	12. 254
12·2·2	0. 9940	7	12. 255
11·6·1	. 9749	<1	12. 254
11·6·3	. 9511	1	12. 254
13·2·1	. 9289	1	12. 253
12·4·4	. 9239	4	12. 257
12·6·0	. 9135	7	12. 256
13·3·2	. 9087	<1	12. 259
12·6·2	. 9036	4	12. 257
888	. 8845	3	12. 256
14·3·1	. 8539	2	12. 256
12·8·0	. 8498	3	12. 256
14·4·0	. 8417	7	12. 255
14·4·2	. 8339	7	12. 256
15·2·1	. 8081	2	12. 255
15·4·1	. 7879	3	12. 257
12·10·0	. 7845	8	12. 254
Average value of last five lines			12. 255

References

[1] S. Schneider, R. Roth, and J. L. Waring, Solid state reactions involving oxides of trivalent cations, J. Research NBS **65A**, 345 (1961).

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

Europium(III) Chloride, $EuCl_3$ (hexagonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of europium chloride was received as a hydrate from Lindsay Chemical Co., West Chicago, Ill. It was dried for 2 hr in a hydrogen chloride atmosphere at 400 °C and 30 mm total pressure and transferred in a dry box to a dry atmosphere sample holder which was used to prepare the patterns. An analysis from Lindsay Chemical Co. showed the following impurities: less than 0.2 percent combined of other rare earths, largely samarium, gadolinium, and neodymium.

The sample was very pale yellow. The indices of refraction could not be determined because the material was too hygroscopic.

The *d*-values of the three strongest lines are: 2.526, 2.084, and 3.469 A.

Structural data. The structure of europium chloride has not been reported. It is assumed to have the uranium chloride-type structure, the space group C_{6h}^2-$P6_3/m$ (No. 176) and $2(EuCl_3)$ per unit cell.

Lattice constants

		a	*c*
		A	*A*
1961	National Bureau of Standards.	7. 375	4.134 at 25 °C

The density of europium chloride calculated from the NBS lattice constants is 4.405 g/cm^3 at 25 °C.

hkl	1961 National Bureau of Standards Co, 1.7889 A at 25 °C	
	d	*I*
	A	
100	6. 40	65
110	3. 687	39
101	3. 469	78
200	3. 193	23
111	2. 750	41
201	2. 526	100
210	2. 413	26
300	2. 128	40
211	2. 084	82
002	2. 066	29
102	1. 966	24
220	1. 843	12
112	1. 803	17
310	1. 770	15
202	1. 735	16
311	1. 628	13
400	1. 596	10
212	1. 570	31
302	1. 483	27
410	1. 394	23
321	1. 381	29
312	1. 346	12
402	1. 264	17
501	1. 2204	6
213	1. 1967	16
322	1. 1952	16
421	1. 1582	7
412	1. 1559	15
511	1. 1053	10

Europium Oxychloride, EuOCl (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of europium oxychloride was prepared at NBS by heating at 700 °C for 5 min a sample of europium chloride from the Lindsay Chemical Co., West Chicago, Ill. Their spectrographic analysis showed the following impurities: a maximum as rare earth oxides of 0.2 percent (largely Sm, Gd, and Nd).

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

The *d*-values of the three strongest lines are: 2.559, 2.804, and 3.41 A.

Structural data. The structure of EuOCl has not been determined; it is apparently isostructural with PbFCl, with the space group D_{4h}^7-$P4/nmm$ (No. 129) and 2 (EuOCl) per unit cell.

Lattice constants

		a	*c*
		A	*A*
1961	National Bureau of Standards	3. 964	6. 696 at 25 °C

The density of europium oxychloride calculated from the NBS lattice constants is 6.420 g/cm^3 at 25 °C.

Europium Oxychloride, EuOCl (tetragonal)—Continued

hkl	1961 National Bureau of Standards Co, 1.7889 *A* at 25 °C	
	d	*I*
	A	
001	6.70	16
101	3.41	63
002	3.35	10
110	2.804	74
111	2.586	8
102	2.559	100
003	2.232	6
112	2.150	24
200	1.9817	41
103	1.9459	4
201	1.9012	6
113	1.7460	20
211	1.7143	21
202	1.7043	5
004	1.6750	2
212	1.5669	38
104	1.5420	13
203	1.4820	7
114	1.4362	7
220	1.4012	9
213	1.3880	3
221	1.3718	3
005	1.3393	3
301	1.2963	5
222	1.2929	3
204	1.2791	2
105	1.2687	2
310	1.2534	10
311	1.2320	5
302	1.2291	9
214	1.2166	12
115	1.2085	2
223	1.1870	3
312	1.1739	5
303	1.1371	4
006	1.1163	2
205	1.1091	2
313	1.0928	5
321	1.0848	3
106, 224	1.0740	<1
215	1.0684	1
322	1.0446	8
304, 116	1.0364	5
314	1.0031	5
400	0.9909	3

Gadolinium Fluoride, GdF_3 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
5-0747 5-0748	1.25 3.24 2.97	Chromium	Zalkin [1] 1951

Additional published patterns. None.

NBS sample. The sample of gadolinium fluoride was prepared at NBS by the reaction of a solution of gadolinium chloride and hydrofluoric acid. It was heated at 750 °C for 10 min for additional crystal growth. The gadolinium chloride was obtained from the Lindsay Chemical Co., West Chicago, Ill. Their spectrographic analysis showed the presence of the following impurities in the chloride: a maximum as oxides of 0.1 percent samarium and europium plus a trace of terbium. Spectrographic analysis at NBS showed the following additional impurities in the fluoride: 0.01 to 0.1 percent of calcium, and 0.001 to 0.01 percent each of aluminum, iron, magnesium, manganese, lead, and silicon.

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

The *d*-values of the three strongest lines are: 3.236, 1.962, and 3.494 A.

Structural data. Zalkin and Templeton [2] in 1953 determined that gadolinium fluoride has yttrium fluoride-type structure, the space group D_{2h}^{16} Pnma (No. 62) and 4(GdF_3) per unit cell.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1953	Zalkin and Templeton [2]	6.570	6.984	4.393
1961	National Bureau of Standards	6.571	6.985	4.393 26 °C

The density of gadolinium fluoride calculated from the NBS lattice constants is 7.056 g/cm^3 at 26 °C.

Gadolinium Fluoride, GdF_3 (orthorhombic)—Continued

hkl	1961 National Bureau of Standards Co, 1.7889 A at 25 °C	
	d	*I*
	A	
011	3. 72	31
101	3. 65	57
020	3. 494	62
111	3. 236	100
210	2. 974	60
201	2. 633	3
121	2. 523	18
211	2. 461	3
220	2. 393	2
002	2. 195	11
221	2. 102	17
102	2. 083	4
112	1. 9959	25
131, 301	1. 9615	63
230	1. 8993	36
311	1. 8876	18
022	1. 8590	12
122	1. 7881	18
212	1. 7662	17
040	1. 7455	11
321	1. 7094	16
400	1. 6423	6
141	1. 5756	6
132, 302	1. 5514	6
312	1. 5137	8
411	1. 5025	9
331	1. 4997	12
420	1. 4869	6
241	1. 4553	5
232	1. 4362	11
013	1. 4329	9
103	1. 4295	<1
322	1. 4170	2
421	1. 4079	<1
113	1. 4000	3
042	1. 3669	5
430	1. 3427	5
142, 203	1. 3375	8
051	1. 3315	4
402, 213	1. 3146	4
151, 341	1. 3046	11
412	1. 2928	1
332	1. 2911	2
250	1. 2855	5
431	1. 2832	4
501	1. 2591	3
223	1. 2485	11
033, 511	1. 2394	7
422	1. 2312	5
303, 133	1. 2179	<1
313	1. 1993	2
440	1. 1967	5
521	1. 1847	5
060	1. 1643	6
152, 233, 342	1. 1601	7
323	1. 1496	2
432	1. 1449	<1
351	1. 1378	4
502	1. 1274	1
512	1. 1127	<1
252, 161	1. 1092	8
531	1. 1075	10
143	1. 1056	6
403	1. 0922	2
104, 610	1. 0822	7
413, 333	1. 0798	12
522	1. 0730	6
114	1. 0704	6
261, 450	1. 0638	2
601	1. 0627	5
243	1. 0615	8
442, 611	1. 0506	4
024	1. 0485	3
352	1. 0378	5
124, 451	1. 0341	7
062	1. 0284	4
541	1. 0214	3
621, 162	1. 0162	2
532	1. 0146	3
053	1. 0104	5
361	1. 0010	5
630	0. 9911	6
433	. 9892	8
134	. 9818	4
304, 262	. 9814	6

References

[1] Zalkin, Thesis U. California, Berkeley (1951).

[2] Allan Zalkin and D. H. Templeton, The crystal structures of YF_3 and related compounds, J. Am. Chem. Soc. **75**, 2453–2458 (1953).

Gadolinium Oxide, Gd_2O_3 (cubic)

ATSM cards. None.

Additional published patterns. None.

NBS sample. The sample of gadolinium oxide was prepared by the Lindsay Chemical Co., West Chicago, Ill. The sample was heated in air to 1,200 °C for 48 hr. Their analysis showed the following impurities: a total of less than 0.1 percent of samarium and europium, and a trace of terbium.

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

The *d*-values of the three strongest lines are: 3.122, 1.912, and 2.704 A.

Structural data. Pauling and Shappell [1] in 1930 determined that gadolinium oxide has the thallium-oxide type structure (rare earth type C), the space group T_h^7—Ia3 (No. 206) and 16 (Gd_2O_3) per unit cell. Several unit cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1925	Goldschmidt, Barth, and Ulrich [2]	10. 81
1939	Bommer [3]	10. 819
1947	Iandelli [5]	10. 820
1954	Templeton and Dauben [4]	10. 813
1961	National Bureau of Standards	10. 813 at 25 °C

The density of gadolinium oxide calculated from the NBS lattice constant is 7.616 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Co, 1. 7889 A at 25 °C		
	d	*I*	*a*
	A		A
211	4. 42	12	10. 8
222	3. 122	100	10. 81
321	2. 890	2	10. 81
400	2. 704	35	10. 81
411	2. 548	6	10. 81
420	2. 418	1	10. 81
332	2. 305	5	10. 81
422	2. 206	1	10. 81
431	2. 120	8	10. 81
521	1. 974	2	10. 81
440	1. 912	39	10. 81
433	1. 854	2	10. 81
600	1. 801	<1	10. 81
611	1. 754	5	10. 81
620	1. 709	1	10. 81
541	1. 669	3	10. 82
622	1. 6300	28	10. 812
631	1. 5946	6	10. 815
444	1. 5610	6	10. 815
543	1. 5298	2	10. 817
640	1. 4995	1	10. 813
721	1. 4720	3	10. 817
642	1. 4454	1	10. 816
732	1. 3739	2	10. 818
800	1. 3512	4	10. 810
811	1. 3305	4	10. 809
820	1. 3110	2	10. 811
653	1. 2925	2	10. 814
822	1. 2743	1	10. 813
831	1. 2566	3	10. 810
662	1. 2401	8	10. 811
840	1. 2089	4	10. 813
833	1. 1941	1	10. 813
842	1. 1798	<1	10. 813
921	1. 1663	2	10. 816
851	1. 1397	2	10. 812
932	1. 1153	2	10. 813
844	1. 1035	5	10. 812
941	1. 0923	3	10. 813
10·0·0	1. 0815	1	10. 815
10·1·1	1. 0706	<1	10. 813
10·2·0	1. 0601	4	10. 811
943	1. 0502	1	10. 812
10·2·2	1. 0405	5	10. 813
10·3·1	1. 0310	2	10. 813
871	1. 0127	2	10. 813
10·4·0	1. 0039	3	10. 812
10·3·3	0. 9953	2	10. 812
10·4·2	. 9870	2	10. 812
954	. 9789	2	10. 812
11·2·1	. 9633	3	10. 813
880	. 9557	1	10. 812
10·4·4	. 9411	2	10. 813
11·3·2	. 9341	2	10. 813
10·6·0	. 9271	1	10. 812
11·4·1	. 9204	3	10. 813
10·6·2	. 9138	6	10. 812
965	. 9074	1	10. 813
Average value of last five lines			10. 813

References

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

[2] V. M. Goldschmidt, T. Barth, and F. Ulrich, Geochemische Verteilungsgesetze der Element IV—Zur Krystallstruktur der Oxyde der seltenen Erdmetalle, Skrifter Norske Videnskaps-Akad. Oslo Math. Naturv. Kl. 1925.

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

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

[5] A. Iandelli, Sulle modificazioni dei sesquiossidi delle terre rare, Gazz. chim. ital. **77,** 312–318 (1947).

Gadolinium Oxychloride, GdOCl (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of gadolinium oxychloride was prepared at NBS by heating at 500 °C a sample of $GdCl_3$ obtained from the Lindsay Chemical Co., West Chicago, Ill. Their analysis showed the following total impurities to be less than 0.1 percent oxides of samarium, neodymium, and yttrium, and traces of other rare earths.

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

The *d*-values of the three strongest lines are: 2.550, 3.403, and 2.795 A.

Structural data. A reference to the structure of gadolinium oxychloride was not found; however, is is apparently isostructural with PbFCl, with the space group D_{4h}^{7}—P4/nmm (No. 129) and 2(GdOCl) per unit cell.

Lattice constants

		a	*c*
		A	*A*
1961	National Bureau of Standards	3. 950	6. 673 at 26 °C

The density of gadolinium oxychloride calculated from the NBS lattice constants is 6.656 g/cm^3 at 26 °C.

hkl	1961 National Bureau of Standards Cu, 1.7889A at 26 °C	
	d	*I*
	A	
001	6. 68	30
101	3. 403	85
002	3. 339	11
110	2. 795	78
111	2. 584	6
102	2. 550	100
003	2. 222	7
112	2. 141	27
200	1. 9746	41
103	1. 9387	3
201	1. 8940	7
113	1. 7397	20
211	1. 7070	25
202	1. 6981	8
004	1. 6661	1
212	1. 5610	41
104	1. 5362	11
203	1. 4772	8
114	1. 4320	8
220	1. 3967	11
213	1. 3826	1
221	1. 3675	2
005	1. 3349	3
301	1. 2918	5
222	1. 2882	3
204	1. 2744	3
105	1. 2642	2
310	1. 2492	9
311	1. 2283	2
302	1. 2247	8
214	1. 2126	11
115	1. 2043	3
223	1. 1821	5
312	1. 1697	6
303	1. 1334	2
006	1. 1124	<1
205	1. 1059	3
313	1. 0890	7
321	1. 0811	5
224, 106	1. 0708	1
215	1. 0648	2
322	1. 0407	9
304, 116	1. 0332	6
314	1. 0001	4
400	0. 9872	4
323	. 9834	1

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

ASTM cards. None.

Additional published patterns. None.

MBS sample. The sample of holmium ethylsulfate nonahydrate was prepared at NBS by R. S. Kaeser from solutions of holmium hydroxide and diethyl sulfate. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent zirconium and 0.0001 to 0.001 percent each of calcium and lead.

The color of the sample was pink. It is optically negative with the indices of refraction N_e=1.481 and N_0=1.495.

The *d*-values of the three strongest lines are: 4.96, 4.58, and 6.09 A.

Structural data. Ketelaar [1] in 1937 determined the structure of some of the rare earth ethylsulfates. Holmium ethylsulfate nonahydrate is isostructural with neodymium ethylsulfate nonahydrate, having the space group C_{6h}^2—$P6_3/m$ (No. 176) with $2\{Ho[(C_2H_5)SO_4]_3 \cdot 9H_2O\}$ per unit cell.

