Cop 2

NBS MONOGRAPH 25—SECTION 5

Standard X-ray Diffraction Powder Patterns

U.S.

U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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Standard X-ray Diffraction Powder Patterns

H. E. Swanson, H. F. McMurdie, M. C. Morris,
and E. H. Evans

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Standard x-ray powder patterns:

Calculated powder patterns (cubic):

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*Not previously listed in Powder Diffraction File.

**A mineral name in parentheses indicates a synthetic sample.

Errata

Monograph 25, Section 5

Circular 539

Vol. 1, p. 55; In the last column, the 7th entry should be I = 17, (for *d* = 1.675).
Vol. 2, p. 28; The space group should be T_h^7-Ia3; the reference for it is:

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

Vol. 3, p. 27; The space group should be T_h^7-Ia3, from Pauling and Shappell, (ibid).
Vol. 3, p. 28; The space group should be T_h^7-Ia3, from Pauling and Shappell, (ibid).
Vol. 6, p. 12; The space group should be D_{2h}^{16}-Pmcn.
Vol. 8, p. 23; The line in the table reading: 503 1.5386 10 should follow the line: 610 1.5532 7.
Vol. 8, p. 25; The space group should be Ia3 (No. 206), from the reference:

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

Monograph 25

Sec. 2, p. 23; The first two *hkl* entries for the pattern should be 002 and 102.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Information on ten volumes in this series listed as follows is available from Mr. Howard E. Swanson, Room A221, Materials Building, National Bureau of Standards, Washington, D. C., 20234:

NBS Circular 539, Volume 1, Standard X-ray Diffraction Powder Patterns (Data for 54 substances).
NBS Circular 539, Volume 2, Standard X-ray Diffraction Powder Patterns (Data for 30 substances).
NBS Circular 539, Volume 3, Standard X-ray Diffraction Powder Patterns (Data for 34 substances).
NBS Circular 539, Volume 4, Standard X-ray Diffraction Powder Patterns (Data for 42 substances).
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NBS Circular 539, Volume 6, Standard X-ray Diffraction Powder Patterns (Data for 44 substances).
NBS Circular 539, Volume 7, Standard X-ray Diffraction Powder Patterns (Data for 53 substances).
NBS Circular 539, Volume 8, Standard X-ray Diffraction Powder Patterns (Data for 61 substances).
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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 5.—Data for 80 substances

Howard E. Swanson, Howard F. McMurdie,[1] Marlene C. Morris,[1] and Eloise H. Evans[1]

Standard x-ray diffraction powder patterns are presented for 80 substances. Thirty-nine of these patterns represent experimental data and 41 are calculated. The experimental x-ray powder diffraction patterns are made with a Geiger counter x-ray diffractometer, using samples of high purity. All d-values were assigned Miller indices determined by comparison with theoretical interplanar spacings and from consideration of space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were obtained from published crystal structure data. The reported peak height intensities for calculated patterns were converted from integrated intensities.

Reference intensity values based upon the strongest line of corundum (113) in a 50 percent weight mixture are given for 73 materials.

Keywords: standard, x-ray diffraction, powder-patterns, crystal, structure, measurements, lattice, constants, reference-intensities

INTRODUCTION

The X-ray Powder Diffraction File (1965)[2] is a compilation of diffraction patterns, gathered from many sources and produced under the auspices of the Joint Committee on Chemical Analysis by Powder Diffraction Methods.[3] The File is used for the identification of unknown crystalline materials by matching d-spacings and intensity measurements. Under the partial sponsorship of the Joint Committee, a program at the National Bureau of Standards contributes new data for this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents data for 80 compounds, 39 experimental and 41 calculated patterns. This compilation is the fifteenth of the series of "Standard X-ray Diffraction Powder Patterns."[4]

Experimental Powder Patterns

Powder Diffraction File Cards. Under this heading are given the Powder Diffraction File card numbers and the literature reference for each card. Cards listed through the 1965 index to the Powder Diffraction File are included.

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

NBS sample. Many of the samples used to make NBS patterns were special preparations of high purity obtained from a variety of sources or prepared in small quantities in our laboratory. Treating the sample by appropriate annealing, recrystallizing, or heating in hydrothermal bombs improved the definition of most of the patterns.

Unless otherwise noted, the spectrographic analyses were done at NBS after preparation of the sample was completed. The limit of detection for the alkali elements was 0.05 percent for the spectrographic analyses. A check of phase purity was usually provided by the x-ray pattern itself, when it was indexed by comparison with theoretical d-values. A microscopic inspection for phase purity was also made on the nonopaque materials during the refractive index determination. The latter was done by grain-immersion methods in white light, with oils standardized in sodium light, in the range 1.40 to 2.1.

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts (1965).

Structural data. For cubic materials a value for the lattice constant was calculated for each d-value. However, the constant reported is that obtained by averaging the constants for the last five lines because of the greater accuracy of calculation in the high-angle region of the pattern. The unit cell values for noncubic substances were determined by means of a least-squares calculation made on the IBM 7094, using those d-values for which only one set of Miller indices could be assigned. The number of significant figures reported for the d-values in the NBS patterns varies slightly with the symmetry and crystallinity of each sample. The indexing and cell refinement calculation was performed using a program developed by Evans, Appleman, and Handwerker (1963). Lattice constant errors are given only for data refined on that program and are based on least-squares refinement of the variance-covariance matrix derived from the unweighted $\Delta\theta$ residuals.

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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] Dates in brackets indicate the literature references at the end of each section of this paper.

[3] This committee is composed of members from the American Society for Testing and Materials, the American Crystallographic Association, and the British Institute of Physics. Financial support is also provided by the National Bureau of Standards.

[4] See previous page for listing of other published volumes.

Published unit cell data in kX units and data given in angstrom units prior to 1947 were converted to angstrom units using the factor 1.00202 as recommended by an international conference of crystallographers reported in J. Sci. Instr. (1947).

The space groups are listed with both the Schoenflies and short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography (1952).

Orthorhombic cell dimensions are presented according to the Dana convention b>a>c (Dana System of Mineralogy, 1944).

The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter and are computed from the Avogadro number (6.02252×10^{23}) and from atomic weights based on carbon 12 (Chem. Eng. News, 1961).

Intensity measurements. At least three patterns for intensity measurements were prepared to check reproducibility. Samples that gave satisfactory intensity patterns usually had an average particle-size smaller than 10 μ (Alexander et al., 1948). In order to avoid the orientation effects which occur when samples are packed or pressed, a sample holder was made that had an extended rectangular cavity opened on its top face and at one end. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see fig. 1). The powdered sample was then drifted into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample surface could be exposed to the x-ray beam (as shown in fig. 2). To powders that did not flow readily, or were prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the intensity of the strongest line.

Interplanar spacings. Specimens for the interplanar spacing patterns were prepared by packing into a shallow holder a sample containing approximately 5 wt. percent tungsten powder that served as an internal standard. When tungsten lines were found to interfere, 25 percent silver was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used for the regions between the peaks of the standard. For low values of 2θ, the pattern peak was measured in the center, at a place averaging about 75 percent of the peak height. For higher values of 2θ, where α_1 and α_2 peaks were resolved, the α_1 peak was measured in the same way. The internal standard correction appropriate to each region was then applied to the measurement of 2θ. The new internal standard lattice constants used were 3.16504 Å for tungsten and 4.08625 Å for silver at 25°C, as determined by Swanson, Morris, and Evans (1966). These changes increase d-values by a factor of 1.00004 when compared to the d-values obtained with the older standard samples. All of the NBS patterns, unless otherwise noted, are made on a diffractometer at 25°C using filtered copper radiation ($K\alpha_1$), having the wavelength 1.5405 Å. A curved lithium fluoride crystal monochromator was used in the preparation of some patterns.

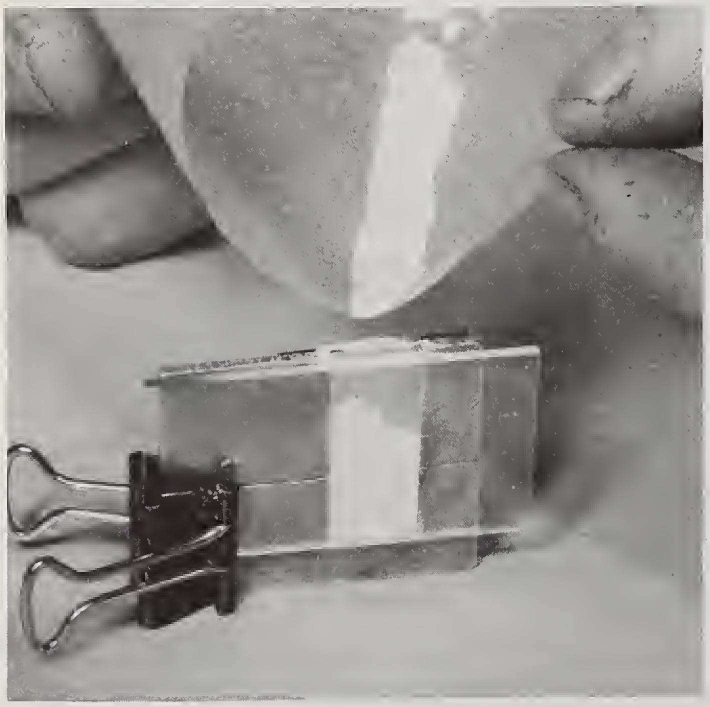

Figure 1

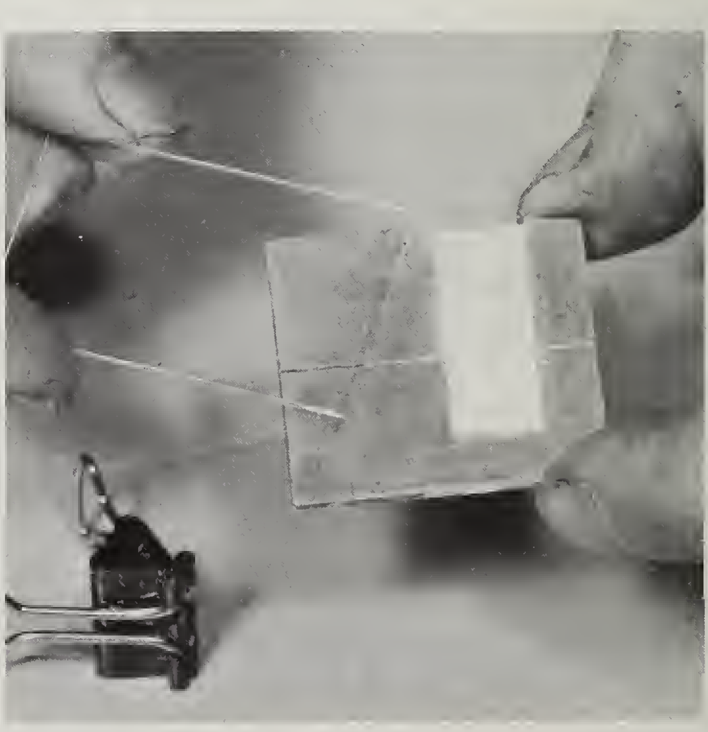

Figure 2

Since some substances are not readily available for experimental work, calculated powder patterns were made. These were based on published crystal structure data, using a FORTRAN program developed by Smith (1963).

Lorentz-polarization corrections are included. No corrections were made for temperature factors or absorption factors. Scattering factor values without ionization were taken from table 3.3.1A of the International Tables (1962a) for the following elements: beryllium, boron, calcium, cobalt, hydrogen, magnesium, nitrogen, oxygen, phosphorus, selenium, silver, and sulfur. All other scattering factor values used were taken from table 3.3.1B, International Tables (1962b).

Intensity calculations were based upon copper wavelength, 1.5405 Å. The integrated intensities printed out from the computer program were converted to peak height values by means of a graph from Swanson, Morris, Stinchfield, and Evans (1962). The peak height intensities are tabulated as percentages of the peak intensity of the strongest line. Peak height intensities from 0.1 to 0.9 were recorded as < 1; data with peak height intensities < 0.1 were omitted. When adjacent 2θ values were nearly equal, resolution of individual peaks in the powder pattern would be unlikely. In that case, only one angle and its d-spacing are listed, with multiple *hkl's* and with the sum of the intensities of the peaks involved.

Literature references for calculated patterns are compiled at the end of that section.

The authors are indebted to J. H. deGroot for the preparation of many samples used, and to S. J. Carmel for his assistance on the work particularly in performing intensity measurements.

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ISCC-NBS Centroid Color Charts, Standard Sample No. 2106, obtained from the Office of Standard Reference Materials, Room B328, Chemistry Building, National Bureau of Standards, Washington, D. C. 20234. $3.00 per set.

Smith, D. K. (1963). A FORTRAN program for calculating x-ray powder diffraction patterns, UCRL-7196, University of California, Lawrence Radiation Laboratory, Livermore, California.

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Swanson, H. E., Morris, M. C., Stinchfield, R. P., and Evans, E. H. (1962). Standard X-ray Diffraction Powder Patterns, Natl. Bur. Std. U.S. Monograph 25, Sec. 1, 3.

The conversion factor for kX units to angstrom units (1947). J. Sci. Instr. 24, 27.

REFERENCE INTENSITY VALUES

The format of the first Powder Diffraction Cards issued by the Joint Committee had a space for a reference intensity in which NaCl was used. This original attempt to establish absolute values started by the Dow Chemical Co. however was not continued.

In 1961 de Wolff in Holland proposed that a variation of this idea be reconsidered as a help in evaluating mixtures. We expressed a desire to cooperate in the development of this project. After several reference materials were examined in both Delft and NBS labs, αAl_2O_3 was chosen as an internal standard to be mixed 1:1 by weight. Corundum was picked partly because it is available commercially as Linde "A" in approximately one micron particle size from Union Carbide Corp., East Chicago, Ind., and partly because of its chemical stability and freedom from shape orientation in sample preparation.

The 1:1 mixture is mounted in our regular intensity sample holder (illust. p. 2) and it is necessary to run only the portion of the x-ray pattern that includes the strongest line of each compound; corundum (113), d= 2.085 Å was used. The direct ratio of the heights of the two lines is then reported as $I/I_{corundum}$. In a few instances the strongest line of one of the materials may fall on a line of the other. In this case the second strongest line is measured, and based upon previous knowledge of the relative peak heights, a correction is made thus enabling one to reconstruct the value for the strongest line.

In this report we are listing 35 $I/I_{corundum}$ values for some samples we have worked with in the past. Data reported from July 1965 has the $I/I_{corundum}$ value included in the text for each compound. We expect to continue measuring this value for new data submitted to the PDF.

$I/I_{corundum}$ Values for Some Previously Reported Powder Patterns

Aluminum 3:2 Silicate (mullite), $3Al_2O_3 \cdot 2SiO_2$ (orthorhombic)	1.7
Ammonium Fluoberyllate, $(NH_4)_2BeF_4$ (orthorhombic)	0.6
Ammonium Fluoborate, NH_4BF_4 (orthorhombic)	0.7
Barium Stannate, $BaSnO_3$ (cubic)	6.1
Bismuth Orthophosphate, $BiPO_4$ (monoclinic)	4.7
Bismuth Sulfide (bismuthinite), Bi_2S_3 (orthorhombic)	2.1
Cadmium Telluride, CdTe (cubic)	6.5
Calcium Fluoride Phosphate (fluorapatite), $Ca_5F(PO_4)_3$ (hexagonal)	1.5
Cesium Chromate, Cs_2CrO_4 (orthorhombic)	1.4
Cesium Fluoantimonate, $CsSbF_6$ (trigonal)	2.7
Cobalt Silicate, Co_2SiO_4 (orthorhombic)	0.9
Cobalt Tungstate, $CoWO_4$ (monoclinic)	5.6
Cobalt Titanate, $CoTiO_3$ (trigonal)	1.5
Erbium Arsenate, $ErAsO_4$ (tetragonal)	3.1
Europium(III) Vanadate, $EuVO_4$ (tetragonal)	1.6

Holmium Arsenate, $HoAsO_4$ (tetragonal)	3.5
Iridium Dioxide, IrO_2 (tetragonal)	7.9
Lead Boron Oxide, PbB_4O_7 (orthorhombic)	2.5
Lithium Phosphate, low form, (lithiophosphate), Li_3PO_4 (orthorhombic)	1.1
Lithium Phosphate, high form, Li_3PO_4 (orthorhombic)	1.2
Magnesium Ammonium Phosphate Hexahydrate (struvite), $MgNH_4PO_4 \cdot 6H_2O$ (orthorhombic)	1.0
Neodymium Arsenate, $NdAsO_4$ (monoclinic)	1.3
Potassium Acid Phthalate, C_6H_4 (COOH) (COOK) (orthorhombic)	1.4
Potassium Zinc Decavanadate 16 Hydrate, $K_2Zn_2V_{10}O_{28} \cdot 16H_2O$ (triclinic)	0.8
Rubidium Chromate, Rb_2CrO_4 (orthorhombic)	1.6
Samarium Arsenate, $SmAsO_4$ (tetragonal)	5.0
Scandium Arsenate, $ScAsO_4$ (tetragonal)	4.9
Strontium Boron Oxide, SrB_2O_4 (orthorhombic)	3.1
Strontium Boron Oxide, SrB_4O_7 (orthorhombic)	1.9
Thallium Chromate, Tl_2CrO_4 (orthorhombic)	3.0
Tin Arsenide, SnAs (cubic)	3.5
Tin Fluoride, SnF_2 (monoclinic)	2.7
Titanium Dioxide, brookite, TiO_2 (orthorhombic)	1.1
Zinc Antimony Oxide, $ZnSb_2O_4$ (tetragonal)	4.2
Zinc Telluride, ZnTe (cubic)	9.3

Ammonium Cadmium Trichloride, NH_4CdCl_3 (orthorhombic)

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium cadmium chloride was precipitated at NBS from stoichiometric solutions of ammonium chloride and cadmium chloride.