Lattice constants

		a	c
		A	A
1961	National Bureau of Standards	13.928	7.052 at 25 °C

The density of holmium ethylsulfate nonahydrate calculated from NBS lattice constants is 1.969 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
100	12.13	78
110	6.98	22
101	6.09	85
200	6.03	53
111	4.96	100
201	4.58	87
300	4.019	53
211	3.827	69
002	3.526	27
301	3.495	19
310	3.346	20
221	3.123	22
202	3.044	15
311	3.024	16
400	3.018	10
212	2.790	36
320	2.769	19
302	2.651	16
410	2.633	17
321	2.578	24
222	2.481	9
312	2.428	7
500	2.409	5
330	2.322	7
103	2.305	3
501	2.282	28
203	2.190	19
322	2.177	25
421	2.170	28
412	2.109	20
213	2.088	15
511	2.071	28
303	2.030	2
600	2.010	8
502	1.991	5
430	1.985	7
332	1.938	10
313	1.923	8
422, 431	1.911	7
512	1.845	10
610	1.838	10
323	1.791	8
611	1.779	8
004	1.764	7
602	1.7460	7
440	1.7390	5
432	1.7284	7
114	1.7092	5
522, 204	1.6934	8
441	1.6899	8
701	1.6737	5

Reference

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

Iron Arsenide, FeAs (orthorhombic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of iron arsenide was made at the Geophysical Laboratory in Washington, D.C., by L. Clark. A mixture of iron and arsenic was melted at 1,060 °C in an evacuated quartz tube and quenched at 900 °C. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of cobalt, chromium, copper, manganese, molybdenum, and nickel.

The sample was a gray opaque powder.

The *d*-values of the three strongest lines are: 2.588, 1.996, and 2.635 A.

Structural data. Hägg [1] in 1929 determined that iron arsenide has the manganese phosphide-type structure, the space group D_{2h}^{16}—Pnam (No. 62) and 4(FeAs) per unit cell. The unit-cell measurements reported by Hägg have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1929	Hägg [1]	5. 439	6. 028	3. 373
1957	Heyding and Calvert [2].	5. 432	6. 023	3. 372
1961	National Bureau of Standards.	5. 4361	6. 0242	3. 3724 at 25 °C

The density of iron arsenide calculated from NBS lattice constants is 7.861 g/cm³ at 25 °C.

References

[1] G. Hägg, Röntgenographische Studien über das System Eisen-Arsen, Z. Krist. **71**, 134 (1929).

[2] R. D. Heyding and L. D. Calvert, Arsenides of transition metals: The arsenides of iron and cobalt, Can. J. Chem. **35**, 449 (1957).

hkl	1961 National Bureau of Standards Co, 1.7889 A at 25 °C	
	d	*I*
	A	
011	2. 942	5
120	2. 635	58
111	2. 588	100
210	2. 478	6
*201	2. 116	17
121	2. 076	34
220	2. 019	33
211	1. 996	59
130	1. 884	10
310	1. 735	12
031	1. 725	32
002	1. 686	17
230	1. 616	6
320	1. 553	5
311	1. 543	9
231	1. 457	8
140	1. 452	8
122	1. 421	12
321	1. 410	6
400	1. 3590	5
410	1. 3255	4
222	1. 2942	6
*401	1. 2605	5
132	1. 2564	5
411	1. 2337	<1
312	1. 2093	7
150	1. 1763	<1
232	1. 1663	3
421	1. 1629	4
322	1. 1423	3
430	1. 1253	5
151	1. 1107	<1
341	1. 0954	13
113	1. 0829	5
510	1. 0699	3
402	1. 0582	6
251	1. 0469	2
123	1. 0341	3
213	1. 0235	6

*Contrary to space group.

Lanthanum Borate, $LaBO_3$ (orthorhombic)

ASTM cards. None.

Additional published patterns. Goldschmidt and Hauptmann [1] 1932.

NBS sample. The sample of lanthanum borate was prepared by E. Levin [2] at NBS from lanthanum oxide and boric oxide. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, and silicon; and 0.0001 to 0.001 percent each of silver, copper, and magnesium.

The color of the sample was white. It is optically negative with the indices of refraction N_α=1.800, N_β=1.877, and N_γ=1.822. 2V≈20°.

The *d*-values of the three strongest lines are: 3.492, 3.377, and 2.037 A.

Structural data. Goldschmidt and Hauptmann [1] in 1932 determined that lanthanum borate has the aragonite-type structure, the space group D_{2h}^{16}-Pnam (No. 62) and 4($LaBO_3$) per unit cell. The unit cell measurements reported by Goldschmidt

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
011	4.339	20
020	4.130	10
111	3.492	100
120	3.377	53
200	2.936	19
121	2.822	1
210	2.767	8
002	2.553	21
201	2.547	11
130	2.493	1
211	2.433	40
031	2.424	25
220	2.394	13
112	2.252	10
022	2.173	12
040	2.066	7
122	2.037	42
140	1.947	19
202	1.927	20
212	1.875	3
231	1.869	27
311	1.785	22
320	1.768	13
222	1.746	8
240	1.690	5
013	1.6676	5
113, 241	1.6039	13
142	1.5482	11
151	1.5176	10
400	1.4679	5
322	1.4539	5
213	1.4497	12
340	1.4207	4
242	1.4084	5
411	1.3906	8
420	1.3832	4
060	1.3764	3
233	1.2985	9
004	1.2769	5
402	1.2727	10
313	1.2695	9
431	1.2556	8
260	1.2461	7
342	1.2412	3
351	1.2254	6
422	1.2163	4
062	1.2117	2
440	1.1963	2
124	1.1944	7
204	1.1710	6
153	1.1620	5
511	1.1339	6
520	1.1294	6
262	1.1199	6
413	1.1020	3
361, 253	1.0994	3
442	1.0834	2
451	1.0725	2
149	1.0675	7
512	1.0581	3
324	1.0351	6
522	1.0329	8
433	1.0307	11
540	1.0207	4
244	1.0183	5
353, 015	1.0137	5
370	1.0098	5
452	1.0080	3
460	1.0038	6
115	0.9991	6
371	.9913	6
600	.9785	2
404	.9634	2
513	.9602	7
035	.9577	5
254	.9550	2
542	.9478	6
182	.9445	3
551	.9406	4
064, 621	.9356	2
462	.9344	4

and Hauptmann have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	c
		A	A	A
1932	Goldschmidt and Hauptmann [1]	5.84	8.24	5.11
1961	National Bureau of Standards	5.872	8.257	5.107 at 25 °C

The density of lanthanum borate calculated from NBS lattice constants is 5.303 g/cm³ at 25 °C.

References

[1] V. M. Goldschmidt and H. Hauptmann, Isomorphie von Boraten und Carbonaten, Nachr. Ges. Wiss. Göttingen **1932**, 53–72 (1932).

[2] E. Levin, C. Robbins, and J. Waring, Immiscibility and the system lanthanum oxide-boric acid, J. Am. Ceram. Soc. **44**, No. 2, 87–91 (1961).

Lanthanum Chloride, $LaCl_3$ (hexagonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of lanthanum chloride was received as a hydrate from Lindsay Chemical Co., West Chicago, Ill. It was dried for 30 min in vacuum at 400 °C and transferred in a dry box to a dry atmosphere sample holder which was used to prepare the patterns. An analysis from Lindsay Chemical Co., showed the following impurities: less than 0.01 percent praseodymium and less than 0.001 percent cerium.

The sample was colorless. The indices of refraction could not be determined because the material was too hygroscopic.

The *d*-values of the three strongest lines are: 2.603, 6.49, and 2.137A.

Structural data. Zachariasen [1] in 1948 determined that lanthanum chloride has the uranium chloride-type structure, the space group C_{6h}^2-$P6_3/m$ (No. 176) and 2 ($LaCl_3$) per unit cell.

Lattice constants

		a	c
		A	A
1948	Zachariasen [1]	7.483	4.375
1961	National Bureau of Standards.	7.483	4.364 at 25 °C

The density of lanthanum chloride calculated from the NBS lattice constants is 3.848 g/cm³ at 25 °C.

References

[1] W. H. Zachariasen, Crystal chemical studies of the 5-f series of elements, Acta Cryst. **1**, 265–268 (1948).

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	I
	A	
100	6.49	79
110	3.742	49
101	3.622	70
200	3.243	20
111	2.844	33
201	2.603	100
210	2.450	18
002	2.184	26
300	2.159	44
211	2.137	75
102	2.071	13
112	1.886	15
220	1.871	9
202	1.810	10
310	1.797	2
311	1.662	11
212	1.627	11
302	1.536	20
320	1.486	3
222, 103	1.419	17
321	1.408	23
312	1.388	5
203	1.327	8
402	1.299	4
213	1.251	11
501	1.244	5
412	1.187	8
421	1.1794	4
511	1.1250	5
520, 323	1.0383	8

Lanthanum Magnesium Nitrate 24-Hydrate, $La_2Mg_3(NO_3)_{12}{\cdot}24H_2O$ (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of lanthanum magnesium nitrate hydrate was prepared at NBS by Robert Kaeser from stoichiometric mixtures of lanthanum nitrate and magnesium nitrate. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent strontium; and 0.0001 to 0.001 percent each of calcium, copper, iron, and manganese.

The sample is colorless and optically negative. The indices of refraction are $N_e=1.516$ and $N_o=1.521$.

The *d*-values of the three strongest lines are: 8.35, 3.994, and 6.43 A.

hkl (hex.)	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
101	9. 24	<1
012	8. 35	100
104	6. 43	82
006	5. 77	14
015	5. 60	16
110	5. 521	54
113	4. 984	4
202	4. 607	6
107	4. 397	10
024	4. 185	58
116	3. 994	94
018	3. 945	19
009	3. 854	6
122	3. 538	16
027	3. 437	4
214	3. 335	57
1·0·10	3. 261	<1
208	3. 211	16
300	3. 187	3
303	3. 076	2
217	2. 920	4
0·2·10	2. 806	45
128	2. 775	75
132	2. 622	55
1·1·12	2. 557	32
134	2. 538	12
2·1·10	2. 501	35
226	2. 491	52
0·1·14	2. 398	26
042	2. 370	1
137	2. 340	5
404	2. 306	9
318, 045	2. 261	16
232	2. 177	12
3·0·12	2. 140	45
324	2. 125	40
1·0·16	2. 113	16
1·3·10	2. 107	22
410	2. 086	15
413	2. 054	9
1·2·14	2. 043	9
327	2. 004	12
2·2·12	1. 997	23
0·2·16	1. 974	14
4·0·10	1. 966	30
416	1. 962	33
238	1. 958	22
0·0·18	1. 927	3
2·0·17	1. 875	1
2·1·16	1. 858	14
330	1. 841	8
1·1·18	1. 819	9
422	1. 797	8
2·2·15	1. 772	5
336	1. 752	8
0·1·20	1. 706	7
4·1·12	1. 692	13
1·3·16	1. 679	8
428	1. 669	5
0·0·21	1. 6502	6
2·0·20	1. 6294	1
2·4·10	1. 6024	9
600	1. 5940	7
1·2·20	1. 5647	5
1·0·22	1. 5546	8
0·4·17	1. 5513	5
5·1·10	1. 5391	5
345	1. 5335	6
0·2·22	1. 4964	3
526	1. 4801	4
2·1·22	1. 4461	4
2·0·23	1. 4369	1
0·5·16	1. 4334	<1
1·5·14	1. 4112	5
1·1·24	1. 3972	1
2·4·16	1. 3873	2
440	1. 3801	<1
5·2·12	1. 3532	1
704	1. 3496	1
4·0·22 3·0·24	1. 3153	1
0·6·15	1. 3123	1
538	1. 3028	1
627	1. 2807	<1
0·4·23	1. 2741	<1
7·0·10	1. 2712	1

Lanthanum Magnesium Nitrate 24-Hydrate, $La_2Mg_3(NO_3)_{12}\cdot 24H_2O$ (trigonal)—Continued

Structural data. Culvahouse and Sapp [1] in 1959 determined the structure of cerium zinc nitrate hydrate and other rare earth magnesium nitrate hydrates. Due to the similarity of this pattern and cerium magnesium nitrate hydrate we believe the two compounds to be isostructural, having the space group D^5_{3d}-$R\bar{3}m$ (No. 166) and $1[La_2Mg_3(NO_3)_{12}\cdot 24H_2O]$ per unit rhombohedral cell or $3[La_2Mg_3(NO_3)_{12}\cdot 24H_2O]$ per unit hexagonal cell.

Lattice constants

		a	c
		A	A
1961	National Bureau of Standards.	11.042	34.66 at 25 °C

The density of lanthanum magnesium nitrate 24-hydrate calculated from NBS lattice constants is 2.079 g/cm³ at 25 °C.

References

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

Lithium Molybdate, Li_2MoO_4 (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of lithium molybdate was prepared at NBS by crystallization from a solution of stoichiometric quantities of lithium hydroxide and ammonium molybdate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, silicon, and sodium, and 0.001 to 0.01 percent each of aluminum and potassium.

The sample was colorless and optically negative with the indices of refraction $N_e=1.433$ and $N_o=1.570$.

The *d*-values of the three strongest lines are: 4.22, 2.920, and 4.47 A.

Structural data. Zachariasen [1] in 1926 determined that lithium molybdate has phenacite-type structure, the space group C^2_{3i}—$R\bar{3}$ (No. 148) and $18(Li_2MoO_4)$ per unit hexagonal cell or $6(Li_2MoO_4)$ per unit rhombohedral cell. According to Goldschmidt [2], there also exists at high temperatures a cubic form with spinel-type structure. Zachariasen's unit cell "a" measurement was multiplied by $\sqrt{3}$ as suggested by Goldschmidt [3]. The cell measurements were then converted from kX to angstrom values for comparison.

Lattice constants

		a	c
		A	A
1926	Zachariasen [1]	14. 23	9.47
1961	National Bureau of Standards.	14. 338	9.588 at 25 °C.

The density of lithium molybdate calculated from the NBS lattice constants is 3.043 g/cm³ at 25 °C.

References

[1] W. H. Zachariasen, Note on the crystal structure of phenacite, willemite and related compounds, Norsk geol. tidsskr. **9**, 65–73 (1926).

[2] V. M. Goldschmidt, Die Gesetze der Krystallochemie, Geochemische Verteilungsgesetze der Elemente VII (1926), Skrifter Norske Videns.-Akad. Oslo I. Mat.-Nat. Kl. No. 2, 1–117 (1926).

[3] V. M. Goldschmidt, Untersuchungen über Bau und Eigenschaften von Krystallen, Geochemische Verteilungsgesetze VIII (1927), Skrifter Norske Videns.-Akad. Oslo I. Mat.-Nat. Kl. (1926), 1–156 (1927).