Spectrographic analysis showed the major impurities to be less than 0.001 percent each of aluminum, barium, calcium, copper, magnesium, and silicon.

The sample was colorless and optically positive with a small 2V. $N_\alpha = 1.711$, $N_\beta = 1.714$, and $N_\gamma = 1.748$.

$I/I_{corundum} = 2.5$.

Structural data. Brasseur and Pauling (1938) determined that ammonium cadmium chloride has the space group D_{2h}^{16}-Pnam (No. 62) and 4(NH_4CdCl_3) per unit cell. Ammonium cadmium chloride is used as a structure type.

Lattice constants

	a(Å)	b(Å)	c(Å)
Brasseur and Pauling (1938)	8.98	14.90	3.98
MacGillavry, et.al. (1939)	9.02	14.93	3.97
NBS, sample at 25°C	9.017	14.911	3.9896

The density of ammonium cadmium chloride calculated from the NBS lattice constants is 2.932 g/cm^3 at 25° C.

Internal standard W, a = 3.16504 Å

CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.71	89	110	11.47
7.44	100	020	11.87
5.745	65	120	15.41
4.509	15	200	19.67
4.348	5	130	20.41
4.316	6	210	20.56
3.857	10	220,011	23.04
3.728	4	040	23.85
3.541	43	111	25.13
3.445	17	140	25.84
3.340	27	230	26.67
3.110	5	031	28.68
2.987	30	201	29.89
2.945	8	310,131	30.32
2.930	36	211	30.48
2.873	15	240	31.10
2.833	15	150	31.55
2.787	12	320	32.08
2.773	58	221	32.25
2.608	2	141	34.35
2.573	10	330	34.84
2.487	10	250,060	36.09
2.396	25	160	37.51
2.340	2	340	38.44
2.285	16	321	39.40
2.255	1	400	39.95
2.158	6	420	41.83
2.117	3	350	42.68
2.111	6	251	42.80
2.073	4	170	43.62
2.053	14	161,430	44.07
2.018	24	341	44.87
1.994	11	002	45.45
1.963	4	401	46.21
1.929	9	440	47.07
1.927	9	022,270	47.12
1.915	1	360	47.44
1.9110	1	261	47.54
1.8978	13	421	47.89
1.8794	6	071	48.39
1.8642	2	080	48.81
1.8394	15	171	49.51
1.8253	7	431,180	49.92
1.7987	3	450	50.71
1.7533	2	520	52.12

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Brasseur, H. and Pauling, L. (1938). The crystal structure of ammonium cadmium chloride, NH_4CdCl_3, J. Am. Chem. Soc. 60, 2886-2890.

MacGillavry, C.H., Nijveld, H., Dierdorp, S. and Karsten, J. (1939). Die Kristallstruktur von NH_4CdCl_3 und $RbCdCl_3$, Rec. trav. chim. 58, 193-200.

Ammonium Cadmium Trichloride, NH_4CdCl_3 (orthorhombic)—continued

<table>
<tr><th colspan="4">Internal standard W, a = 3.16504 Å
CuKα₁ λ = 1.5405 Å; temp. 25 °C</th></tr>
<tr><th><i>d</i> (Å)</th><th><i>I</i></th><th><i>hkl</i></th><th>2θ(°)</th></tr>
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<tr><td>1.7262</td><td>4</td><td>142,361</td><td>53.00</td></tr>
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<tr><td>1.4371</td><td>3</td><td>172</td><td>64.82</td></tr>
</table>

Ammonium Manganese(II) Trifluoride, NH_4MnF_3 (cubic)

Powder diffraction cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium manganese trifluoride was prepared at NBS by R.A. Forman from saturated solutions of ammonium fluoride and manganese chloride. The first 10 percent of the crystals were collected and washed in alcohol. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, calcium, iron, and magnesium.

The color of the sample was pinkish white. The index of refraction was 1.490.

$I/I_{\text{corundum}} = 3.2$.

Structural data. Simanov, Batsanova, and Kovba (1957) determined that ammonium manganese trifluoride has the perovskite structure, the space group O_h^1-Pm3m (No. 221) and 1 (NH_4MnF_3) per unit cell.

Lattice constants

	a(Å)
Simanov, Batsanova, and Kovba (1957)---------------	4.239
Hoppe, Liebe, and Dahne (1961)--	4.241
NBS, sample at 25°C-------------	4.2410

The density of ammonium manganese trifluoride calculated from the NBS lattice constant is 2.829 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)	*a* (Å)
4.243	100	100	20.92	4.243
3.000	63	110	29.76	4.243
2.449	5	111	36.66	4.242
2.120	57	200	42.60	4.240
1.896	33	210	47.93	4.240
1.731	16	211	52.85	4.240
1.4994	18	220	61.82	4.241
1.4135	10	300	66.04	4.240
1.3414	5	310	70.09	4.242
1.2245	5	222	77.96	4.242
1.1763	3	320	81.81	4.241
1.1334	6	321	85.62	4.241
1.0605	3	400	93.16	4.242
1.0287	5	410	96.96	4.2414
0.9996	7	411	100.80	4.2409
.9484	4	420	108.61	4.2414
.9254	3	421	112.68	4.2407
.9042	3	332	116.82	4.2411
.8657	3	422	125.69	4.2410
.8482	2	500	130.48	4.2410
.8317	4	510	135.67	4.2409
.8162	2	511	141.37	4.2411
.7875	3	520	155.94	4.2408

References

Hoppe, R., Liebe, W., and Dähne, W. (1961). Über Fluoromanganate der Alkalimetalle, Z. anorg. u. allgem. Chem. 307, 276-289.

Simanov, Yu. P., Batsanova, L.P., and Kovba, L.M. (1957). X-ray investigation of the binary fluorides of bivalent manganese, Russ. J. Inorg. Chem. 2, 207. (Translated from Zh. Neorgan. Khim. II, No. 10, 2410-2415).

Ammonium Mercury(II) Trichloride, NH_4HgCl_3 (tetragonal)

Powder diffraction cards. None.

Additional published patterns. None

NBS sample. The sample of ammonium mercury trichloride was precipitated at NBS from solutions of ammonium chloride and mercury chloride.

Spectrographic analysis showed the only impurity greater than 0.001 percent to be 0.01 to 0.1 percent silicon.

The sample was light gray to colorless, and optically positive with the indices of refraction $N_o = 1.793$ and $N_e = 1.84$. The higher index could not be measured accurately because the liquid and sample reacted.

$I/I_{corundum} = 3.1$.

Structural data. Harmsen (1938) reported that ammonium mercury trichloride has one of several tetragonal space groups P*** and 1 (NH_4HgCl_3) per unit cell. Ammonium mercury trichloride is used as a structure type.

Lattice constants

	a(Å)	c(Å)
Harmsen (1938)-----------	4.20	7.96
NBS, sample at 25°C------	4.1977	7.9353
	±0.0001	±0.0002

The density of ammonium mercury trichloride calculated from the NBS lattice constants is 3.859 g/cm³ at 25°C.

Reference

Harmsen, E.J. (1938). The crystal structure of NH_4HgCl_3, Z. Krist. **100A**, 208-211.

Internal standard Ag, a = 4.08625 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
7.93	100	001	11.15
4.200	56	100	21.14
3.967	23	002	22.39
3.711	38	101	23.96
2.969	44	110	30.07
2.883	47	102	30.99
2.782	22	111	32.15
2.645	18	003	33.86
2.377	33	112	37.81
2.239	18	103	40.25
2.099	13	200	43.06
2.029	9	201	44.62
1.983	18	004	45.71
1.974	17	113	45.93
1.877	8	210	48.45
1.855	6	202	49.06
1.827	13	211	49.88
1.793	10	104	50.88
1.6966	2	212	54.00
1.6491	11	114	55.69
1.6444	9	203	55.86
1.5868	2	005	58.08
1.5308	6	213	60.42
1.4843	3	105,220	62.52
1.4588	4	221	63.74
1.4417	4	204	64.59
1.3994	4	115,300	66.79
1.3899	5	222	67.31
1.3780	3	301	67.96
1.3635	4	214	68.79
1.3274	2	310	70.94
1.3227	2	006	71.23
1.3092	3	311	72.08
1.2943	5	223	73.04
1.2658	2	205	74.96
1.2616	4	106	75.25
1.2587	4	312	75.46
1.2366	2	303	77.05
1.2116	1	215	78.95
1.2081	2	116	79.22

Internal standard Ag, a = 4.08625 Å

CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
1.1881	4	224	80.83
1.1865	3	313	80.96
1.1646	2	320	82.81
1.1518	3	321	83.94
1.1434	2	304	84.70
1.1333	1	007	85.63
1.1190	2	206	87.00
1.1032	2	314	88.56
1.0944	2	107	89.47
1.0837	2	225	90.59
1.0810	2	216	90.88
1.0656	2	323	92.58
1.0590	2	117	93.33
1.0496	2	305,400	94.42
1.0184	3	315,410	98.29
1.0095	3	411	99.46
1.0043	2	324	100.16
0.9975	2	207	101.10
.9920	1	008	101.88
.9893	2	330	102.26
.9874	3	226	102.54
.9756	3	403	104.28
.9706	3	217	105.05
.9655	3	108	105.84
.9612	3	306	106.51
.9502	1	413	108.32
.9408	3	118	109.91

Barium Aluminum Oxide, $BaAl_2O_4$ (hexagonal)

Powder Diffraction File cards. No. 2-0545, Wallmark and Westgren (1937).

Additional published patterns. None.

NBS sample. The sample of barium aluminum oxide was prepared at NBS from gamma alumina and barium carbonate. The mixture was heated at 1200°C for 1 and 1/2 hrs.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium, silicon, and vanadium.

The sample was colorless and had very low double refraction. The average index of refraction was approximately 1.675.

$I/I_{corundum} = 4.4$.

Structural data. Wallmark and Westgren (1937) determined that barium aluminum oxide has the space group D_6^6-$P6_322$ (No. 182).

Arlett, White, and Robbins (1967) found a doubling of the *a* axis and $8(BaAl_2O_4)$ per unit cell.

Lattice constants

	a(Å)	c(Å)
Wallmark and Westgren [1937]----------------	5.220	8.779
Glasser and Dent Glasser [1963]----------------	5.228	8.756
Do Dinh and Bertaut [1965]----------------	5.227	8.802
Arlett et al. [1967]-----	10.444	8.793
NBS, sample at 25°C------	10.4470 ±.0001	8.7940 ±.0002

The density of barium aluminum oxide, calculated from the NBS lattice constants is 4.080 g/cm³ at 25°C.

Additional published patterns. Do Dinh and Bertaut (1965).

Internal standard Ag, a = 4.08625 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.525	45	200	19.60
4.001	6	002	20.16
4.022	10	201	22.08
3.153	100	202	28.28
2.611	40	220	34.31
2.505	3	221	35.81
2.461	2	203	36.48
2.413	<1	311	37.23
2.262	11	400	39.81
2.246	25	222	40.11
2.199	10	004	41.01
2.136	<1	104	42.28
2.0111	19	402	45.04
1.9774	12	204	45.85
1.9505	<1	223	46.52
1.7911	<1	403	50.94
1.7098	5	420	53.55
1.6822	10	224	54.50
1.6391	1	205	56.06
1.5935	18	422	57.81
1.5764	7	404	58.50
1.5078	8	600	61.44
1.4771	<1	423	62.86
1.4660	1	431,006	63.39
1.4263	1	602	65.37
1.3944	3	206	67.06
1.3890	1	405	67.36
1.3628	<1	611	68.83
1.3496	6	424	69.60
1.3057	3	440	72.30
1.2782	5	531,226	74.11
1.2547	1	620	75.74
1.2516	2	442	75.96
1.2435	4	604	76.55
1.2299	1	406	77.55
1.2262	1	425	77.83
1.2063	6	622	79.36
1.1536	<1	623	83.78
1.1308	<1	800,631	85.87
1.1228	2	444	86.63
1.1129	2	426	87.59
1.0952	2	802	89.38
1.0898	2	624	89.95
1.0683	2	208	92.27
1.0549	<1	803	93.80

Internal standard Ag, a = 4.08625 Å
CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
1.0511	1	811,606	94.24
1.0379	1	640	95.83
1.0216	<1	625	97.87
1.0132	<1	228	98.97
1.0100	2	642	99.39
1.0056	<1	804	99.98
0.9885	1	408	102.38
.9872	2	820	102.57
.9783	<1	643	103.87
.9750	1	446	104.37
.9632	1	822	106.20
.9532	1	626	107.82
.9431	<1	911	109.52
.9386	1	644	110.30
.9247	2	428	112.81
.9048	<1	10.0.0	116.71
.9005	1	824	117.59
.8953	<1	806	118.71
.8938	<1	645	119.04
.8883	<1	608	120.25
.8861	1	10.0.2	120.74
.8794	<1	0.0.10	122.29
.8728	<1	905	123.89
.8706	1	660	124.43
.8632	<1	2.0.10	126.33
.8547	<1	10.1.1	128.63
.8470	1	646	130.85
.8410	<1	448	132.66
.8391	2	842	133.25
.8367	1	10.0.4	134.03
.8334	1	2.2.10	135.11
.8268	2	628	137.36
.8188	2	826	140.34
.8125	<1	10.2.0	142.90
.8094	1	664	144.19
.7989	2	10.2.2	149.21
.7968	2	844	150.35
.7882	<1	808	155.50

References

Arlett, R. H., White, J. G., and Robbins, M. (1967). Single crystals of $BaAl_2O_4$, Acta Cryst **22**, 315.

Do Dinh, C. and Bertaut, E.-F. (1965). Parametres de $BaAl_2O_4$ et etudes des solutions solides $BaFe_xAl_{2-x}O_4$ et $BaGa_xAl_{2-x}O_4$, Bull. Soc. Franc. Mineral. Crist. **88** 413-6.

Glasser, F. P. and Dent Glasser, L. S. (1963). Crystal chemistry of some AB_2O_4 compounds, J. Am. Chem. Soc. **46**, 377-380.

Hoppe, R. and Schepers, B. (1960). Crystal structure of $BaGa_2O_4$ and $BaAl_2O_4$, Naturwissenschaften **47**, 376.

Wallmark, S. and Westgren, A. (1937). X-ray analysis of barium aluminates, Arkiv Kemi, Mineral. Geol. **B12**, No. 35.

Bismuth Sulfide (bismuthinite), Bi_2S_3 (orthorhombic) (revised)

Powder Diffraction File cards. No. 6-0333, National Bureau of Standards (1955). The following data is essentially the same as that reported on the above card: however, A. Glatz, Carrier Research and Development Co. suggested that if the pattern were remeasured, using his sample, it would be interesting to see the effect of back reflection lines on the lattice constants. The sharper pattern produced by this new sample also added weak front reflection lines.

Additional published patterns. None.

NBS sample. The high purity sample of bismuth sulfide, furnished by A. C. Glatz, was prepared by the method described in a paper by Glatz and Meikleham (1963). In addition, he also ground, sieved to -50 mesh, and annealed this sample at 400°C for one month.

The sample was a dark gray opaque powder.

$I/I_{corundum} = 2.1$.

Structural data. Hofmann (1933) determined that bismuth sulfide has the antimony sulfide structure, the space group D_{2h}^{16}-Pbnm (No. 62) and $4(Bi_2S_3)$ per unit cell.

Lattice constants

	a(Å)	b(Å)	c(Å)
NBS (1955), sample at 26°C	11.150	11.300	3.981
NBS, sample at 25°C	11.149	11.304	3.981

The density of bismuth sulfide calculated from NBS (1965) lattice constants is 6.806 g/cm³ at 25°C.

References

Glatz, A. and Meikleham, V. (1963). The preparation and electrical properties of bismuth trisulfide, J. Electrochem. Soc. **110**, 1231-1234.

Hofmann, W. (1933). Die Struktur der Minerale der Antimonitgruppe, Z. Krist. **86**, 225-245.

Swanson, H. E., Fuyat, R. K., and Ugrinic, G. M. (1955). Standard X-ray Diffraction Powder Patterns, Natl. Bur. Standards (U.S.), Circ. 539, **IV**, 23-25.