Lithium Molybdate, Li_2MoO_4 (trigonal)—Continued

hkl (hex.)	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
110	7.17	12
021	5.21	5
012	4.47	38
211	4.22	100
300	4.14	15
202	3.794	5
220	3.584	29
122	3.353	26
131	3.241	17
401	2.954	2
113	2.920	39
312	2.797	7
321	2.730	2
410	2.708	30
042	2.605	8
303	2.529	2
232	2.449	3
330	2.390	12
223	2.386	12
104	2.354	3
241	2.279	10
502	2.205	11
511	2.173	<1
214	2.136	5
422	2.108	2
600	2.070	3
152	2.022	6
431	1.997	11
520	1.988	10
333	1.914	14
404, 015	1.897	4
342	1.878	2
161	1.858	3
324	1.835	<1
205	1.834	<1
125	1.775	8
612	1.761	<1
701	1.744	5
603	1.737	5
054	1.724	6
621	1.695	5
244, 315	1.676	2
072	1.664	1
710	1.645	4
514, 045	1.632	2
262	1.620	2
006	1.598	6
541	1.568	2
630, 443	1.564	4
116	1.560	1
434	1.554	2
081	1.532	<1
452	1.509	4
271	1.498	2
164, 425	1.485	1
713	1.462	12
226	1.460	5
722	1.446	1
811	1.436	<1
550	1.434	2
704	1.427	<1
633	1.4052	6
624, 345	1.3979	4
182	1.3906	2
900	1.3792	5
416	1.3764	7
642	1.3651	1
820	1.3546	<1
615	1.3473	<1
544	1.3247	1
217	1.3148	2
084, 075	1.3022	1
191	1.2892	1
740	1.2872	1
274, 265	1.2811	2
137	1.2727	1
903, 606	1.2652	<1
912	1.2561	3
381	1.2499	3
823	1.2469	3
526	1.2449	2
464, 455	1.2242	2
921	1.2138	1
0·10·2	1.2019	1
660, 743	1.1941	3
018, 446	1.1928	2
725	1.1894	2
292	1.1855	2
247	1.1829	2
571	1.1801	2
10·1·0	1.1780	2
208	1.1771	2
841	1.1644	1

Lithium Oxide, Li_2O (cubic)

ASTM cards. None.

Additional published patterns. Bijvoet and Karssen [1] 1924, Bijvoet, Claassen, and Karssen [2] 1926, Zintl, Harder, and Dauth [3] 1934, and Rode, Dobrynina, and Gol'der [4] 1955.

NBS sample. The sample of lithium oxide was prepared at NBS by heating in a vacuum furnace overnight at 650 °C a sample of lithium hydroxide obtained from Fisher Scientific Co. To prevent decomposition it was necessary to protect the lithium oxide from atmospheric moisture and carbon dioxide. A silver boat was used. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of calcium; 0.01 to 0.1 percent of sodium; and 0.001 to 0.01 percent each of aluminum, silicon, and vanadium.

The sample was a very fine white powder. The index of refraction was not determined because the sample reacted with index liquids.

The *d*-values of the three strongest lines are: 2.664, 1.6307, and 1.3906 A.

Structural data. Bijvoet and Karssen [1] in 1924 determined that lithium oxide has fluorite-type structure, the space group O_h^5-Fm3m (No. 225), and 4(Li_2O) per unit cell.

Lattice constants

		A
1924	Bijvoet and Karssen [1]	4.62
1934	Zintl, Harder, and Dauth [3]	4.628
1955	Rode, Dobrynina, and Gol'der [4].	4.619
1961	National Bureau of Standards	4.6114 at 25 °C

The density of lithium oxide calculated from the NBS lattice constant is 2.023 g/cm^3 at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		A
111	2.664	100	4.614
200	2.306	8	4.613
220	1.6307	41	4.612
311	1.3906	15	4.612
400	1.1531	3	4.612
331	1.0580	3	4.6117
422	0.9413	8	4.6116
511	.8875	4	4.6117
440	.8151	3	4.6110
531	.7794	5	4.6111
Average value of last five lines			4.6114

References

[1] J. M. Bijvoet and A. Karssen, X-ray investigation of the crystal structure of lithium oxide, Rec. Trav. Chim. Pays-Bas **43,** 680–684 (1924).

[2] J. M. Bijvoet, A. Claassen, and A. Karssen, The scattering power of lithium and oxygen, determined from the diffraction-intensities of powdered lithium oxide, Proc. Amsterdam **29,** 1286–1292 (1926).

[3] E. Zintl, A. Harder, and B. Dauth, Gitterstruktur der Oxyde, Sulfide, Selenide und Telluride des Lithiums, Natriums und Kaliums, Z. Elektrochem. **40,** 588–593 (1934).

[4] T. V. Rode, T. A. Dobrynina, and G. A. Gol'der, Fizikokhimicheskoye izucheniye perekisi litiya, Izvest. Akad. Nauk S.S.S.R., Otdel. Khim. Nauk, 611–621 (1955).

Lithium Tungstate, Li_2WO_4 (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of lithium tungstate was obtained from the City Chemical Co., New York, N.Y. As received, the sample was hydrated. After heating to fusion and cooling the sample was found to be the 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 with the refractive index N_o=1.658. N_e was not determined because of orientation of the particles under the microscope.

The *d*-values of the three strongest lines are: 4.23, 4.49, and 2.714 A.

Structural data. Zachariasen [1] in 1926 determined that lithium tungstate has phenacite-type structure, the space group C_{3i}^2-R$\bar{3}$ (No. 148) and 18(Li_2WO_4) per unit hexagonal cell or 6(Li_2WO_4) per unit rhombohedral cell. According to Goldschmidt [2] the substance converts to a cubic spinel-type structure at high temperatures. In addition, there exists at room temperature a cubic hydrate. The "a" unit-cell measurement of

Lattice constants

		a	*c*
		A	A
1926	Zachariasen [1]	14.23	9.47
1961	Zachariasen and Plettinger [37]	14.361	9.602
1961	National Bureau of Standards	14.361	9.603 at 25 °C.

Lithium Tungstate, Li_2WO_4 (trigonal)—Continued

hkl (hex.)	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
110	7.2	12
021	5.23	6
012	4.49	46
211	4.23	100
300	4.15	10
202	3.803	6
220	3.594	23
122	3.361	33
131	3.246	18
113	2.926	33
312	2.802	3
410	2.714	35
042	2.610	17
232	2.454	5
223	2.390	21
104	2.358	7
241	2.283	12
024	2.240	3
502	2.209	12
511	2.176	2
214	2.138	7
422	2.111	3
600	2.072	3
152	2.025	7
431	2.000	10
134	1.971	1
333	1.918	17
404	1.9004	4
342	1.8816	3
161	1.8610	3
324, 205	1.8367	1
125	1.7781	9
612	1.7640	2
701	1.7474	7
603	1.7403	4
054	1.7278	6
621	1.6972	7
523	1.6914	8
244, 315	1.6783	3
072	1.6661	4
710	1.6474	4
514, 045	1.6350	4
262	1.6228	1
006	1.6004	5
541	1.5710	3
630, 443	1.5668	4
434	1.5567	2
081	1.5347	2
452	1.5116	4
271	1.5009	2
306	1.4927	<1
164, 425	1.4879	3
802	1.4794	<1
713	1.4650	10
226	1.4617	8
811	1.4395	2
550	1.4363	1
704	1.4279	1
461	1.4118	1
633	1.4071	8
624, 345	1.4003	4
182	1.3930	2
731	1.3846	<1
900	1.3816	4
416	1.3785	10
642	1.3674	2
820	1.3570	1
615	1.3498	<1
372	1.3429	<1
027	1.3401	<1
336	1.3302	<1
544	1.3267	5
217	1.3166	4
084, 075	1.3044	2
191	1.2916	1
740	1.2897	<1
274, 265	1.2833	2
137	1.2748	2
606	1.2672	<1
912	1.2583	4
407	1.2546	3
381	1.2516	2
823	1.2493	2
526	1.2475	2
814	1.2446	2
464, 455	1.2265	2
832	1.2215	1
921	1.2156	2
734, 805	1.2088	2
0·10·2	1.2040	<1

Zachariasen [1] was multiplied by $\sqrt{3}$ to give the smallest hexagonal cell measurements, which were converted from kX to angstrom units for comparison.

The density of lithium tungstate calculated from the NBS lattice constants is 4.560 g/cm^3 at 25 °C.

References

[1] W. H. Zachariasen, Note on the crystal structure of phenacite, willemite and related compounds, Norsk geol. tidsskr. **9,** 65–73 (1926).

[2] V. M. Goldschmidt, Die Gesetze der Krystallochemie, Geochemische Verteilungsgesetze der Elemente VII (1926), Skrifter Norske Videns.-Akad. Oslo I, Mat.-Nat. Kl. No. 2, 1–117 (1926).

[3] W. H. Zachariasen and H. A. Plettinger, The crystal structure of lithium tungstate, Acta Cryst. **14,** 229–230 (1961).

Lutetium Oxide, Lu_2O_3 (cubic)

ASTM cards. None.

Additional published patterns. Zachariasen [1] 1926.

NBS sample. The sample of lutetium oxide was prepared by the Lindsay Chemical Co., West Chicago, Ill. The sample was heated in air to 1,200 °C for 60 hr. Their analysis showed the following impurities: a total of less than 0.1 percent of ytterbium and thulium and traces of other rare earths.

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

The *d*-values of the three strongest lines are: 3.001, 2.598, and 1.837 A.

Structural data. Pauling and Shappell [2] in 1930 determined that lutetium oxide has the thallium-oxide type structure (rare earth type C), the space group T_h^7-Ia3 (No. 206) and 16(Lu_2O_3) per unit cell. Several unit cell measurements have been converted from kX to angstrom units for comparison.

Lattice constants

		A
1925	Goldschmidt, Barth, and Ulrich [3].	10.39
1939	Bommer [4]	10.396
1954	Templeton and Dauben [5]	10.391
1961	National Bureau of Standards	10.390 at 25 °C.

The density of lutetium oxide calculated from the NBS lattice constant is 9.424 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Co, 1.7889 A at 25 °C		
	d	*I*	*a*
	A		A
211	4. 25	12	10. 41
222	3. 001	100	10. 40
321	2. 778	3	10. 40
400	2. 598	37	10. 39
411	2. 449	6	10. 39
420	2. 325	1	10. 40
332	2. 216	5	10. 40
422	2. 121	1	10. 39
431	2. 038	9	10. 39
521	1. 898	3	10. 40
440	1. 837	34	10. 39
433	1. 782	2	10. 39
600	1. 731	1	10. 38
611	1. 686	5	10. 39
620	1. 643	1	10. 39
541	1. 604	4	10. 39
622	1. 567	28	10. 40
631	1. 532	5	10. 39
444	1. 500	6	10. 39
543	1. 470	2	10. 40
640	1. 4413	1	10. 393
721	1. 4143	3	10. 393
642	1. 3886	2	10. 391
732	1. 3199	3	10. 393
800	1. 2989	3	10. 391
811	1. 2791	3	10. 391
820	1. 2601	2	10. 391
653	1. 2420	2	10. 391
822	1. 2246	1	10. 391
831	1. 2080	3	10. 392
662	1. 1921	7	10. 392
840	1. 1619	5	10. 392
833	1. 1477	1	10. 393
842	1. 1338	1	10. 392
921	1. 1204	2	10. 390
851	1. 0954	2	10. 392
932	1. 0719	2	10. 392
844	1. 0605	5	10. 391
941	1. 0497	3	10. 392
10·0·0	1. 0392	2	10. 392
10·1·1	1. 0290	1	10. 392
10·2·0	1. 0189	5	10. 391
943	1. 0092	1	10. 390
10·2·2	0. 9999	5	10. 391
10·3·1	. 9907	4	10. 390
871	. 9732	3	10. 391
10·4·0	. 9648	3	10. 391
10·3·3	. 9566	2	10. 391
10·4·2	. 9486	3	10. 391
954	. 9407	2	10. 390
11·2·1	. 9256	3	10. 390
880	. 9184	1	10. 390
Average value of last five lines			10. 390

References

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

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

[3] V. M. Goldschmidt, T. Barth, and F. Ulrich, Geochemische Verteilungsgesetze der Elemente IV—Zur Krystallstruktur der Oxyde der seltenen Erdmetalle, Skrifter Norske Videnskaps-Akad. Oslo Math. Nat. Kl. (1925).

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

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

Magnesium Aluminum Silicate (low-cordierite),** $Mg_2Al_4Si_5O_{18}$ (orthorhombic)

ASTM cards. None. Cards numbered 9–326 and 9–472 give crystallographic data for orthorhombic cordierite; however, the *d*-values listed compare more favorably with the hexagonal cordierite.

Additional published patterns. Byström [1] 1942; Iiyama [2] 1956; Miyashiro, Iiyama, Yamasaki, and Miyashiro [4] 1954.

NBS sample. The sample of low temperature cordierite was prepared at the Geophysical Laboratory in Washington, D.C., by W. Schreyer and J. F. Schairer from stoichiometric mixtures of the oxides as a glass devitrified at 1,000 °C for 3 days, and 1,380 °C for 7 days. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, iron, sodium, and platinum; and 0.001 to 0.01 percent each of barium, chromium, copper, nickel, and silver.

The sample is colorless. The mean index of refraction, using a phase contrast microscope with white light, is slightly less than 1.528.

The *d*-values of the three strongest lines are: 8.45, 8.52, and 3.039 A.

Structural data. Byström [1] in 1942 determined that orthorhombic cordierite has the space group D_{2h}^{20}-Cccm (No. 66) and $4(Mg_2Al_4Si_5O_{18})$ per unit cell. According to Byström [1], the pseudo-hexagonal structure ($a \sim b\sqrt{3}$) is almost identical with that of beryl. The unit cell data reported by Gossner and by Byström have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	b	c
		A	A	A
1928	Gossner [3]	9.80	17.13	9.35
1941	Byström [1]	9.69	17.06	9.37
1954	Miyashiro Iiyama, Yamasaki, and Miyashiro [4].	9.7	17.1	9.3
1956	Iiyama [2]*	9.76	17.12	9.33
1961	National Bureau of Standards.	9.721	17.062	9.339 at 25 °C

*This data is an average of 6 sets from 6 different locations.

References

[1] A. Byström, The crystal structure of cordierite, Arkiv. Kemi. Mineral. Geol. **15B,** No. 12, 7 (1941–42).

[2] Iiyama, Optical properties and unit cell dimensions of cordierite and indialite, Mineral. J. **1,** No. 6, 372–394 (1956).

[3] B. Gossner, Structural relation between beryl and cordierite, Central. Mineral. Geol. **1928A,** 204–207 (1928).

[4] A. Miyashiro, T. Iiyama, M. Yamasaki, and T. Miyashiro, The polymorphism of cordierite and indialite, Am. J. Sci. **253,** 185–208 (1955).

[5] W. Schreyer and J. F. Schairer, Compositions and structural states of anhydrous Mg-cordierite: A re-investigation of the central part of the system $MgO–Al_2O_3–SiO_2$, J. Petrology **2,** No. 3, 324–406 (1961).

The density of low cordierite calculated from NBS lattice constants is 2.505 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
020	8.52	98
110	8.45	100
130	4.91	28
200	4.86	10
002	4.67	13
040	4.27	1
112	4.09	52
221	3.84	1
132	3.381	51
202	3.369	38
042	3.149	25
222	3.132	56
151	3.039	64
241	3.035	64
311	3.012	56
152	2.650	22
242	2.644	22
312	2.637	12
260	2.454	4
400	2.430	5
332	2.409	3
261	2.373	1
004	2.334	11
171	2.293	2
351	2.278	2
243	2.234	4
313	2.225	5
262	2.173	5
402	2.156	2
080	2.132	<1
172	2.107	11
204, 352	2.102	11
422	2.091	8
224	2.044	2
280	1.954	4
370	1.948	6
082	1.942	5
510	1.932	3
263, 442	1.925	4
281	1.912	<1
314, 173	1.882	8
353	1.876	11
423	1.870	10
460	1.848	1
530	1.839	2
115	1.825	<1
461	1.811	4
064	1.804	7
334	1.798	8
225, 0·10·0	1.706	6
264	1.691	18

** According to Schreyer and Schairer [5].

Magnesium Aluminum Silicate (high-cordierite),* $Mg_2Al_4Si_5O_{18}$ (hexagonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
[a] 9–326	8. 54 4. 09 3. 37	Cobalt___	Richardson and Rigby [2] 1949.
[a] 9–472	8. 58 3. 38 3. 04	Copper___	Claringbull, British Museum.

[a] These two cards give crystallographic data for the orthorhombic form but the pattern contains only hexagonal spacing.

Additional published patterns. Miyashiro and Iiyama [3] 1954 and Miyashiro, Iiyama, Yamasaki, and Miyashiro [4] 1955.

NBS sample. The sample of hexagonal cordierite was prepared at the Geophysical Laboratory in Washington, D.C., by W. Schreyer and J. F. Schairer from stoichiometric mixtures of the oxides as a glass devitrified at 1,000 °C for 16 days. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of iron, nickel, sodium, and platinum; and 0.001 to 0.01 percent each of calcium, chromium, copper, and silver.

The sample is colorless. The mean index of refraction, using a phase contrast microscope with white light, is 1.528.

The *d*-values of the three strongest lines are: 8.46, 3.027, and 3.138 A.

Structural data. Miyashiro and Iiyama [3] in 1954 determined that hexagonal cordierite has the beryl-type structure, the space group D^2_{6h}–P6/mcc (No. 192) and $2(Mg_2Al_4Si_5O_{18})$ per unit cell. Miyashiro and Iiyama [3] call hexagonal cordierite, indialite.

Lattice constants

		a	*c*
		A	*A*
1954	Miyashiro and Iiyama [3] (natural-α)____________	9. 812	9. 351
1954	Miyashiro and Iiyama (synthetic-α)___________	9. 782	9. 365
1954	Miyashiro and Iiyama (synthetic-β)___________	9. 792	9. 349
1956	Iiyama [5]_______________	9. 742	9. 394 [b]
1956	Iiyama__________________	9. 777	9. 358 [c]
1961	National Bureau of Standards_________________	9. 770	9. 352 at 25 °C

[b] Synthesized at 1,000 °C.
[c] Synthesized above 1,200 °C.

The density of hexagonal cordierite calculated from NBS lattice constants is 2.512 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
100	8. 48	100
110	4. 89	32
002	4. 679	15
102	4. 094	51
112	3. 379	57
202	3. 138	66
211	3. 027	86
212	2. 640	26
220	2. 441	6
302	2. 414	4
004	2. 338	12
311	2. 276	5
213	2. 231	5
222	2. 165	6
114	2. 108	8
312	2. 098	12
204	2. 046	3
320	1. 941	8
402	1. 927	6
321	1. 901	3
313	1. 875	15
410	1. 846	6
411	1. 811	7
304	1. 800	9
412	1. 718	3
224	1. 6882	28
314	1. 6559	3
323	1. 6472	4
330	1. 6286	4
215	1. 6150	3
420	1. 5988	6
413	1. 5885	9
404	1. 5690	2
006	1. 5584	3
332	1. 5377	3
324	1. 4935	8
116	1. 4852	5
315, 206	1. 4625	5

References

[1] W. Schreyer and J. F. Schairer, Compositions and structural states of anhydrous Mg-cordierite: A reinvestigation of the central part of the system $MgO-Al_2O_3-SiO_2$, J. Petrology **2**, No 3, 324–406 (1961).

[2] H M. Richardson and G. M. Rigby, The occurrence of iron-cordierite in blast furnace linings, Min. Mag. **28**, 547–554 (1949).

[3] A. Miyashiro and T. Iiyama, A preliminary note on a new mineral, indialite, polymorphic with cordierite, Proc. Japan Acad. **30**, 746–751 (1954).

[4] A. Miyashiro, T. Iiyama, M. Yamasaki, and T. Miyashiro, The polymorphism of cordierite and indialite, Am. J. Sci. **253**, 185–208 (1955).

[5] T. Iiyama, Optical properties and unit cell dimensions of cordierite and indialite, Mineral. J. **1**, No. 6, 372–394 (1956).

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* According to Schreyer and Schairer [1].

Magnesium Silicate Fluoride (humite), $3Mg_2SiO_4 \cdot MgF_2$(orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
[a]7–167 7–168	1. 74 2. 45 1. 48	Copper	Gillery, Pennsylvania State University

Additional published patterns. Sahama [1] 1953.

NBS sample. The sample of humite was prepared by A. Van Valkenburg at NBS by a solid state reaction using magnesium fluoride, quartz, and magnesium carbonate. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent nickel; 0.01 to 0.1 percent each of aluminum, calcium, iron, and titanium; and 0.001 to

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
020	10. 42	5
040	5. 17	9
200	5. 11	9
210	4. 97	18
220	4. 59	19
111	4. 20	1
121	3. 97	5
031	3. 90	12
131	3. 66	5
240	3. 64	49
201	3. 47	5
060	3. 453	32
211	3. 430	25
141	3. 312	32
051	3. 119	7
231	3. 102	7
151	2. 980	6
241	2. 885	6
301	2. 770	23
311	2. 744	32
161	2. 691	50
321	2. 674	5
080	2. 589	7
331	2. 572	38
420	2. 490	4
261	2. 453	4
341	2. 443	30
171	2. 438	70
430	2. 399	21
022	2. 308	8
351	2. 304	12
440	2. 297	7
271	2. 256	100
401, 122	2. 251	35
181	2. 218	17
132	2. 189	7
361	2. 158	6
142	2. 107	38
222	2. 103	30
460	2. 057	6
2·10·0, 291	1. 920	5
501	1. 881	7
1·10·1	1. 867	8
521	1. 850	1
531	1. 814	6
471	1. 794	2
2·10·1	1. 779	6
391	1. 772	5
082	1. 7477	6
272	1. 7387	65
182	1. 7229	5
490, 551	1. 7117	4
481	1. 6995	3
432	1. 6859	12
3·10·1, 630	1. 6581	10
442	1. 6486	1
372	1. 6256	2
640	1. 6213	15
452	1. 6032	4
621	1. 5863	5
3·11·1	1. 5575	4
462	1. 5525	13
1·10·2, 123	1. 5419	3
2·13·0	1. 5223	10
----	1. 5192	8
4·11·0	1. 5176	5
1·13·1	1. 4948	1
----	1. 4895	16
670	1. 4786	69
3·12·1	1. 4644	1
1·11·2	1. 4588	1
303	1. 4326	1
163, 2·14·0	1. 4223	<1

0.01 percent each of barium, chromium, copper, manganese, lead, and vanadium.

The color of the sample was cream. It is optically positive with indices of refraction $N_\alpha=1.598$, $N_\beta=1.606$, and $N_\gamma=1.630$.

The *d*-values of the three strongest lines are: 2.256, 2.438, and 1.4786 A.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1928	Taylor and West [2][a]	10. 23	20. 86	4.738 [b]
------	Gillery [a]	10. 25	20. 84	4.734
1961	National Bureau of Standards.	10. 243	20. 72	4.735 at 25 °C

[a] Natural mineral.

[b] Unspecified angstrom units.

Structural data. Taylor and West [2] in 1928 determined that humite has the space group D_{2h}^{16}-Pnma (No. 62) and $4(3Mg_2SiO_4 \, . \, MgF_2)$ per unit cell.

The density of humite calculated from NBS lattice constants is 3.201 g/cm^3 at 25 °C.

References

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

[2] W. H. Taylor and J. West, The crystal structure of the chondrodite series, Proc. Roy. Soc. (London) **117A,** 517–532 (1927–28).

Neodymium Borate, $NdBO_3$ (orthorhombic)

ASTM cards. None.
Additional published patterns. None.

NBS sample. The sample of neodymium borate was prepared at NBS by E. Levin from neodymium oxide and boric oxide. A well-crystallized material was obtained by heating at 1,075 °C for 18 hr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent europium and 0.001 to 0.01 percent each of holmium, lanthanum, silicon, and ytterbium.

The color of the sample was light 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: 3.427, 3.300, and 2.377 A.

Structural data. According to Levin, Roth, and Martin [1], neodymium borate is isostructural with calcium carbonate, aragonite-type structure, the space group D_{2h}^{16}-Pnam (No. 62) and $4(NdBO_3)$ per unit cell.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1961	National Bureau of Standards.	5. 729	8. 080	5.041 at 25 °C

The density of neodymiun borate calculated from NBS lattice constants is 5.779 g/cm³ at 25 °C.

Reference

[1] E. Levin, R. Roth, and J. Martin, Polymorphism of ABO_3 type rare earth borates, **46**, 1030–1055 (1961). Am. Mineralogist.

Neodymium Borate, $NdBO_3$ (orthorhombic)

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
011	4. 273	18
020	4. 039	10
111	3. 427	100
120	3. 300	51
200	2. 865	18
121	2. 763	5
210	2. 701	5
002	2. 520	18
130	2. 438	6
211, 031	2. 377	46
220	2. 336	11
112	2. 217	5
022	2. 138	11
040	2. 019	8
122	2. 003	39
140	1. 094	22
202	1. 893	19
231	1. 828	30
311	1. 744	21
320	1. 727	12
222	1. 714	6
240	1. 650	6
013	1. 646	8
113	1. 581	13
142	1. 519	11
151	1. 4860	10
033	1. 4257	15
410	1. 4102	3
340	1. 3877	4
242	1. 3812	7
411	1. 3585	6
251	1. 3558	7
060	1. 3467	5
233	1. 2766	11
004	1. 2604	5
313	1, 2465	11
252, 431	1. 2273	10
260	1, 2182	12
114, 342	1, 2162	12
351	1, 1986	7
062	1. 1881	6
243	1. 1778	7
204	1. 1541	4
153	1. 1414	5
352	1. 1077	8
171	1. 1041	8
262	1. 0974	6

Neodymium Chloride, $NdCl_3$ (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
3-0078	6. 40 2. 55 2. 10	Molybdenum	Dow Chemical Co.

Additional published patterns. None.

NBS sample. The sample of neodymium chloride was received as a hydrate from Lindsay Chemical Co., West Chicago, Ill. It was dried for 45 min in vacuum at 400 °C and transferred in a dry box to a dry atmosphere sample holder which was used to prepare the patterns. An analysis from Lindsay Chemical Co., showed the following impurities: less than 0.1 percent combined of other rare earths, largely praseodymium and samarium.

The sample was colorless. The indices of refraction could not be determined because the material was too hygroscopic.

The *d*-values of the three strongest lines are: 2.556, 2.105, and 3.535A.

Structural data. Zachariasen [1] in 1948 determined that neodymium chloride has the uranium chloride-type structure, the space group C^2_{6h} $P6_3/m$ (No. 176) and $2(NdCl_3)$ per unit cell.

Lattice constants

		a	*c*
		A	*A*
1948	Zachariasen [1	7. 396	4.240
1961	National Bureau of Standards.	7. 400	4.240 at 25 °C.

The density of neodymium chloride calculated from the NBS lattice constants is 4.138 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
100	6. 42	67
110	3. 702	41
101	3. 535	68
200	3. 208	22
111	2. 788	31
201	2. 556	100
210	2. 422	22
300	2. 137	45
002	2. 122	45
211	2. 105	77
102	2. 014	27
220	1. 851	15
112	1. 840	17
310	1. 778	9
202	1. 769	9
311	1. 639	14
212	1. 595	14
302	1. 504	22
320	1. 471	6
410	1. 3985	20
222	1. 3937	20
321	1. 3890	25
312	1. 3625	6
203	1. 2927	9
213	1. 2210	16
412	1. 1671	16
511	1. 1108	8
323, 114	1. 0187	11

References

[1] W. H. Zachariasen, Crystal chemical studies of the 5-f series of elements, Acta Cryst. **1,** 265–268 (1948).

Neodymium Gallium Oxide 3:5, $Nd_3Ga_2(GaO_4)_3$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of neodymium oxide and gallium oxide. The samples were pressed into pellets and heated at 1,000 °C for 12 hr, then ground, remixed, and again pressed into pellets and heated at 1,350 °C for 6 hr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent europium and 0.001 to 0.01 percent each of aluminum, holmium, lanthanum, silicon, and ytterbium.

The color of the sample was light purple. The index of refraction is 1.985.

The *d*-values of the three strongest lines are: 2.796, 2.553, and 1.6712 A.

Structural data. Keith and Roy [1] in 1954 showed that double oxides of trivalent elements in these proportions may have the garnet-type structure. Neodymium gallium oxide is isostructural with other double oxides of trivalent elements, having the space group O_h^{10}—Ia3d (No. 230) with $8[Nd_3Ga_2(GaO_4)_3]$ per unit cell.

Lattice constants

		A
1961	National Bureau of Standards	12.506 at 25 °C.

The density calculated from the NBS lattice constant is 6.609 g/cm^3 at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		*A*
211	5. 107	15	12. 51
220	4. 420	6	12. 50
321	3. 342	11	12. 50
400	3. 128	29	12. 51
420	2. 796	100	12. 50
332	2. 669	1	12. 52
422	2. 553	46	12. 51
431	2. 452	3	12. 50
521	2. 283	11	12. 50
440	2. 211	4	12. 51
611	2. 029	13	12. 51
620	1. 977	2	12. 51
631	1. 843	4	12. 50
444	1. 805	16	12. 51
640	1. 735	29	12. 51
721	1. 701	6	12. 50
642	1. 6712	37	12. 505
732	1. 5883	9	12. 504
800	1. 5630	15	12. 504
840	1. 3982	9	12. 507
842	1. 3646	20	12. 507
921	1. 3489	3	12. 509
664	1. 3333	8	12. 507
10·2·0	1. 2267	5	12. 510
10·3·1	1. 1923	4	12. 505
10·4·0	1. 1614	17	12. 509
10·3·3	1. 1513	2	12. 506
10·4·2	1. 1417	10	12. 507
11·2·1	1. 1143	3	12. 508
880	1. 1056	9	12. 508
11·3·2	1. 0801	2	12. 503
12·0·0	1. 0422	7	12. 506
12·2·0	1. 0281	9	12. 507
11·5·2	1. 0212	6	12. 507
12·2·2	1. 0146	10	12. 509
11·6·3	0. 9707	3	12. 503
13·2·1	. 9482	1	12. 507
12·4·4	. 9425	7	12. 504
12·6·0	. 9321	13	12. 505
13·3·2	. 9272	2	12. 509
12·6·2	. 9219	6	12. 505
888	. 9025	6	12. 505
14·3·1	. 8715	3	12. 508
12·8·0	. 8670	4	12. 504
14·4·0	. 8589	13	12. 506
14·4·2	. 8510	10	12. 507
15·2·1	. 8245	4	12. 504
15·3·2	. 8107	2	12. 507
12·10·0	. 8007	13	12. 507
14·7·1	. 7973	2	12. 505
14·6·4	. 7941	10	12. 507
Average value of last five lines			12. 506

References

[1] M. L. Keith and R. Roy, Structural relations among double oxides of trivalent elements, Am. Mineralogist **39** Nos. 1 and 2, 1–23 (1954).

Nickel Arsenic Sulfide (gersdorffite), NiAsS (cubic)

ASTM cards. None.

Additional published patterns

Source	Radiation
Olshausen [1] 1925	Copper
Harcourt [2] 1942	Copper

NBS sample. The sample of gersdorffite was prepared by R. Yund of the Geophysical Laboratory at 725 °C. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, copper, and iron; and 0.0001 to 0.001 percent each of silver and magnesium.

The sample was a gray opaque powder.

The *d*-values of the three strongest lines are: 2.545, 2.325, and 1.7163A.