Internal standard W, a = 3.16504 Å
CuKα₁ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.936	1	110	11.14
5.654	22	020	15.66
5.566	6	200	15.91
5.040	22	120	17.58
3.967	42	220	22.39
3.748	17	101	23.72
3.569	100	130	24.93
3.530	58	310	25.21
3.253	16	021	27.39
3.118	80	230,211	28.60
2.824	14	040	31.65
2.812	51	221	31.80
2.717	28	301	32.94
2.709	4	410	33.04
2.641	18	311	33.91
2.521	40	240	35.58
2.499	12	420	35.91
2.456	10	231	36.55
2.305	20	041	39.04
2.258	32	141	39.90
2.241	12	430	40.20
2.188	5	510	41.22
2.130	7	241	42.39
2.118	11	421	42.65
2.096	9	250	43.13
2.075	10	520	43.59
1.990	18	002	45.54
1.985	16	440	45.66
1.953	39	431	46.45
1.945	31	501	46.66
1.937	16	151	46.87
1.932	10	350	47.00
1.919	18	530	47.32
1.884	23	060	48.26
1.857	13	600,160	49.00
1.853	16	251	49.11
1.834	10	610	49.67
1.785	4	260	51.13
1.780	8	222	51.28
1.765	5	620	51.74
1.750	8	540	52.21
1.738	33	132	52.60
1.734	14	312	52.74
1.703	11	061	53.77
1.683	4	161	54.46
1.680	4	360	54.58
1.665	2	611	55.12
1.606	4	451	57.30
1.603	2	541	57.45
1.587	2	550	58.07

Internal standard W, a = 3.16504 Å
CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.562	11	242	59.09
1.552	7	640	59.49
1.548	7	361	59.69
1.537	4	631	60.14
1.5328	7	720	60.33
1.4828	11	171	62.59
1.4809	17	370,152	62.68
1.4451	6	271	64.42
1.4431	6	252	64.52
1.4359	8	522	64.88
1.4306	12	721	65.15
1.4127	1	080	66.08
1.4052	4	442	66.48
1.4018	4	180	66.66
1.3974	6	470	66.90
1.3862	4	352	67.51
1.3830	4	810	67.69
1.3814	8	532	67.78
1.3682	5	062	68.52
1.3580	2	162	69.11
1.3534	11	820,561	69.38
1.3498	5	651	69.59
1.3225	6	660	71.24
1.3184	4	471	71.50
1.3145	4	542	71.74
1.3101	10	741	72.02
1.3062	5	811	72.27
1.2950	6	281	72.99
1.2828	4	213	73.81
1.2587	4	223	75.46
1.2554	3	661	75.69
1.2482	10	190	76.21
1.2425	2	571	76.62
1.2310	1	910	77.47
1.2250	3	290	77.92
1.2145	4	722	78.72
1.2014	5	481,043	79.75
1.1938	3	143,580	80.36
1.1909	3	191	80.60
1.1880	7	372	80.83
1.1861	3	850,333	80.99
1.1830	4	901	81.25
1.1766	2	930,911	81.78
1.1656	4	671	82.73
1.1449	3	490	84.56
1.1432	8	472,581	84.72
1.1406	6	433,802	84.95
1.1380	2	153	85.19
1.1246	2	680	86.46
1.1093	1	10·1·0	87.95

Internal standard W, a = 3.16504 Å
CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.1079	4	2·10·0	88.09
1.1006	5	382,491	88.83
1.0940	1	590,10·2·0	89.50
1.0875	5	0·10·1	90.19
1.0823	2	681	90.74
1.0794	2	163	91.06
1.0570	6	192,780	93.55
1.0548	2	10·2·1	93.81
1.0475	2	912,4·10·0	94.67
1.0436	2	292,3·10·1	95.14
1.0410	1	363	95.45
1.0374	2	10·4·0	95.89
1.0350	2	960	96.18
1.0324	4	10·3·1	96.50
1.0236	1	582	97.61
1.0213	5	781,392	97.91
1.0196	5	871,703	98.13
1.0131	3	932	98.98
1.0106	4	463,2·11·0	99.31
1.0082	5	273	99.63
1.0040	2	10·4·1	100.20
1.0016	3	961	100.53
0.9953	2	004	101.41
.9926	5	492	101.79
.9910	2	1·11·1	102.02
.9862	2	790	102.71
.9830	2	970	103.18
.9823	1	0·10·2,11·0·1	103.28
.9794	3	2·11·1	103.71
.9767	3	124,862	104.12
.9761	3	214	104.21
.9695	2	10·5·1,10·1·2	105.21
.9681	3	11·2·1,2·10·2	105.43
.9612	6	3·11·1	106.51
.9590	4	743,592	106.87
.9542	3	971,11·4·0	107.65
.9480	1	234	108.68
.9420	1	10·3·2,0·12·0	109.70
.9385	5	1·12·0,6·10·1	110.31
.9369	3	663,4·11·1	110.60
.9336	1	782	111.19
.9314	3	573,980,+	111.58
.9258	2	12·1·0,244	112.60
.9250	2	11·5·0	112.75
.9184	1	962	114.00
.9168	4	12·2·0	114.31
.9011	4	11·5·1,2·11·2	117.48
.8995	5	5·10·2	117.81
.8982	5	7·10·1	118.09
.8933	2	10·5·2,12·2·1	119.14

Bismuth Sulfide (bismuthinite), Bi_2S_3 (orthorhombic) (revised)—continued

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
0.8865	1	3·11·2	120.37
.8845	2	354,853	121.10
.8826	3	12·4·0	121.56
.8800	1	064,12·3·1	122.16
.8774	1	8·10·0,604,+	122.78
.8710	1	11·6·1	124.33
.8678	2	4·11·2,520	125.13
.8670	4	624,493	125.35
.8605	3	11·4·2,0·10·3	127.04
.8583	3	11·7·0	127.64
.8575	3	1·10·3,8·10·1	127.87
.8515	1	10·1·3,0·12·2	129.52
.8490	1	1·12·2	130.24
.8480	3	13·2·0	130.56
.8471	4	1·13·1	130.80
.8420	1	12·0·2	132.34
.8417	1	714,2·12·2	132.44
.8402	1	12·5·1	132.92
.8398	2	6·12·0,12·1·2	133.02
.8384	3	13·0·1	133.45
.8364	2	7·10·2,13·3·0	134.11
.8350	3	9·10·0	134.57
.8337	2	10·9·0	134.99
.8327	2	12·2·2,10·3·3	135.35
.8303	5	4·13·0	136.16
.8294	5	3·12·2,13·2·1	136.46
.8281	2	3·13·1	136.92
.8273	4	8·11·0	137.21
.8260	3	374,873	137.64
.8222	2	4·10·3	139.03
.8200	2	6·11·2	140.01
.8162	4	963,10·9·1	141.36
.8127	2	4·13·1	142.79
.8105	3	7·12·0,474	143.72
.8070	3	0·14·0,12·4·2	145.30
.8054	3	11·0·3,12·7·0	146.01
.8035	2	11·1·3,8·10·2,+	146.94
.7964	2	14·0·0	150.55
.7955	3	664,5·12·2	151.07
.7939	5	105,10·10·0	151.97
.7893	2	973,12·7·1	154.74
.7890	1	1·14·1,12·5·2	154.98
.7884	2	14·2·0,2·13·2,+	155.37
.7864	3	125,215	156.70
.7836	3	2·14·1	158.82
.7802	2	8·12·0,13·2·2	161.67

Cadmium Chromite, $CdCr_2O_4$ (cubic)

Powder Diffraction File cards. No. 2-1000, Holgersson (1930).

Additional published patterns. None.

NBS sample. The sample of cadmium chromite was prepared at NBS from cadmium oxide and chromium trioxide, dried before weighing, and heated in vacuum at 300°C for 17 hrs. The substance was ground, compressed into a pellet, and heated at 1050°C for 1 and 1/2 hrs.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium and magnesium, and 0.001 to 0.01 percent each of aluminum, barium, copper, iron, manganese, nickel, antimony, and silicon.

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

$I/I_{corundum} = 2.8$.

Structural data. Holgersson (1930) determined that cadmium chromite has the spinel structure with the space group O_h^7-Fd3m (No. 227) and 8($CdCr_2O_4$) per unit cell.

Lattice constants

	a(Å)
Holgersson (1930)	8.61
Krause and Thiel (1934)	8.59
Verwey and Heilmann (1947)	8.584
NBS, sample at 25°C	8.597

The density of cadmium chromite calculated from the NBS lattice constants is 5.862 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
4.959	3	111	17.87
3.036	74	220	29.39
2.589	100	311	34.61
2.480	4	222	36.19
2.146	2	400	42.06
1.972	6	331	45.98
1.755	22	422	52.08
1.654	32	511	55.50
1.519	30	440	60.93
1.3592	7	620	69.04
1.3107	9	533	71.98
1.2956	2	622	72.95
1.1486	10	642	84.23
1.1188	12	731	87.02
1.0745	3	800	91.59
1.0131	4	822	98.98
0.9926	8	751	101.79
.9164	3	664	114.38
.9012	6	931	117.44
.8775	8	844	122.75
.8311	8	951	135.88

References

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Krause, O. and Thiel, W. (1934). Über Keramische Farbkörper I, Ber. deut. keram. Ges. 15, 101-110.