Structural data. Peacock and Henry [3] in 1947 determined that gersdorffite has the pyrite type structure, the space group T_h^6—Pa3 (No. 205), and 4(NiAsS) per unit cell. Several unit cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1925	Olshausen [1]	5.731
1925	Ramsdell [4]	5.69
1926	Goldschmidt [5]	5.72
1947	Peacock and Henry [3]	5.66
1961	National Bureau of Standards	5.692 at 25 °C

The density of gersdorffite calculated from the NBS lattice constant is 5.966 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		A
111	3.285	5	5.690
002	2.848	59	5.696
021	2.545	100	5.692
112	2.325	88	5.694
022	2.013	33	5.693
113	1.7163	79	5.692
222	1.6436	10	5.694
023	1.5786	10	5.692
123	1.5214	37	5.693
004	1.4232	6	5.693
133	1.3057	3	5.691
024	1.2730	6	5.693
124	1.2422	15	5.692
233	1.2138	7	5.693
224	1.1616	6	5.691
115	1.0955	20	5.692
025	1.0571	14	5.693
125	1.0393	8	5.692
044	1.0063	20	5.692
006	0.9485	1	5.691
061	.9357	2	5.692
116	.9233	18	5.692
026	.8998	4	5.691
126	.8888	4	5.691
335	.8680	8	5.692
226	.8580	4	5.692
063	.8485	10	5.692
136	.8393	7	5.692
444	.8215	1	5.692
236	.8131	3	5.691
117	.7970	1	5.692
046	.7893	8	5.692
146	.7819	14	5.692
Average value of last five lines			5.692

References

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

[2] G. A. Harcourt, Tables for the identification of minerals by X-ray Powder Patterns, Am. Mineralogist **27,** 63 (1942).

[3] M. A. Peacock and W. G. Henry, The crystal structures of cobaltite (CoAsS), gersdorffite (NiAsS), and ullmannite (NiSbS), Univ. Toronto Studies, Geol. Series **52,** 71 (1947).

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

[5] V. M. Goldschmidt, Geochemische Verteilungsgesetze VIII, Skrifter Norske Vidensk. Akad. Oslo, Math. Nat. Kl. **8,** 390 (1926–27).

Nickel(II) Carbonate, $NiCO_3$ (trigonal)

ASTM cards. None.

NBS sample. The sample of nickel carbonate was prepared by Thelma Isaacs at NBS by heating basic nickelous carbonate (Fischer's reagent), solid CO_2, and distilled water in a Morey bomb at 270 °C for two weeks. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium; 0.001 to 0.01 percent each of aluminum, copper, platinum, and silicon.

The color of the sample was green. It was optically negative with the indices of refraction $N_o=1.913$ and $N_e=1.696$.

The *d*-values of the three strongest lines are: 2.708, 3.512, and 1.6811 A.

Structural data. Bizette and Langlès [1] in 1950 determined that nickel carbonate has calcite-type structure, the space group D_{3d}^6—$R\bar{3}c$ (No. 167) and $6(NiCO_3)$ per unit cell.

The rhombohedral cell reported by Bizette and Langlès was converted to hexagonal for comparison.

Lattice constants

		a	*c*
		A	*A*
1950	Bizette and Langlès	4. 596	14.622
1961	National Bureau of Standards.	4. 609	14.737 at 25 °C.

The density of nickel carbonate calculated from the NBS lattice constants is 4.362 g/cm³ at 25 °C.

hkl (hex.)	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
012	3. 512	48
104	2. 708	100
110	2. 304	27
113	2. 086	34
202	1. 926	28
024	1. 7546	15
116	1. 6811	43
018	1. 6734	37
211	1. 5001	2
122	1. 4782	17
214	1. 3961	13
1·0·10	1. 3834	3
208	1. 3542	6
119	1. 3351	9
300	1. 3310	14
0·0·12	1. 2287	5
217	1. 2262	3
0·2·10	1. 1857	2
128	1. 1672	6
220	1. 1526	1
1·1·12	1. 0843	4
134	1. 0606	4
2·1·10	1. 0546	3
226	1. 0435	4
0·1·14	1. 0175	<1
1·2·11	1. 0010	9
404	0. 9633	3
318	. 9490	5
2·0·14	. 9310	<1
232	. 9088	2
2·1·13	. 9067	1
1·1·15	. 9036	1
3·0·12	. 9027	4
407	. 9006	2

References

[1] H. Bizette and R. de Saint-Léon Langlès, Préparation d'un carbonate de nickel neutre rhomboédrique, Bull. soc. chim. France 1041, (1950).

Nickel Sulfide, millerite, NiS (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
3-0760	2.77 1.85 2.50	Copper	Harcourt [1] 1942

Additional published patterns. Alsen [2] 1925; Kolkmeijer and Moseveld [3]; Levi and Baroni [4].

NBS sample. The sample of millerite was obtained from the National Museum, catalog #113065. Spectrographic analysis showed the following impurities: 5 percent iron; 0.1 to 1.0 percent arsenic, cobalt, copper, and silicon; 0.01 to 0.1 percent each of aluminum, calcium, magnesium, manganese, and zinc; and 0.001 to 0.01 percent each of silver and barium. A small amount of chalcopurite, CuFcS, was present as an impurity in the physical mixture.

The sample was a gray opaque powder.

The *d*-values of the three strongest lines are: 2.777, 1.8631, and 2.513 A.

Structural data. Alsen [2] in 1925 determined that millerite has the space group C^5_{3v}—R3m (No. 160) and 9(NiS) per unit hexagonal cell or 3(NiS) per unit rhombohedral cell. Several unit cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		a	*c*
		A	*A*
1925	Alsen [2]	9.62	3.16
1926	Ott [5]	9.63	3.161
1931	Kolkmeijer and Moseveld [3].	9.609	3.171
1935	Levi and Baroni [4]	9.63	3.16
1947	Lundqvist [6]	9.610	3.151
1961	National Bureau of Standards.	9.620	3.149 at 25 °C

The density of millerite calculated from the NBS lattice constant is 5.374 g/cm^3 at 25 °C.

hkl (hex.)	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
110	4.807	62
101	2.946	41
300	2.777	100
021	2.513	64
220	2.406	12
211	2.228	56
131	1.8631	97
410	1.8178	43
401	1.7372	42
321	1.6340	17
330	1.6037	35
012	1.5470	27
600	1.3884	8
520	1.3343	4
312	1.3008	9
042	1.2560	8
440	1.2023	6
161	1.1783	4
502	1.1447	5
422, 701	1.1133	15
710	1.1033	7
152, 621	1.0846	8
342	1.0333	12
541	1.0104	6
612, 081	0.9888	6
303	.9820	8
262, 811	.9316	8
461	.9143	<3
413, 820	.9090	6
731	.8984	8
740	.8640	5

References

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

[2] N. Alsen, Röntgenographische Untersuchung der Kristallstructuren von Magnetkies, Breithauptit, Pentlandit, Millerit, und verwandten Verbindungen, Geol. Fören. i. Stockholm Förh. **47**, 19–72 (1925).

[3] N. H. Kolkmeijer and A. L. Th. Moseveld, Über die Dichte und Struktur des Millerits (rhomboedrischen Nickelsulfids), Z. Krist. **80**, 91 (1931).

[4] G. R. Levi and A. Baroni, Struttura ed alterazioni di struttura di NiS e di NiSe, Z. Krist. **A92**, 210–215 (1935).

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[6] D. Lundqvist, X-Ray studies on the binary system Ni-S, Arkiv. Kemi Mineral. Geol. **24A**, No. 21, 1–12 (1947).

Potassium Dihydrogen Arsenate, KH_2AsO_4 (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. Potassium dihydrogen arsenate was prepared at NBS by dissolving arsenic trioxide in nitric acid and then adding a solution of potassium carbonate. The purity of the sample was improved by several recrystallizations. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of sodium and lead, and 0.001 to 0.01 percent each of aluminum, antimony, calcium, copper, iron, magnesium, and silicon.

The sample was colorless and optically negative with the refractive indices $N_o=1.562$ and $N_e=1.519$.

The *d*-values of the three strongest lines are: 3.810, 2.980, and 2.000 A.

Structural data. Helmholtz and Levine [1] in 1942 discovered that potassium dihydrogen arsenate is an isotype of potassium dihydrogen phosphate, with the space group D_{2d}^{12}–$I\bar{4}2d$ (No. 122) and $4(KH_2AsO_4)$ per unit cell. Several unit cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1942	Helmholtz and Levine [1]	7.67	7.18
1946	Frevel, Rinn and Anderson [2].	7.63	7.13
1950	Dickson and Ubbelohde [3]	7.624	7.163 at 18 °C
1961	National Bureau of Standards.	7.630	7.163 at 25 °C

The density of potassium dihydrogen arsenate calculated from the NBS lattice constants is 2.866 g/cm^3 at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
101	5.21	65
200	3.810	100
211	3.078	28
112	2.980	87
220	2.697	31
202	2.610	6
310	2.412	4
301	2.397	<1
321	2.029	8
312	2.000	72
213	1.956	4
400	1.908	9
411, 004	1.792	4
303	1.741	5
420	1.707	18
204	1.622	14
332	1.6070	18
323	1.5833	3
422	1.5405	1
501, 224	1.4925	13
413	1.4629	2
314	1.4379	1
105	1.4071	<1
521	1.3897	3
512	1.3808	16
440	1.3491	3
215	1.3209	<1
404	1.3054	6
503	1.2852	1
600	1.2716	22
305	1.2482	1
611, 424	1.2353	8
532	1.2291	12
523	1.2184	<1
620	1.2066	10
602	1.1985	<1
325	1.1865	1
541	1.1754	2
116	1.1656	3
415	1.1331	<1
631	1.1232	1
613	1.1103	1
701, 444	1.0776	2
316	1.0700	4
640	1.0581	2
721, 604	1.0369	2
712	1.0332	10
642, 107	1.0142	1
406	1.0118	<1
624	1.0004	2
336	0.9944	1
426	.9774	<1
651	.9679	<1
732	.9648	6
800	.9538	1
615	.9435	<1

References

[1] L. Helmholtz and R. Levine, A determination of parameters in potassium dihydrogen arsenate and silver arsenate, J. Am. Chem. Soc. **64**, 354–358 (1942).

[2] L. K. Frevel, H. W. Rinn, and H. C. Anderson, Tabulated diffraction data for tetragonal isomorphs, Ind. Eng. Chem. Anal. Ed. **18**, 83–93 (1946).

[3] D. H. W. Dickson and A. R. Ubbelohde, The hydrogen bond in crystals. VIII. The isotope effect in KH_2AsO_4, Acta Cryst. **3**, 6–9 (1950).

Praseodymium Chloride, $PrCl_3$ (hexagonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of praseodymium chloride was received as a hydrate from Lindsay Chemical Co. Chicago, Ill. It was dried for 2 hr in vacuum at 400 °C and transferred in a dry box to a dry atmosphere sample holder which was used to prepare the patterns. An analysis from Lindsay Chemical Co., showed the following impurities: less than 1 percent combined of lathanum, neodymium, and smaller amounts of cerium and samarium.

The sample was very pale green. The indices of refraction could not be determined because the material was too hygroscopic.

The *d*-values of the three strongest lines are: 2.571, 2.112, and 3.56A.

Structural data. Zachariasen [1] in 1948 determined that praseodymium chloride has the uranium chloride-type structure, the space group C_{6h}^2–$P6_3/m$ (No. 176) and 2 ($PrCl_3$) per unit cell.

Lattice constants

		a	*c*
		A	*A*
1948	Zachariasen [1]	7. 42	4. 26
1961	National Bureau of Standards	7. 423	4. 272 at 25 °C

The density of praseodymium chloride calculated from the NBS lattice constants is 4.027 g/cm^3 at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
100	6. 46	56
110	3. 72	41
101	3. 56	65
200	3. 22	16
111	2. 81	28
201	2. 571	100
210	2. 429	19
300	2. 140	58
211	2. 112	79
102	2. 027	31
112	1. 853	25
310	1. 782	17
202	1. 779	
311	1. 645	15
212	1. 604	18
302	1. 512	23
320	1. 475	4
222	1. 402	22
321	1. 394	30
312	1. 369	8
203	1. 302	11
213	1. 229	17
412	1. 173	14
421	1. 169	
511	1. 1148	10
323	1. 0241	12

References

[1] W. H. Zachariasen, Crystal chemical studies of the 5–f series of elements, Acta Cryst. **1**, 265–268 (1948)

Samarium Chloride, $SmCl_3$ (hexagonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of samarium chloride was received as a hydrate from Lindsay Chemical Co., West Chicago, Ill. It was dried for one and one-half hours in vacuum at 400 °C and transferred in a dry box to a dry atmosphere sample holder which was used to prepare the patterns. An analysis from Lindsay Chemical Co., showed the following impurities: less than 0.1 percent combined of other rare earths, largely neodymium, gadolinium, and europium.

The sample was colorless. The indices of refraction could not be determined because the material was too hygroscopic.

The *d*-values of the three strongest lines are: 2.538, 2.090, and 3.494A.

Structural data. The structure of samarium chloride has not been reported. It is assumed to have the uranium chloride-type structure, the space group C_{6h}^2–$P6_3/m$ (No. 176) and 2($SmCl_3$) per unit cell.

Lattice constants

		a	*c*
		A	*A*
1961	National Bureau of Standards.	7. 380	4. 169 at 25 °C

The density of samarium chloride calculated from the NBS lattice constants is 4.334 g/cm^3 at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
100	6. 393	66
110	3. 694	49
101	3. 494	75
200	3. 198	21
111	2. 764	34
201	2. 538	100
210	2. 416	20
300	2. 131	36
211	2. 090	90
102	1. 983	16
220	1. 845	12
112	1. 814	1
310	1. 772	13
202	1. 746	10
311	1. 630	13
400	1. 5973	10
212	1. 5783	15
302	1. 4895	21
410	1. 3946	14
321	1. 3833	30
312	1. 3506	9
203	1. 2744	10
501	1. 2224	14
213	1. 2046	12
412	1. 1594	18
511	1. 1066	9
323	1. 0087	14

Samarium Fluoride, SmF_3 (hexagonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
3–1046	2. 02 1. 97 1. 16	Copper	Oftedal [1] 1929
5–0563	3. 12 2. 00 1. 96	Chromium	Zalkin [2] 1951

Additional published patterns. None.

NBS sample. The sample of samarium fluoride was prepared at NBS by reacting samarium oxide with hydrofluoric acid. It was heated at 900 °C for 5 min to improve the pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, and silicon; and 0.001 to 0.01 percent each of iron and magnesium.

The color of the sample was very light gray. The indices of refraction could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are: 3.13, 1.960, and 2.008 A.

Structural data. Oftedal [3] in 1931 determined that samarium fluoride has the sapce group D^3_{6h} $P6_3/mcm$ (No. 193) with $6(SmF_3)$ per unit cell. Samarium fluoride is isomorphous with lanthanum fluoride, which is used as a structure type. At high temperatures, hexagonal samarium fluoride converts to an orthorhombic form. The unit-cell measurements of Oftedal have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1929	Oftedal [1]	6. 994	7. 164
1953	Zalkin and Templeton [4]	6. 956	7. 120
1961	National Bureau of Standards.	6. 952	7. 122 at 26 °C

The density of samarium fluoride calculated from the NBS lattice constants is 6.928 g/cm³ at 26 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 26 °C	
	d	*I*
	A	
002	3. 56	49
110	3. 48	30
111	3. 13	100
112	2. 487	10
300	2. 008	54
113	1. 960	58
004	1. 779	9
302	1. 748	36
221	1. 689	19
114	1. 584	9
222	1. 562	8
223, 214	1. 4022	17
304	1. 3316	10
115	1. 3180	12
411	1. 2921	17
224	1. 2436	5
412	1. 2333	1
006	1. 1870	6
330	1. 1588	9
413, 404	1. 1497	12
116	1. 1233	5
332, 225	1. 1019	12
414	1. 0569	2
306	1. 0216	8
600	1. 0032	5
226	0. 9803	<1
117	. 9765	1
334	. 9711	3
415, 602	. 9657	10
521	. 9555	8

References

[1] I. Oftedal, Über die Kristallstruktur von Tysonit und eignigen künstlich dargestellten Lanthanidenfluoriden, Z. physik. Chem. **B5**, 272–291 (1929).

[2] Zalkin, Thesis, U. California, Berkeley (1951).

[3] I. Oftedal, Zur Kristallstruktur von Tysonit (Ce, La, . . .)F_3, Z. physik. Chem. **B13,** 190–200 (1931).

[4] A. Zalkin and D. H. Templeton, The crystal structures of YF_3 and related compounds, J. Am. Chem. Soc. **75,** 2453–2458 (1953).

Samarium Gallium Oxide 3:5, $Sm_3Ga_2(GaO_4)_3$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
8–188	2. 76 2. 53 1. 66	Copper	Keith and Roy [1] 1954.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of samarium oxide and gallium oxide. The samples were pressed into pellets and heated at 1,350 °C for 6 hr, then ground, remixed, and again pressed into pellets and heated at 1,650 °C for 6 hr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent dysprosium and 0.001 to 0.01 percent each of aluminum, gadolinium, lanthanum, silicon, and thulium.

The color of the sample was yellowish white. The index of refraction is >2.00.

The *d*-values of the three strongest lines are: 2.781, 2.540, and 1.6614 A.

Structural data. Keith and Roy [1] in 1954 showed that double oxides of trivalent elements had the garnet structure. The garnets have the space group O_h^{10}–Ia3d (No. 230) with $8[Sm_3Ga_2(GaO_4)_3]$ per unit cell.

Lattice constants

		A
1954	Keith and Roy [1]	12.355
1961	National Bureau of Standards	12.432 at 25 °C

The density calculated from the NBS lattice constant is 6.854 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		*A*
211	5. 081	13	12. 45
220	4. 403	5	12. 45
321	3. 321	10	12. 43
400	3. 108	31	12. 43
420	2. 781	100	12. 44
422	2. 540	44	12. 44
431	2. 440	3	12. 44
521	2. 271	13	12. 44
440	2. 199	4	12. 44
611	2. 016	11	12. 43
631	1. 834	3	12. 44
444	1. 794	17	12. 43
640	1. 724	33	12. 43
721	1. 692	5	12. 44
642	1. 661	35	12. 43
732	1. 579	4	12. 44
800	1. 5543	15	12. 434
840	1. 3902	10	12. 434
842	1. 3568	20	12. 435
921	1. 3402	3	12. 429
664	1. 3254	7	12. 433
932	1. 2825	3	12. 434
10·2·0	1. 2190	3	12. 431
10·3·1	1. 1852	4	12. 431
10·4·0	1. 1543	18	12. 432
10·3·3	1. 1444	1	12. 431
10·4·2	1. 1348	7	12. 431
11·2·1	1. 1073	9	12. 429
880	1. 0988	2	12. 432
11·3·2	1. 0740	3	12. 432
12·0·0	1. 0359	4	12. 431
12·2·0	1. 0220	5	12. 433
11·5·2	1. 0154	3	12. 436
12·2·2	1. 0084	9	12. 432
11·6·3	0. 9646	4	12. 428
12·4·4	. 9369	5	12. 429
12·6·0	. 9264	13	12. 429
13·3·2	. 9214	5	12. 430
12·6·2	. 9163	5	12. 429
888	. 8971	7	12. 430
14·2·0	. 8786	2	12. 426
14·3·1	. 8660	4	12. 430
12·8·0	. 8620	5	12. 432
14·4·0	. 8538	11	12. 431
14·4·2	. 8459	10	12. 432
15·2·1	. 8197	3	12. 431
14·6·0	. 8161	3	12. 431
15·3·2	. 8059	2	12. 433
12·10·0	. 7959	13	12. 432
14·6·4	. 7895	12	12. 433
Average value of last five lines			12. 432

References

[1] M. L. Keith and R. Roy, Structural relations among double oxides of trivalent elements, Am. Mineralogist **39** Nos. 1 and 2, 1–23 (1954).

Samarium Oxychloride, SmOCl (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of samarium oxychloride was prepared at NBS by heating at 900 °C for 30 min a sample of samarium chloride from the Lindsay Chemical Co., West Chicago, Ill. Their spectrographic analysis showed the following impurities: a maximum as rare earth oxides of 0.1 percent (largely Nd, Gd, and Eu).

The sample was a very pale yellow-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: 2.569, 3.43, and 2.816 A.

Structural data. The structure of SmOCl has not been determined; however, it is apparently isostructural with PbFCl, with the space group D_{4h}^{7}–P4/nmm (No. 129) and 2(SmOCl) per unit cell.

Lattice constants

		a	*c*
		A	*A*
1961	National Bureau of Standards	3. 982	6. 721 at 26 °C

The density of samarium oxychloride calculated from the NBS lattice constants is 6.287 g/cm^3 at 26 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 26 °C	
	d	*I*
	A	
001	6. 73	27
101	3. 43	91
002	3. 36	10
110	2. 816	78
111	2 595	13
102	2. 569	100
003	2. 239	8
112	2. 158	28
200	1. 9905	38
103	1. 9540	6
201	1. 9087	9
113	1. 7530	22
211	1. 7211	30
202	1. 7131	15
004	1. 6814	6
212	1. 5734	39
104	1. 5477	19
203	1. 4884	10
114	1. 4431	4
220	1. 4080	12
213	1. 3948	<1
221	1. 3781	4
005	1. 3439	5
301	1. 3023	6
222	1. 2994	5
204	1. 2836	4
105	1. 2742	8
310	1. 2592	10
311	1. 2383	10
302	1. 2346	12
214	1. 2221	10
115	1. 2130	6
223	1. 1926	5
312	1. 1790	10
303	1. 1423	8
006	1. 1201	3
205	1. 1143	9
313	1. 0978	7
321	1. 0900	7
224, 106	1. 0794	5
215	1. 0726	7
322	1. 0494	10
304, 116	1. 0415	8
314	1. 0078	6
400	0. 9957	14

Silver Carbonate, Ag_2CO_3 (monoclinic)

ASTM cards

Card number	Index lines	Radiation	Source
1–1071	2. 65 2. 73 2. 27	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of silver carbonate was prepared at NBS from solutions of silver nitrate and potassium carbonate. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum and silicon, and 0.0001 to 0.001 percent each of calcium, copper, iron, and magnesium.

The color of the sample was a greenish 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: 2.66, 2.74, and 2.27 A.

Structural data. Donohue and Helmholz [2] reported that Eldridge [3] in 1943 determined the structure of silver carbonate, having the space group C_2^2—$P2_1$ (No. 4) and 2 (Ag_2CO_3) per unit cell. The unit cell measurements reported by Eldridge have been converted from kX to angstrom units for comparison with the NBS values

The density of silver carbonate calculated from the NBS lattice constants is 6.131 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
100	4. 85	15
020	4. 78	34
110	4. 32	32
120	3. 41	2
001	3. 25	3
011	3. 08	8
$\bar{1}01$	2. 74	60
130	2. 66	100
111	2. 56	6
200	2. 42	20
040	2. 39	11
$\bar{1}21$	2. 38	13
210	2. 35	8
121	2. 32	14
031	2. 27	36
220	2. 16	11
131	2. 04	10
$\bar{2}01$	1. 976	2
$\bar{2}11$	1. 934	6
230	1. 929	9
041	1. 912	4
201, 211	1. 875	6
$\bar{1}41$	1. 801	3
150	1. 777	13
240	1. 700	3
$\bar{2}31$	1. 678	9
051	1. 639	10
231	1. 626	6
002	1. 616	1
012, 060	1. 591	9
310	1. 587	4
$\bar{1}12$	1. 538	2
022	1. 530	3
$\bar{2}41$	1. 526	3
160	1. 511	2
102	1. 507	3
$\bar{3}01$	1. 468	<1
$\bar{3}11$	1. 450	1
122, 032	1. 441	2
061	1. 428	1
$\bar{3}21$	1. 411	1
311	1. 400	5
$\bar{1}32$	1. 398	5
$\bar{2}51$	1. 3747	7
$\bar{2}02$	1. 3723	7
132	1. 3654	3
260	1. 3299	4
$\bar{2}22$	1. 3192	<1
$\bar{1}42$	1. 3023	3

References

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

[2] J. Donohue and L. Helmholz, The crystal structure of potassium silver carbonate, $KAgCO_3$, J. Am. Chem. Soc. **66**, 295–298 (1944).

[3] J. E. Eldridge, Thesis, Dartmouth College (1943).

Lattice constants

		a	*b*	*c*	*β*
		A	*A*	*A*	
1943	Eldridge [2, 3]	4. 84	9. 54	3. 24	92.7°
1961	National Bureau of Standards	4. 836	9. 555	3. 235	92.64° at 25 °C

Silver Oxide, Ag_2O (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–1041	2. 72 2. 36 1. 67	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. Wyckoff [2] 1922, Levi and Quilico [3] 1924, and P. Niggli [5] 1922.

NBS sample. The sample of silver oxide was obtained from the Fisher Scientific Co., Washington, D. C. The sample was heated between 250 and 280 °C to sharpen the pattern. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of iron, magnesium, lead, and silicon.

The sample was a very dark brown, opaque powder.

The *d*-values of the three strongest lines are: 2.734, 2.367, and 1.674 A.

Structural data. Wyckoff [2] in 1922 determined that silver oxide has the cuprous oxide structure-type, the space group O_h^4— Pn3m (No. 224) and $2(Ag_2O)$ per unit cell.

Faivre [4] reported that the lattice constants vary from 4.697 to 4.736 A, depending on the amount of heat and the length of time applied. Several unit cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1922	Wyckoff [2]	4. 778
1922	Niggli [5]	4. 728
1924	Levi and Quilico [3]	4. 70–4. 78
1926	Goldschmidt [6]	4. 73
1944	Faivre [4]	4. 734 [a]
1961	National Bureau of Standards	4. 736 at 25 °C

[a] Constant for sample heated to 250 °C.

The density of silver oxide calculated from NBS lattice constants is 7.243 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		*A*
110	3. 348	3	4. 735
111	2. 734	100	4. 735
200	2. 367	33	4. 734
220	1. 674	17	4. 734
311	1. 427	12	4. 734
222	1. 367	6	4. 734
400	1. 184	<1	4. 736
331	1. 086	3	4. 736
420	1. 059	2	4. 735
422	0. 9667	2	4. 736
511	. 9115	2	4. 736
Average value of last five lines			4. 736

References

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

[2] R. W. G. Wyckoff, The crystal structure of silver oxide (Ag_2O), Am. J. Sci. **3,** 184–188 (1922).

[3] G. R. Levi and A. Quilico, Sulla non esistenza del sottossido di argento, Gazz. chim. Ital. **54,** 598–604 (1924).

[4] R. Faivre, Contribution à l'étude des oxydes actifs et du problème des sous-oxydes métalliques, Ann. chim., XI **19,** 58–101 (1944).

[5] P. Niggli, Die Kristallstruktur einiger Oxyde I, Z. Krist. **57,** 253–299 (1922–1923).

[6] V. M. Goldschmidt, Geochemische Verteilungsgesetze der Elemente; VII, Die Gesetze der Krystallochemie, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1926,** No. 2 (1926).

Sodium Molybdate, Na_2MoO_4 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of sodium molybdate was made at NBS by heating at 100 °C a sample of sodium molybdate dihydrate obtained from the Mallinckrodt Chemical Works, New York. Spectrographic analysis showed the presence of the following impurities: 0.001 to 0.01 percent each of aluminum and sodium.

The sample was colorless with the refractive index 1.714.

The *d*-values of the three strongest lines are: 2.746, 3.220, and 5.26 A.

Structural data. According to Lindqvist [1], sodium molybdate is isomorphous with sodium tungstate, with the spinel-type structure, the space group O_h^7-Fd3m (No. 227), and 8(Na_2MoO_4) per unit cell.

Lattice constants

		A
1950	Lindqvist [1]	8.99
1958	Becka and Poljak [2]	8.99
1961	National Bureau of Standards	9.108 at 25 °C

The density of sodium molybdate calculated from the NBS lattice constants is 3.620 g/cm^3 at 25 °C.

References

[1] I. Lindqvist, Crystal structure studies on anhydrous sodium molybdates and tungstates, Acta Chem. Scand. **4**, 1066–1074 (1950).

[2] L. N. Becka and R. J. Poljak, Estructura cristalina del MoO_4Na_2 y del WO_4Na_2, Anales asoc. quím. arg. **46**, 204–209 (1958).

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		A
111	5. 26	63	9. 106
220	3. 220	87	9. 108
311	2. 746	100	9. 108
331	2. 090	7	9. 108
422	1. 8588	33	9. 106
511	1. 7533	33	9. 110
440	1. 6106	38	9. 111
531	1. 5391	12	9. 105
620	1. 4403	14	9. 109
533	1. 3888	10	9. 107
711	1. 2756	6	9. 110
642	1. 2171	14	9. 108
731	1. 1857	18	9. 108
800	1. 1386	5	9. 109
822	1. 0734	8	9. 108
751	1. 0519	8	9. 110
840	1. 0184	1	9. 109
911	0. 9999	4	9. 109
664	. 9709	4	9. 108
931	. 9549	4	9. 109
844	. 9295	7	9. 107
933	. 9154	2	9. 108
10·2·0	. 8930	8	9. 107
951	. 8805	6	9. 108
953	. 8494	3	9. 109
10·4·2	. 8315	7	9. 108
11·1·1	. 8213	5	9. 108
880	. 8051	3	9. 108
11·3·1	. 7957	4	9. 107
10·6·0	. 7810	4	9. 108
Average value of last five lines			9. 108

Sodium Tungstate, Na_2WO_4 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
5–0247	5. 19 3. 18 2. 72	Copper	Lindqvist [1] 1950.

Additional published patterns

Source	Radiation
Becka and Poljak [2]	Copper

NBS sample. The sample of sodium tungstate was prepared at NBS by heating at 100 °C a sample of sodium tungstate dihydrate obtained from the Allied Chemical and Dye Corp., New York. Spectrographic analysis showed the presence of the following impurities: 0.01 to 0.1 percent of silicon; and 0.001 to 0.01 percent aluminum.

The sample was colorless with the refractive index 1.679.

The *d*-values of the three strongest lines are: 2.753, 3.23, and 5.28 A.

Structural data. Lindqvist [1] in 1950 determined that sodium tungstate has spinel-type structure, the space group O_h^7–Fd3m (No. 227), and 8(Na_2WO_4) per unit cell.

Lattice constants

		A
1950	Lindqvist [1]	8.99
1958	Becka and Poljak [2]	9.11
1961	National Bureau of Standards	9.1297 at 25 °C.

The density of sodium tungstate calculated from the NBS lattice constant is 5.128 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		*A*
111	5. 28	89	9. 15
220	3. 23	98	9. 14
311	2. 753	100	9. 132
400	2. 282	5	9. 126
331	2. 094	20	9. 126
422	1. 8642	42	9. 133
511	1. 7574	38	9. 132
440	1. 6142	35	9. 131
531	1. 5430	20	9. 128
620	1. 4435	23	9. 130
533	1. 3921	14	9. 129
444	1. 3177	2	9. 129
711	1. 2786	10	9. 131
642	1. 2202	19	9. 131
731	1. 1887	19	9. 131
800	1. 1412	6	9. 130
733	1. 1154	3	9. 130
822	1. 0759	10	9. 129
751	1. 0543	9	9. 130
840	1. 0206	3	9. 128
911	1. 0020	7	9. 129
664	0. 9732	5	9. 1297
931	. 9571	5	9. 1299
844	. 9318	7	9. 1300
933	. 9176	4	9. 1298
10·2·0	. 8952	13	9. 1296
951	. 8826	7	9. 1301
953	. 8514	3	9. 1299
10·4·2	. 8334	8	9. 1298
11·1·1	. 8232	6	9. 1298
880	. 8069	3	9. 1295
11·3·1	. 7977	8	9. 1296
10·6·0	. 7829	9	9. 1296
Average value of last five lines			9. 1297

References

[1] I. Lindqvist, Crystal structure studies on anhydrous sodium molybdates and tungstates, Acta Chem. Scand. **4,** 1066–1074 (1950).