Verwey, E. J. W. and Heilmann, E. L. (1947). Physical properties and cation arrangement of oxides with spinel structures, J. Chem. Phys. 15, 174-180.

Calcium Magnesium Silicate (diopside), $CaMg(SiO_3)_2$ (monoclinic)

Powder Diffraction File cards. No. 3-0860 (synthetic), Clark (1946) and No. 11-654 (natural), deWolff (1961).

Additional published patterns. Kuno and Hess (1953).

NBS sample. The sample of diopside was obtained from Tem-pres Research Inc., State College, Pa.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of aluminum, nickel, and strontium; and 0.01 to 0.1 percent each of iron, sodium, and titanium.

The sample was colorless and optically positive with indices of refraction N_α = 1.674, N_β = 1.680, and N_γ = 1.700. 2V is medium.

$I/I_{corundum}$ = 1.0.

Structural data. Wyckoff and Merwin (1925) determined that diopside has the space group C^6_{2h}-C2/c (No. 15) and 4 [$CaMg(SiO_3)_2$] per unit cell.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.462	5	020	19.88
4.407	1	$\bar{1}11$	20.13
3.660	3	111	24.30
3.343	11	021	26.64
3.231	28	220	27.58
2.992	100	$\bar{2}21$	29.84
2.951	32	310	30.26
2.894	42	$\bar{3}11$	30.87
2.838	3	130	31.50
2.566	25	$\bar{1}31$	34.93
2.524	64	002	35.53
2.518		$\bar{1}12$,221	35.63
2.389	3	131	37.61
2.301	16	311	39.12
2.215	13	112	40.70
2.198	13	$\bar{2}22$,022	41.02
2.156	12	330	41.87
2.133	18	$\bar{3}31$	42.34
2.108	10	$\bar{4}21$	42.86
2.075	1	420	43.57
2.042	19	041	44.33
2.014	14	240,$\bar{4}02$	44.97
2.006	10	202	45.15
1.968	8	$\bar{1}32$	46.07
1.860	3	331	48.93
1.835	9	510,$\bar{4}22$	49.64
1.831		222	49.76
1.813	3	132	50.29
1.774	2	421	51.46
1.754	13	150	52.10
1.720	2	$\bar{5}12$	53.22
1.684	2	$\bar{1}51$	54.45
1.673	6	042,$\bar{2}42$	54.83
1.658	6	$\bar{3}13$	55.37
1.624	33	$\bar{5}31$,$\bar{2}23$	56.61
1.617		440	56.90
1.586	1	530	58.11
1.562	3	600	59.08
1.550	5	350	59.59
1.529	3	$\bar{6}02$	60.49
1.523	6	402	60.75
1.5096	2	$\bar{5}32$	61.36
1.5034	11	$\bar{1}33$	61.64
1.4918	2	242	62.17
1.4877	5	060	62.36
1.4750	1	620	62.96
1.4609	2	441	63.64
1.4469	3	$\bar{6}22$	64.33
1.4267	8	061	65.35
1.4225	17	531	65.57

References

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

Futergendler, S.I. (1958). X-ray study of solid inclusions in diamonds, Soviet Phys.-Cryst. 3, 494.

Kuno, H. and Hess, H.H. (1953). Unit cell dimensions of clinoenstatite and pigeonite in relation to other common clinopyroxenes, Am. J. Sci. 251, 741-752.

Wyckoff, R.W.G. and Merwin, H.E. (1925). The space group of diopside [$CaMg(SiO_3)_2$], Am. J. Sci. 9, 379-394.

Calcium Magnesium Silicate (diopside), $CaMg(SiO_3)_2$ (monoclinic)—continued

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
1.4086	10	$\bar{3}52$	66.30
1.4072		152	66.37
1.3895	3	223	67.33
1.3755	2	$\bar{7}11$	68.11
1.3439	1	043	69.94
1.3305	7	$\bar{7}12$	70.75
1.3269	7	621,512	70.97
1.3168	3	$\bar{5}33$	71.60
1.2824	7	$\bar{2}62$,062	73.83
1.2624	5	$\bar{4}61$,004	75.20
1.2480	4	352	76.22
1.2362	2	$\bar{1}71$	77.08
1.2222	1	532	78.13
1.2174	2	$\bar{4}24$	78.50
1.2147	2	171,024	78.71

Lattice constants

	a(Å)	*b(Å)*	*c(Å)*	*β(°)*
Wyckoff and Merwin (1925)	9.73	8.91	5.25	105.83°
Kuno and Hess (1953)	9.731	8.930	5.249	105.43°
Futergendler (1958)	9.70	8.91	5.22	105°
deWolff (1961)	9.761	8.926	5.258	105.79°
NBS, sample at 25°C	9.748	8.926	5.250	105.86°

The density of diopside calculated from the NBS lattice constants is 3.273 g/cm^3 at 25° C.

Cesium Cadmium Trichloride, CsCdCl (hexagonal)

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium cadmium trichloride was made at NBS by fusing stoichiometric amounts of cesium chloride and cadmium chloride.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent sodium, and 0.01 to 0.1 percent each of barium, calcium, potassium, rubidium, and strontium.

The sample was colorless. It was optically positive with indices of refraction $N_o = 1.737$ and $N_e = 1.750$.

$I/I_{corundum} = 2.6$.

Structural data. Siegel and Gebert (1964) determined that cesium cadmium trichloride has the hexagonal barium titanate structure, the space group D^4_{6h}-$P6_3/mmc$ (No. 194) and 6($CsCdCl_3$) per unit cell. Ferrari and Baroni (1927) reported that there also exists a pseudocubic perovskite form of cesium cadmium trichloride.

Lattice constants

	a(Å)	c(Å)
Siegel and Gebert (1964)	7.418	18.39
NBS, sample at 25°C	7.416	18.440

The density of cesium cadmium trichloride calculated from the NBS lattice constants is 3.989 g/cm^3 at 25°C.

Internal standard Ag, a = 4.08625 Å

CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.070	18	101	14.58
5.266	4	102	16.82
4.440	20	103	19.98
3.743	92	104	23.75
3.708	100	110	23.98
3.198	19	105	27.87
3.072	9	006	29.04
3.032	11	202	29.43
2.846	35	203	31.40
2.635	62	204	33.99
2.438	12	107	36.84
2.422	18	205	37.08
2.259	4	213	39.88
2.170	6	108	41.58
2.147	30	214	42.04
2.142	33	300	42.16
2.037	10	207	44.43
2.027	12	215	44.66
1.958	5	118	46.33
1.952	4	109	46.48
1.873	14	208	48.57
1.853	24	220	49.11
1.785	8	217	51.12
1.774	3	311	51.48
1.727	8	209	52.98
1.710	2	313	53.53
1.672	6	218	54.88
1.6614	8	314,307	55.24
1.6218	2	1·0·11	56.71
1.6034	4	315	57.42
1.5880	3	226	58.03
1.5652	4	219	58.96
1.5530	4	403	59.47
1.5370	4	0·0·12	60.15
1.5158	7	404	61.08
1.4752	5	317	62.95
1.4721	6	405	63.10
1.4324	2	323	65.06
1.4200	5	1·11·2	65.70
1.4095	3	318	66.25

References

Ferrari, A. and Baroni, A. (1927). On the crystalline structure of the double chloride of cadmium and cesium ($CsCdCl_3$), Atti accad. nazl. Lincei Rend. Classe sci. fis. mat. e nat. 6, 418.

Siegel, S. and Gebert, E. (1964). The structure of hexagonal $CsCdCl_3$ and tetragonal Cs_2CdCl_4, Acta Cryst. 17, 790.

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.4015	9	410	66.68
1.3794	3	2·1·11	67.89
1.3712	3	407	68.35
1.3679	3	325	68.54
1.3446	3	319	69.90
1.3410	2	414	70.11
1.3177	3	408	71.54
1.2860	1	327	73.59
1.2636	3	409	75.11
1.2482	6	3·0·12	76.21
1.2412	3	328	76.71
1.2373	4	504,417	77.00
1.2205	2	3·1·11	78.26
1.1961	3	329	80.18
1.1906	3	423	80.62
1.1830	6	2·2·12	81.25
1.1737	5	424	82.03
1.1528	4	425	83.85

Cesium Calcium Trichloride, $CsCaCl_3$ (cubic)

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium calcium trichloride was prepared by fusing cesium chloride and anhydrous calcium chloride at approximately 900°C.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent strontium; and 0.01 to 0.1 percent each of potassium, sodium, and rubidium.