[2] L. N. Becka and R. J. Poljak, Estructura cristalina del MoO_4Na_2 y del WO_4Na_2, Anales asoc. quím. arg. **46,** 204–209 (1958).

Thallium(I) Tungstate, Tl_2WO_4 (hexagonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of thallium tungstate was prepared at NBS by reaction of solutions of thallium (I) sulfate and sodium tungstate. The slightly soluble precipitate was recrystallized from a boiling aqueous solution and then fused at approximately 700 °C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of arsenic and calcium.

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

The *d*-values of the three strongest lines are: 3.25, 3.14, and 2.260 A.

Structural data. No reference was found for the structure of thallium tungstate; however, by means of Bunn Charts, the pattern was tentatively indexed with a hexagonal cell containing $2(Tl_2WO_4)$. Observed with an optical microscope, thallium tungstate appears as hexagonal platelets.

Lattice constants

		a	*c*
		A	A
1961	National Bureau of Standards.	6.288	8.103 at 25 °C.

The density of thallium tungstate calculated from the NBS lattice constants is 7.857 g/cm³ at 25 °C. The average density obtained with a Berman balance is 7.841 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
002	4.05	1
102	3.25	100
110	3.14	83
003	2.702	<1
103	2.420	2
202	2.260	48
004	2.025	2
104	1.899	29
212	1.836	38
300	1.816	22
114	1.703	2
204	1.625	14
220	1.572	9
105	1.553	1
214	1.4437	18
312	1.4152	12
006	1.3503	2
106	1.3109	1
402	1.2904	4
116	1.2405	9
314	1.2108	5
322	1.1938	5
410	1.1884	7
107	1.1318	1
404	1.1298	2
306	1.0834	4
324	1.0633	1
502	1.0517	2
330	1.0483	2
226	1.0245	3
422	0.9973	2
108	.9958	2
512	.9505	2
208	.9494	2
424	.9173	2
218	.9090	2

Ytterbium Gallium Oxide 3:5, $Yb_3Ga_2(GaO_4)_3$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of ytterbium oxide and gallium oxide. The sample 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: 0.001 to 0.01 percent silicon and 0.0001 to 0.001 percent each of erbium, lutetium, and thulium.

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: 2.725, 2.489, and 1.6920 A.

Structural data. Keith and Roy [1] in 1954 showed that double oxides of trivalent elements in these proportions may have the garnet-type structure. Ytterbium gallium oxide is isostructural with garnet, having the space group O_h^{10}—Ia3d (No. 230) with $8[Yb_3Ga_2(GaO_4)_3]$ per unit cell.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		*A*
211	4. 973	21	12. 18
220	4. 310	6	12. 19
321	3. 260	12	12. 20
400	3. 046	30	12. 18
420	2. 725	100	12. 19
422	2. 489	45	12. 19
431	2. 392	2	12. 20
521	2. 228	12	12. 20
440	2. 156	3	12. 20
611	1. 979	12	12. 199
620	1. 930	1	12. 206
631	1. 799	2	12. 201
444	1. 7609	16	12. 200
640	1. 6920	34	12. 201
721	1. 6603	5	12. 201
642	1. 6307	34	12. 203
732	1. 5494	3	12. 200
800	1. 5253	14	12. 202
653	1. 4582	2	12. 200
822	1. 4377	2	12. 199
752	1, 3816	2	12. 202
840	1. 3642	8	12. 202
842	1. 3311	18	12. 200
921	1. 3155	2	12. 199
664	1. 3006	6	12. 201
932	1. 2584	2	12. 201
941	1. 2326	1	12. 202
10·1·1	1. 2081	1	12. 201
10·2·0	1. 1965	2	12. 202
10·3·1	1. 1630	3	12. 198
	A		
10·4·0	1. 1328	14	12. 201
10·3·3	1. 1229	2	12. 198
10·4·2	1. 1137	6	12. 200
11·2·1	1. 0869	3	12. 200
880	1. 0783	6	12. 200
11·3·2	1. 0539	<1	12. 200
10·6·0	1. 0460	<1	12. 198
965	1. 0238	1	12. 200
12·0·0	1. 0166	4	12. 199
12·2·0	1. 0028	4	12. 200
11·5·2	0. 9961	1	12. 200
12·2·2	. 9896	7	12. 200
11·6·1	. 9706	1	12. 200
11·6·3	. 9469	1	12. 200
13·2·1	. 9248	2	12. 199
12·4·4	. 9196	4	12. 199
12·6·0	. 9094	8	12. 200
13·3·2	. 9044	<1	12. 201
12·6·2	. 8994	5	12. 200
888	. 8805	3	12. 201
14·1·1	. 8671	<1	12. 201
14·2·0	. 8626	<1	12. 200
14·3·1	. 8500	2	12. 200
12·8·0	. 8460	2	12. 200
14·4·0	. 8380	8	12. 201
14·4·2	. 8302	8	12. 201
14·5·1	. 8188	1	12. 200
15·2·1	. 8045	2	12. 201
15·3·2	. 7908	<1	12. 200
Average value of last five lines			12. 200

Lattice constants

		A
1961	National Bureau of Standards	12.200 at 25 °C

The density calculated from the NBS lattice constant is 7.750 g/cm ^{3} at 25 °C.

Reference

[1] M. L. Keith and R. Roy, Structural relations among double oxides of trivalent elements, Am. Mineralogist **39,** Nos. 1 and 2, 1–23 (1954).

Yttrium Gallium Oxide 3:5, $Y_3Ga_2(GaO_4)_3$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of yttrium oxide and gallium oxide. The sample 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 each of calcium and silicon and 0.001 to 0.01 percent each of erbium, molybdenum, potassium, terbium, and titanium.

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: 2.744, 2.507, and 1.6404 A.

Structural data. Keith and Roy [1] in 1954 showed that double oxides of trivalent elements in these proportions may have the garnet-type structure. Yttrium gallium oxide is isostructural with garnet, having the space group O_h^{10}—Ia3d (No. 230) with $8[Y_3Ga_2(GaO_4)_3]$ per unit cell.

Lattice constants

		A
1956	Bertaut and Forrat [2]	12. 30
1961	National Bureau of Standards	12. 277 at 25 °C

The density calculated from the NBS lattice constant is 5.794 g/cm³ at 25 °C.

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C		
	d	*I*	*a*
	A		A
211	5. 009	4	12. 27
400	3. 070	40	12. 28
420	2. 744	100	12. 27
332	2. 617	4	12. 28
422	2. 507	51	12. 28
431	2. 407	5	12. 28
521	2. 242	6	12. 28
440	2. 170	2	12. 28
611	1. 991	6	12. 28
444	1. 772	13	12. 28
640	1. 702	34	12. 28
721	1. 670	2	12. 27
642	1. 6404	43	12. 276
800	1. 5349	16	12. 279
840	1. 3727	11	12. 278
842	1. 3393	18	12. 275
664	1. 3084	7	12. 274
851	1. 2937	1	12. 273
941	1. 2399	1	12. 274
10·1·1	1. 2155	2	12. 276
10·2·0	1. 2035	2	12. 273
10·3·1	1. 1704	3	12. 275
10·4·0	1. 1399	15	12. 277
10·4·2	1. 1207	10	12. 277
11·2·1	1. 0935	2	12. 275
880	1. 0850	8	12. 275
12·0·0	1. 0229	5	12. 275
12·2·0	1. 0091	5	12. 276
12·2·2	0. 9956	10	12. 275
11·6·3	. 9527	2	12. 275
12·4·4	. 9254	5	12. 277
12·6·0	. 9149	12	12. 275
13·3·2	. 9100	1	12. 277
12·6·2	. 9050	6	12. 276
10·9·3	. 8904	1	12. 273
888	. 8859	6	12. 275
14·3·1	. 8553	2	12. 276
12·8·0	. 8513	4	12. 278
14·4·0	. 8431	11	12. 276
14·4·2	. 8354	14	12. 278
14·5·1	. 8239	1	12. 276
15·2·1	. 8095	2	12. 277
Average value of last five lines			12. 277

References

[1] M. L. Keith and R. Roy, Structural relations among double oxides of trivalent elements, Am. Mineralogist **39** Nos. 1 and 2, 1–23 (1954).

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

Yttrium Oxychloride, YOCl (tetragonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of yttrium oxychloride was prepared at NBS by heating for 10 min at 700 °C a sample of YCl_3 obtained from the Lindsay Chemical Co., West Chicago, Ill. Their analysis showed the following impurities: a total as oxides of less than 0.1 percent of dysprosium, gadolinium, terbium, and europium, and traces of other rare earths.

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

The *d*-values of the three strongest lines are: 2.520, 2.759, and 3.358 A.

Structural data. Zachariasen [1] in 1949 determined that yttrium oxychloride has PbFCl-type structure, the space group D_{4h}^7—P4/nmm (No. 129) and 2(YOCl) per unit cell.

Lattice constants

		a	c
		A	A
1949	Zachariasen [1]	3. 900	6.604
1961	National Bureau of Standards.	3. 903	6.596 at 26 °C

The density of yttrium oxychloride calculated from NBS lattice constants is 4.639 g/cm^3 at 26 °C.

References

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

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 26 °C	
	d	I
	A	
001	6. 59	26
101	3. 358	50
002	3. 298	5
110	2. 759	73
102	2. 520	100
003	2. 198	3
112	2. 116	20
200	1. 9505	40
103	1. 9148	3
201	1. 8703	6
113	1. 7196	16
211	1. 6868	17
202	1. 6783	2
004	1. 6488	5
212	1. 5426	37
104	1. 5187	10
203	1. 4592	6
114	1. 4158	8
220	1. 3799	11
213	1. 3660	<1
221	1. 3515	4
005	1. 3198	1
301	1. 2766	3
222	1. 2734	3
204	1. 2597	3
105	1. 2490	4
310	1. 2342	8
311	1. 2135	2
302	1. 2102	5
214	1. 1984	7
115	1. 1903	3
223	1. 1694	3
312	1. 1562	3
006	1. 0996	5
205	1. 0925	5
313	1. 0761	4
321	1. 0681	5
224, 106	1. 0584	2
215	1. 0525	2
322	1. 0284	6
304, 116	1. 0214	4
314	0. 9881	4
400	. 9757	3

Zirconium Iodate, $Zr(IO_3)_4$ (tetragonal)

ASTM cards. None.

NBS sample. The sample of zirconium iodate was contributed by Don T. Cromer, Los Alamos Scientific Laboratory, Los Alamos, N. Mex. The compound was prepared by mixing water solutions of stoichiometric quantities of sodium iodate and zirconium sulfate tetrahydrate. The precipitate was dried at approximately 180 °C. It was refluxed in concentrated nitric acid to encourage crystallization. Their chemical analysis showed 11.66 percent Zr(—Hf) and 64.0 percent I. The source $Zr(SO_4)_2 \cdot 4H_2O$ contained 0.36 atom percent Hf in the Zr (by spectrographic analysis).

The sample was colorless. The indices of refraction are higher than available immersion liquids.

The *d*-values of the three strongest lines are: 4.18, 2.784, and 2.963 A.

Zirconium Iodate, $Zr(IO_3)_4$ (tetragonal)—Continued

hkl	1961 National Bureau of Standards Cu, 1.5405 A at 25 °C	
	d	*I*
	A	
110	5. 92	20
111	4. 64	18
200	4. 18	100
002	3. 729	33
201	3. 651	22
102	3. 406	10
211	3. 349	15
112	3. 157	3
220	2. 963	55
202	2. 784	94
212	2. 644	1
301	2. 616	15
311	2. 497	6
003	2. 489	4
222	2. 319	32
113	2. 293	1
321	2. 219	9
312	2. 159	11
203	2. 137	5
400	2. 094	25
213	2. 071	8
401	2. 020	<1
322	1. 972	4
411	1. 960	14
331	1. 908	3
223	1. 904	8
420	1. 873	12
004	1. 864	8
402	1. 826	16
421	1. 817	4
412	1. 784	2
332	1. 746	<1
204	1. 703	22
323	1. 698	
422	1. 674	37
214	1. 671	
510	1. 643	2
501	1. 635	13
403	1. 602	6
224	1. 578	5
413	1. 575	13
304	1. 551	4
502	1. 527	12
521	1. 523	
512	1. 5040	2
423	1. 4966	2
005	1. 4925	4
440	1. 4815	7
205	1. 4063	7
600	1. 3968	11
503	1. 3902	7
442	1. 3772	4
414	1. 3740	4
611	1. 3551	5
225	1. 3328	3
620	1. 3252	10
424	1. 3224	10
523	1. 3191	5
305	1. 3160	2
602	1. 3084	3
541	1. 2893	5
443	1. 2728	1
622	1. 2489	4
504	1. 2464	4
006	1. 2432	2
631	1. 2323	3
116	1. 2170	<1
405	1. 2156	<1
613	1. 2051	1
415	1. 2026	<1
524	1. 1948	1
206	1. 1919	1
710	1. 1852	1
701	1. 1820	<1
623	1. 1692	1
425	1. 1675	2
444	1. 1597	7
543	1. 1586	4
226	1. 1469	3
721	1. 1378	3
712	1. 1299	1
633	1. 1165	2
505	1. 1142	2
642	1. 1094	3
730	1. 1005	2

Structural data. Larson and Cromer [1] in 1959 determined that zirconium iodate has the space group C_{4h}^3—P4/n (No. 85) with $2[Zr(IO_3)_4]$ per unit cell.

Lattice constants

		a	*c*
		A	*A*
1959	Larson and Cromer [1]----	8. 38	7. 49
1961	National Bureau of Standards.	8. 380	7. 460 at 25 °C

The density of zirconium iodate calculated from the NBS lattice constants is 5.012 g/cm³ at 25 °C.

References

[1] A. C. Larson and Don T. Cromer, The crystal structure of $Zr(IO_3)_4$, Acta Cryst. **14**, 128–132 (1961). (Presented at ACA meeting, Cornell University, Ithaca, N.Y.) (1959).

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

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

m—Monograph 25.

	Vol. or sec.	Page
Cesium bomide, $CsBr$	3	49
Cesium bromoplatinate, Cs_2PtBr_6	8	19
Cesium bromoselenate, Cs_2SeBr_6	8	20
Cesium bromotellurate, Cs_2TeBr_6	9	24
Cesium chlorate, $CsClO_3$	8	20
Cesium chloride, $CsCl$	2	44
Cesium chloroplatinate, Cs_2PtCl_6	5	14
Cesium chlorostannate, Cs_2SnCl_6	5	16
Cesium chromium sulfate dodecahydrate, $CsCr(SO_4)_2\cdot 12H_2O$	8	21
Cesium dichloroiodide, $CsICl_2$	3	50
Cesium fluoborate, $CsBF_4$	8	22
Cesium fluogermanate, Cs_2GeF_6	5	17
Cesium fluoplatinate, Cs_2PtF_6	6	27
Cesium fluosilicate, Cs_2SiF_6	5	19
Cesium gallium sulfate dodecahydrate, $CsGa(SO_4)_2\cdot 12H_2O$	8	23
Cesium iodide, CsI	4	47
Cesium iron sulfate dodecahydrate, $CsFe(SO_4)_2\cdot 12H_2O$	6	28
Cesium nitrate, $CsNO_3$	9	25
Cesium perchlorate, $CsClO_4$, (orthorhombic)	1m	10
Cesium sulfate, Cs_2SO_4	7	17
Cesium vanadium sulfate dodecahydrate, $CsV(SO_4)_2\cdot 12H_2O$	1m	11
Chromium, Cr	5	20
Chromium orthophosphate, beta, β-$CrPO_4$	9	26
Chromium(III) oxide, Cr_2O_3	5	22
Chromium silicide, Cr_3Si	6	29
Cobalt aluminum oxide, $CoAl_2O_4$	9	27
Cobalt arsenide (skutterudite), $CoAs_3$	10	21
Cobalt(II) carbonate (spherocobaltite), $CoCO_3$	10	24
Cobalt diarsenide, $CoAs_2$	10	26
Cobalt gallate, $CoGa_2O_4$	10	27
Cobalt germanate, Co_2GeO_4	10	27
Cobalt iron arsenide (safflorite), $CoFeAs_4$	10	28
Cobalt(II) oxide, CoO	9	28
Cobalt(II, III) oxide, Co_3O_4	9	29
Copper, Cu	1	10
Copper(I) bromide, $CuBr$	4	36
Copper carbonate, basic, (azurite), $Cu_3(OH)_2(CO_3)_2$	10	30
Copper carbonate, basic, (malachite), $Cu_2(OH)_2(CO_3)$	10	31
Copper(I) chloride (nantokite), $CuCl$	4	35
Copper(I) iodide (marshite), CuI	4	38
Copper(I) oxide (cuprite), Cu_2O	2	23
Copper(II) oxide (tenorite), CuO	1	49
Copper(II) sulfide (covellite), CuS	4	13
Dysprosium sesquioxode, Dy_2O_3	9	30
Erbium gallium oxide 3:5, $Er_3Ga_2(GaO_4)_3$	1m	12
Erbium phosphate, $ErPO_4$	9	31
Erbium sesquioxide, Er_2O_3	8	25
Europium(III) chloride, $EuCl_3$	1m	13
Europium oxychloride, $EuOCl$	1m	13
Gadolinium fluoride, GdF_3	1m	14
Gadolinium oxide, Gd_2O_3	1m	16
Gadolinium oxychloride, $GdOCl$	1m	17
Gallium, Ga	2	9
Gallium antimonide, $GaSb$	6	30
Gallium oxide, alpha, Ga_2O_3	4	25
Gallium phosphate, (α-quartz type) $GaPO_4$	8	27
Germanium, Ge	1	18
Germanium dioxide, GeO_2 (hexagonal)	1	51
Germanium dioxide, GeO_2 (tetragonal)	8	28
Germanium(IV) iodide, GeI_4	5	25
Gold, Au	1	33
Gold antimony 1:2 (aurostibite), $AuSb_2$	7	18
Gold(I) cyanide, $AuCN$	10	33
Gold tin 1:1 $AuSn$	7	19
Hafnium, Hf	3	18
Holmium ethylsulfate nonahydrate, $Ho[(C_2H_5)SO_4]_3\cdot 9H_2O$	1m	18
Holmium sesquioxide, Ho_2O_3	9	32

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Indium, In	3	12
Indium antimony, $InSb$	4	73
Indium oxide, In_2O_3	5	26
Indium phosphate, $InPO_4$	8	29
Iodic acid, HIO_3	5	28
Iodine, I_2	3	16
Iridium, Ir	4	9
Iron, Alpha, Fe	4	3
Iron arsenide, $FeAs$	1m	19
Iron arsenide (loellingite), $FeAs_2$	10	34
Iron sulfide (pyrite), FeS_2	5	29
Lanthanum borate, $LaBO_3$	1m	20
Lanthanum chloride, $LaCl_3$	1m	21
Lanthanum fluoride, LaF_3	7	21
Lanthanum magnesium nitrate 24-hydrate, $La_2Mg_3(NO_3)12\cdot 24H_2O$	1m	22
Lanthanum oxide, La_2O_3	3	33
Lahthanum oxychloride, $LaOCl$	7	22
Lead, Pb	1	34
Lead bromide, $PbBr_2$	2	47
Lead carbonate (cerrussite), $PbCO_3$	2	56
Lead chloride (cotunnite), $PbCl_2$	2	45
Lead formate, $Pb(HCO_2)_2$	8	30
Lead fluochloride (matlockite) $PbFCl$	1	76
Lead fluoride, alpha, PbF_2	5	31
Lead fluoride, beta, PbF_2	5	33
Lead(II), iodide, PbI_2	5	34
Lead molybdate (wulfenite), $PbMoO_4$	7	23
Lead monoxide (litharge), PbO (red)	2	30
Lead monoxide (massicot) PbO (yellow)	2	32
Lead nitrate, $Pb(NO_3)_2$	5	36
Lead(II, III) oxide (minium), Pb_3O_4	8	32
Lead, phosphate hydrate (lead hydroxyapatite), $Pb_5(PO_4)_3OH$	8	33
Lead selenide (clausthalite), $PbSe$	5	38
Lead sulfate (anglesite), $PbSO_4$	3	67
Lead sulfide (galena), PbS	2	18
Lead titanate, $PbTiO_3$	5	39
Lead tungstate (stolzite), $PbWO_4$	7	24
Lithium bromide, $LiBr$	4	30
Lithium chloride, $LiCl$	1	62
Lithium fluoride, LiF	1	61
Lithium iodate, $LiIO_3$	7	26
Lithium molybdate, Li_2MoO_4, (trigonal)	1m	23
Lithium oxide, Li_2O	1m	25
Lithium nitrate, $LiNO_3$	7	27
Lithium perchlorate trihydrate, $LiClO_4\cdot 3H_2O$	8	34
Lithium tungstate, Li_2WO_4, (trigonal)	1m	25
Lutetium oxide, Lu_2O_3	1m	27
Magnesium, Mg	1	10
Magnesium aluminate (spinel), $MgAl_2O_4$	2	35
Magnesium aluminum silicate (low-cordierite), $Mg_2Al_4Si_5O_{18}$ (orthorhombic)	1m	28
Magnesium aluminum silicate (high-cordierite), $Mg_2Al_4Si_5O_{18}$ (hexagonal)	1m	29
Magnesium carbonate (magnesite), $MgCO_3$	7	28
Magnesium chromite (picrochromite), $MgCr_2O_4$	9	34
Magnesium fluoride (sellaite), MgF_2	4	33
Magnesium gallate, $MgGa_2O_4$	10	36
Magnesium germanate, Mg_2GeO_4 (cubic)	10	37
Magnesium germanate, Mg_2GeO_4 (orthorhombic)	10	38
Magnesium hydroxide (brucite), $Mg(OH)_2$	6	30
Magnesium oxide (periclase), MgO	1	37
Magnesium silicate (enstatite), $MgSiO_3$	6	32
Magnesium silicate (forsterite), Mg_2SiO_4	1	83
Magnesium silicate fluoride (norbergite) $Mg_2SiO_4\cdot MgF_2$	10	39
Magnesium silicate fluoride (humite), $3Mg_2SiO_4\cdot MgF_2$	1m	30
Magnesium sulfate heptahydrate (epsomite), $MgSO_4\cdot H_2O$	7	30
Magnesium sulfide, MgS	7	31
Magnesium tin, Mg_2Sn	5	41
Magnesium titanate (geikielite), $MgTiO_3$	5	43

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Magnesium tungstate, $MgWO_4$	1	84
Manganese aluminate (galaxite), $MnAl_2O_4$	9	35
Manganese(II) carbonate (rhodochrosite), $MnCO_3$	7	32
Manganese ferrite (jacobsite), $MnFe_2O_4$	9	36
Manganese(II)oxide (manganosite), MnO	5	45
Manganese(III) oxide (partridgeite), Mn_2O_3	9	37
Manganese selenide, $MnSe$	10	41
Manganese sulfide, alpha (alabandite), α-MnS	4	11
Mercury(I) bromide, Hg_2Br_2	7	33
Mercury(I) chloride (calomel), Hg_2Cl_2	1	72
Mercury(II) chloride, $HgCl_2$	1	73
Mercury(II) cyanide, $Hg(CN)_2$	6	35
Mercury(I) iodide, HgI	4	49
Mercury(II) iodide, HgI_2	1	74
Mercury(II) oxide (montroydite), HgO (revised)	9	39
Mercury(II) selenide (tiemannite), $HgSe$	7	35
Mercury(II) sulfide (cinnabar), HgS (hexagonal)	4	17
Mercury(II) sulfide (metacinnabar), HgS (cubic)	4	21
Neodymium borate, $NdBO_3$	1m	32
Neodymium chloride, $NdCl_3$	1m	33
Neodymium ethylsulfate nonahydrate, $Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$	9	41
Neodymium fluoride, NdF_3	8	36
Neodymium gallium oxide 3:5, $Nd_3Ga_2(GaO_4)_3$	1m	34
Neodymium oxide, Nd_2O_3	4	26
Neodymium oxychloride, $NdOCl$	8	37
Nickel, Ni	1	13
Nichel aluminate, $NiAl_2O_4$	9	42
Nickel arsenic 1:2 (rammelsbergite) $NiAs_2$	10	42
Nickel arsenic sulfide (gersdorffite) $NiAsS$	1m	35
Nickel (II) carbonate, $NiCO_3$ (trigonal)	1m	36
Nickel ferrite (trevorite), $NiFe_2O_4$	10	44
Nickel fluosilicate hexahydrate, $NiSiF_6 \cdot 6H_2O$	8	38
Nickel gallate, $NiGa_2O_4$	10	45
Nickel germanate, Ni_2GeO_4	9	43
Nickel (II) oxide (bunsenite), NiO	1	47
Nickel sulfate hexahydrate, $NiSO_4 \cdot 6H_2O$	7	36
Nickel sulfide, millerite, NiS	1m	37
Niobium silicide, $NbSi_2$	8	39
Osmium, Os	4	8
Palladium, Pd	1	21
Palladium oxide, PdO	4	27
Platinum, Pt	1	31
Potassium aluminum sulfate dodecahydrate, $KAl(SO_4)_2 \cdot 12H_2O$	6	36
Potassium borohydride, KBH_4	9	44
Potassium bromate, $KBrO_3$	7	38
Potassium bromide, KBr	1	66
Potassium bromoplatinate, K_2PtBr_6	8	40
Potassium bromoselenate, K_2SeBr_6	8	41
Potassium chloride (sylvite), KCl	1	65
Potassium chloroplatinate, K_2PtCl_6	5	49
Potassium chlororuthenate (IV), K_2RuCl_6	10	46
Potassium chlorostannate K_2SnCl_6	6	38
Potassium chromium sulfate dodecahydrate, $KCr(SO_4)_2 \cdot 12H_2O$	6	39
Potassium cobaltinitrite, $K_3Co(NO_2)_6$	9	45
Potassium cyanate, $KCNO$	7	39
Potassium cyanide, KCN	1	77
Potassium dihydrogen arsenate, KH_2AsO_4	1m	38
Potassium dihydrogen phosphate, KH_2PO_4	3	69
Potassium fluogermanate, K_2GeF_6	6	41
Potassium fluoplatinate, K_2PtF_6	6	42
Potassium fluoride, KF	1	64
Potassium fluosilicate (hieratite), K_2SiF_6	5	50
Potassium fluotitanate, K_2TiF_6	7	40
Potassium heptafluozirconate, K_3ZrF_7	9	46
Potassium hydroxy-chlororuthenate, $K_4Ru_2Cl_{10}O \cdot H_2O$	10	47
Potassium iodide, KI	1	68

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Potassium metaperiodate, KIO_4	7	41
Potassium nitrate (niter), KNO_3	3	58
Potassium perchlorate, $KClO_4$	6	43
Potassium permanganate, $KMnO_4$	7	42
Potassium perrhenate, $KReO_4$	8	41
Potassium phosphomolybdate, tetrahydrate, $K_3PO_4(MoO_3)_{12} \cdot 4H_2O$	8	43
Potassium sulfate (arcanite), K_2SO_4	3	62
Potassium thiocyanate, $KCNS$	8	44
Potassium zinc fluoride, $KZnF_3$	5	51
Praseodymium chloride, $PrCl_3$	1m	39
Praseodymium fluoride, PrF_3	5	52
Praseodymium oxychloride, $PrOCl$	9	47
Rhenium, Re	2	13
Rhodium, Rh	3	9
Rubidium aluminum sulfate dodecahydrate, $RbAl(SO_4)_2 \cdot 12H_2O$	6	44
Rubidium bromate, $RbBrO_3$	8	45
Rubidium bromide, $RbBr$	7	43
Rubidium bromotellurate, Rb_2TeBr_6	8	46
Rubidium chlorate, $RbClO_3$	8	47
Rubidium chloride, $RbCl$	4	41
Rubidium chloroplatinate, Rb_2PtCl_6	5	53
Rubidium chlorostannate, Rb_2SnCl_6	6	46
Rubidium chlorotellurate, Rb_2TeCl_6	8	48
Rubidium chromium sulfate dodecahydrate, $RbCr(SO_4)_2 \cdot 12H_2O$	6	47
Rubidium fluoplatinate, Rb_2PtF_6	6	48
Rubidium fluosilicate, Rb_2SiF_6	6	49
Rubidium iodide, RbI	4	43
Rubidium sulfate, Rb_2SO_4	8	48
Ruthenium, Ru	4	5
Samarium chloride, $SmCl_3$	1m	40
Samarium fluoride, SmF_3	1m	41
Samarium gallium oxide 3:5, $Sm_3Ga_2(GaO_4)_3$	1m	42
Samarium oxychloride, $SmOCl$	1m	43
Scandium oxide, Sc_2O_3	3	27
Scandium phosphate, $ScPO_4$	8	50
Selenium, Se	5	54
Selenium dioxide (selenolite), SeO_2	1	53
Silicon, Si	2	6
Silicon dioxide (alpha or low quartz), SiO_2	3	24
Silicon dioxide (alpha or low cristobalite), SiO_2 (Revised)	10	48
Silicon dioxide (beta or high crisobalite), SiO_2	1	42
Silver, Ag	1	23
Silver arsenate, Ag_3AsO_4	5	56
Silver bromate, $AgBrO_3$	5	57
Silver bromide (bromyrite), $AgBr$	4	46
Silver carbonate Ag_2CO_3	1m	44
Silver chlorate, $AgClO_3$	7	44
Silver chloride (cerargyrite), $AgCl$	4	44
Silver iodide (iodyrite), AgI (hexagonal)	8	51
Silver iodide, gamma, γ-AgI (cubic)	9	48
Silver metaperiodate, $AgIO_4$	9	49
Silver molybdate, Ag_2MoO_4	7	45
Silver nitrate, $AgNO_3$	5	59
Silver nitrite, $AgNO_2$	5	60
Silver oxide, Ag_2O	1m	45
Silver(II) oxynitrate, $Ag_7O_8NO_3$	4	61
Silver perrhenate, $AgReO_4$	8	53
Silver phosphate, Ag_3PO_4	5	62
Silver sulfate, Ag_2SO_4	7	46
Silver sulfide (argentite), Ag_2S	10	51
Sodium acid fluoride, $NaHF_2$	5	63
Sodium borohydride, $NaBH_4$	9	51
Sodium bromate, $NaBrO_3$	5	65
Sodium bromide, $NaBr$	3	47
Sodium carbonate monohydrate (thermonatrite), $Na_2CO_3 \cdot H_2O$	8	54
Sodium chlorate, $NaClO_3$	3	51
Sodium chloride (halite), $NaCl$	2	41
Sodium cyanide, $NaCN$ (cubic)	1	78
Sodium cyanide, $NaCN$ (orthorhombic)	1	79
Sodium fluoride (villiaumite), NaF	1	63

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