$I/I_{corundum} = 3.8$.

The sample was colorless. The index of refraction was 1.599.

Structural data. No structural information was found in the literature on cesium calcium trichloride; however it appears to be cubic and similar to other perovskites, with the space group O_h^1-Pm3m (No. 221) and 1 ($CsCaCl_3$) per unit cell.

This material gave x-ray patterns which showed no splitting and can be considered fully cubic at 25°C.

Lattice constants

	a(Å)
NBS, sample at 25°C	5.396

The density of cesium calcium trichloride calculated from the NBS lattice constant is 2.952 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.394	15	100	16.42
3.819	100	110	23.27
3.115	71	111	28.63
2.698	78	200	33.17
2.413	7	210	37.23
2.203	33	211	40.92
1.908	30	220	47.62
1.798	2	300	50.72
1.706	11	310	53.67
1.627	12	311	56.53
1.538	8	222	59.27
1.497	2	320	61.95
1.4421	9	321	64.56
1.3486	2	400	69.66
1.3085	2	410	72.72
1.2717	3	411	74.55
1.2380	2	331	76.95
1.2063	6	420	79.36
1.1505	2	332	84.05
1.1016	4	422	88.73
1.0794	2	500	91.06
1.0583	3	510	93.41
1.0387	2	511	95.73
0.9852	<1	521	102.85
.9538	<1	440	107.72
.9255	<1	530	112.66
.9119	1	531	115.27
.8993	<1	600	117.85
.8755	<1	611	123.23
.8532	<1	620	129.05
.8327	<1	541	135.35
.8227	<1	533	138.86
.8136	<1	622	142.43

Cesium Copper(II) Trichloride, $CsCuCl_3$ (hexagonal)

Powder diffraction cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium copper trichloride was crystallized from an aqueous solution of cesium chloride and cupric chloride. The crystals formed as dark red hexagonal prisms terminated by bipyramids.

Spectrographic analysis showed the major impurities to be 0.01 to 0.1 percent of barium and 0.001 to 0.01 percent each of aluminum, calcium, chromium, iron, potassium, magnesium, manganese, sodium, nickel, rubidium, silicon and strontium.

The color of the sample was very dark red when unground and dark orange yellow when ground. In the petrographic microscope the sample was strongly dichroic, being brownish red for vibrations along c and yellowish for vibrations perpendicular to c. The crystals were uniaxial positive with $N_o = 1.75$ and $N_e = 1.885$.

$I/I_{corundum} = 3.0$.

Structure data. Wells (1947) determined that cesium copper trichloride is hexagonal with the space group D_6^2-$P6_122$ (No. 178) and 6($CsCuCl_3$) per unit cell.

Lattice constants

	a(Å)	c(Å)
Klug and Sears (1946)	7.189	18.06
Wells (1947)	7.20	18.00
NBS, sample at 25°C	7.2165	18.180
	±0.0004	± 0.002

The density of cesium copper trichloride calculated from the NBS lattice constants is 3.679 g/cm³ at 25°C.

References

Klug, H.P. and Sears, G.W. (1946). A crystal-chemical study of cesium trichlorocuprate, J. Am. Chem. Soc. 68, 1133.

Wells, A.F. (1947). The crystal structure of $CsCuCl_3$ and the crystal chemistry of complex halides ABX_3, J. Chem. Soc. (London) 1947, 1662.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.249	15	100	14.16
5.909	7	101	14.98
4.354	75	103	20.38
3.676	9	104	24.19
3.608	88	110	24.65
3.541	12	111	25.13
3.146	7	105	28.34
3.126	10	200	28.53
3.078	8	201	28.98
3.032	25	006	29.43
2.956	17	202	30.21
2.777	100	203	32.21
2.726	29	106	32.82
2.576	8	204	34.80
2.369	9	205	37.95
2.319	5	116	38.79
2.286	4	212	39.38
2.200	17	213	40.98
2.175	25	206	41.49
2.095	2	214	43.14
2.082	10	300	43.42
2.070	7	301	43.69
2.031	3	302	44.58
1.998	7	207	45.36
1.981	6	215	45.76
1.922	6	109	47.24
1.863	11	216	48.83
1.805	16	220	50.52
1.795	15	221	50.81
1.770	3	222	51.59
1.747	4	217	52.31
1.730	2	223	52.89
1.702	11	312	53.80
1.697	11	209	53.99
1.666	7	313	55.08
1.6163	2	225	56.92
1.5642	5	315	59.00
1.5501	6	226	59.59
1.5396	6	402	60.04
1.5356	5	308	60.21
1.5145	3	0·0·12	61.14
1.5127	7	403	61.22
1.5040	6	316	61.61
1.4777	6	404	62.83
1.4421	2	317	64.57

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	I	hkl	2θ(°)
1.4298	3	321	65.19
1.4163	2	322	65.89
1.3966	5	1·1·12	66.94
1.3882	5	406	67.40
1.3677	4	324	68.55
1.3637	4	410	68.78
1.3599	5	411	69.00
1.3150	5	319	71.71

Cesium Lead(II) Trichloride, $CsPbCl_3$ (tetragonal)

Powder diffraction cards. None.

Additional published patterns. Møller (1959).

NBS sample. The sample of cesium lead trichloride was prepared at NBS by fusion of cesium chloride and lead chloride at about 500° C. Spectrographic analysis showed the major impurities to be 0.01 to 0.1 percent of potassium and 0.001 to 0.01 percent each of aluminum, barium, calcium, lithium, manganese, sodium, rubidium, silicon and strontium.

The color of the sample was yellow white. Cesium lead trichloride has a very low double refraction. The indices were both near 1.930.

$I/I_{corundum} = 8.3$.

Structural data. Møller (1959) determined that cesium lead trichloride at room temperature has a distorted perovskite structure, with the tetragonal space group C^1_{4v}-P4mm (No. 99) and 1 ($CsPbCl_3$) per unit cell. It was also found to go through a readily reversible inversion at 46.9°C, above which it had a cubic pervoskite structure with a = 5.605Å.

Lattice constants

	a(Å)	*c(Å)*
Møller (1959)	5.590	5.630
NBS, sample at 25°C	5.584 ±0.001	5.623 ±0.001

The density of cesium lead trichloride calculated from the NBS lattice constants is 4.224 g/cm^3 at 25° C.

Reference

Møller, C. K. (1959). The structure of perovskite-like cesium plumbo-trihalides, Kgl. Danske Videnskab. Selskab, Mat. fys. Medd. 32 No. 2.

Internal standard W, a = 3.16504 Å

CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
5.60	14	100,001	15.79
3.960	100	101	22.43
2.809	14	002	31.82
2.794	23	200	32.00
2.509	6	102	35.75
2.502	7	201	35.86
2.288	23	112	39.34
2.283	29	211	39.43
1.981	10	202	45.76
1.976	9	220	45.89
1.871	7	003	48.62
1.867	9	212	48.73
1.862	7	221,300	48.86
1.777	5	103	51.38
1.767	7	301,310	51.70
1.685	1	311	54.39
1.616	3	222	56.95
1.557	<1	203	59.32
1.551	<1	302	59.54
1.548	<1	320	59.67
1.4988	5	213	61.85
1.4949	7	312	62.03
1.4934	5	321	62.10
1.4056	<1	004	66.46
1.3965	<1	400	66.95
1.3563	1	322	69.21
1.3541	1	401,410	69.34
1.3245	1	114	71.12
1.3212	1	303	71.32
1.3168	2	411	71.60
1.2556	<1	204	75.68
1.2501	<1	402	76.07
1.2253	<1	214	77.90
1.2200	<1	412	78.30

Chromium Fluoride Trihydrate, $CrF_3 \cdot 3H_2O$ (monoclinic)

Powder Diffraction File cards. No. 1-0300, Hanawalt, Rinn, and Frevel (1938).

Additional published patterns. Thomas (1956).

NBS sample. The sample of chromium fluoride trihydrate was obtained from Fisher Scientific Co., Washington, D.C. The sample was recrystallized from a water solution.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium, iron, magnesium, and silicon; and 0.001 to 0.01 percent each of aluminum, manganese, nickel, and lead.

The color of the sample was deep green. Optically it appeared uniaxially positive with indices of refraction $N_\alpha \cong N_\beta = 1.448$ and $N_\gamma = 1.476$. 2V could not be measured.

$I/I_{corundum} = 2.5$.

Structural data. Through the help of A. Perloff at this laboratory, single crystal work indicates that the compound is monoclinic with the space group either C_2^3-C2 (No. 5) or C_{2h}^3-C2/m (No. 12). Visser (1964) was able to give a rhombohedral configuration for this compound. Our data was indexed on both the monoclinic cell and the pseudo-hexagonal cell.

The density of chromium fluoride trihydrate calculated from the NBS lattice constants is 2.236 g/cm³ at 25 °C using $3(CrF_3 \cdot 3H_2O)$ per unit hexagonal cell or $2(CrF_3 \cdot 3H_2O)$ per unit monoclinic cell.

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Chemical analysis by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. **10**, 457-513.

Thomas, W. G. (1956). The structure of binary crystalline fluorides, Dissertation Abstr. 16, 467.

Visser, J. W. (1964). (private communication).

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl mono.	hkl hex.	2θ(°)
4.704	100	020,111	110	18.85
4.101	60	$\bar{1}11$,001	101	21.65
3.091	4	021,$\bar{2}01$	021	28.86
2.581	53	$\bar{2}21$,111	211	34.27
2.350	2	040,220,+	220	38.27
2.278	2	$\bar{1}12$,$\bar{2}02$	012	39.52
2.050	8	$\bar{2}22$,002	202	44.15
1.879	25	$\bar{3}12$,022	122	48.40
1.871	22	$\bar{2}41$,201	401	48.61
1.777	9	150,240	410	51.38
1.738	8	$\bar{3}31$,221	321	52.60
1.636	14	$\bar{3}32$,112	312	56.18
1.567	4	060,330	330	58.87
1.545	4	042	042	59.80
1.541	2	151,$\bar{4}01$	051	59.98
1.4988	4	$\bar{3}13$,$\bar{1}13$,+	113	61.85
1.4675	5	$\bar{1}52$,132,+	232	63.32
1.4638	4	061,241	241	63.50
1.3972	2	$\bar{3}51$,311	511	66.91
1.3663	3	$\bar{4}03$	303	68.63
1.3568	2	260,400	600	69.18
1.3422	1	202	502	70.04
1.3122	2	$\bar{4}23$	223	71.89
1.3035	4	350,420	520	72.44
1.2907	2	$\bar{3}42$,222	422	73.28
1.2450	2	152	152	76.44
1.2013	2	261,$\bar{5}11$	161	79.76
1.1811	3	$\bar{4}43$,113,+	413	81.41
1.1738	2	$\bar{3}14$,$\bar{2}04$	104	82.02
1.1655	2	$\bar{5}32$	342	82.73
1.1389	2	$\bar{1}81$,$\bar{4}04$	024	85.11
1.1297	2	$\bar{3}71$,351,+	351	85.97
1.1136	2	$\bar{2}63$,133,+	333	87.53

Lattice constants

	a(Å)	b(Å)	c(Å)	β(°)
Thomas* (hex.) (1956)	5.41	---	8.31	---
NBS, sample at 25°C (hex.)	9.402	---	4.745	---
NBS, sample at 25°C (mono.)	6.281	9.404	4.745	120.24°

*proposed cell does not index pattern.

Cobalt Antimony Oxide, $CoSb_2O_6$ (tetragonal)

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of cobalt antimony oxide was prepared at NBS by heating a mixture of cobalt oxalate and antimony pentoxide for 1/2 hour at 1000°C on a gold boat.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of chromium, iron, nickel, and silicon; and 0.001 to 0.01 percent each of aluminum, barium, calcium, copper, manganese, molybdenum, vanadium, and zinc.

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

$I/I_{corundum} = 2.5.$

Structural data. Byström, Hök, and Mason (1941) determined that cobalt antimony oxide is isomorphous with zinc antimony oxide, with the space group D_{4h}^{14}-$P4_2/mnm$ (No. 136) and 2 ($CoSb_2O_6$) per unit cell.

Lattice constants

	a(Å)	c(Å)
Byström, Hök, and Mason (1941)	4.65	9.27
NBS, sample at 25°C	4.6539	9.283

The density of cobalt antimony oxide calculated from the NBS lattice constants is 6.581 g/cm³ at 25°C.

References

Byström, A., B. Hök, and B. Mason (1941). The crystal structure of zinc metantimonate and similar compounds, Arkiv Kemi, Mineral. Geol. **15B**, No. 4, 1-8.

Internal standard Ag, a = 4.08625 Å
CuKα$_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.643	9	002	19.10
4.164	16	101	21.32
3.292	100	110	27.06
2.686	5	112	33.33
2.576	77	103	34.80
2.328	20	200	38.65
2.254	7	113	39.96
2.081	5	210,202	43.44
2.031	6	211	44.58
1.897	2	114	47.91
1.726	62	213	53.00
1.645	19	220,204	55.84
1.547	8	006	59.73
1.529	2	301	60.49
1.472	15	310	63.12
1.4000	16	116	66.76
1.3864	20	303	67.50
1.3422	1	224	70.04
1.2882	6	206	73.44
1.2784	2	321	74.10
1.2754	2	107	74.30
1.2436	2	322	76.53
1.2417	2	216	76.68
1.1914	13	323	80.56
1.1635	3	400	82.91
1.1272	9	226	86.21
1.1207	1	411	86.83
1.0973	4	330	89.17
1.0663	10	316	92.50
1.0606	10	413	93.15
1.0408	5	420	95.47
1.0155	<1	422	98.66
1.0070	4	109	99.80
0.9917	<1	334	101.91
.9840	<1	119	103.02
.9646	<1	415	105.98
.9484	2	228	108.61
.9298	6	406	111.87
.9241	12	219	112.93
.9127	5	510,432	115.11
.9112	3	318	115.40
.8949	6	336	118.80
.8913	10	503	119.58
.8635	7	426	126.26
.8589	6	309	127.47
.8322	10	523	135.49
.8227	2	440	138.87
.8057	6	329	145.87
.7981	5	530	149.64
.7861	9	516	156.96

Copper Antimony Oxide, $CuSb_2O_6$ (monoclinic)

Powder Diffraction File cards. None.

Additional published patterns. Byström, Hök, and Mason (1941).

NBS sample. The sample of copper antimony oxide was prepared at NBS by a solid state reaction of cupric oxide and antimony pentoxide in a silver boat at 945°C in vacuum for 2 hours.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, calcium, nickel, silicon, and zinc, and 0.001 to 0.01 percent each of silver, barium, chromium, iron, magnesium, and lead.

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

$I/I_{corundum} = 4.5$.

Structural data. Byström, Hök, and Mason (1941) determined that copper antimony oxide has a deformed trirutile structure, the space group C_{2h}^{5}-$P2_1/n$ (No. 14), and $2(CuSb_2O_6)$ per unit cell.

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Byström, et.al. (1941)	4.63	4.63	9.30	91.55°
NBS, sample at 25°C	4.6359	4.6339	9.294	91.14°

The density of copper antimony oxide calculated from the NBS lattice constants is 6.704 g/cm³ at 25°C.

Internal standard Ag, a = 4.08625 Å
CuKα$_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.650	7	002	19.07
4.185	7	$\bar{1}01$	21.21
4.152	9	011	21.38
4.120	6	101	21.55
3.274	100	110	27.21
2.694	2	$\bar{1}12$	33.23
2.660	2	112	33.67
2.599	19	$\bar{1}03$	34.48
2.576	37	013	34.80
2.552	17	103	35.13
2.317	21	200,020	38.83
2.266	3	$\bar{1}13$	39.74
2.247	1	021	40.09
2.236	3	113	40.29
2.073	4	022	43.63
2.057	1	202	43.98
2.027	2	$\bar{1}21$	44.66
2.019	2	121	44.85
2.015	2	211	44.95
1.909	1	$\bar{1}14,\bar{2}12$	47.60
1.885	<1	122	48.23
1.736	17	$\bar{2}13,\bar{1}05$	52.68
1.730	19	$\bar{1}23$	52.88
1.715	17	123	53.38
1.709	16	213	53.59
1.638	15	220	56.08
1.549	8	006	59.63
1.539	1	124	60.06
1.524	1	031	60.72
1.518	1	301	60.98
1.4656	15	310	63.41
1.4078	6	$\bar{1}16$	66.34
1.3998	2	$\bar{1}32$	66.77
1.3928	11	116	67.15
1.3826	8	033	67.71
1.3714	5	215,303	68.34
1.3305	1	224	70.75
1.2995	3	$\bar{2}06$	72.70
1.2876	3	026	73.48
1.2759	2	$\bar{3}21$,206	74.27
1.1940	4	$\bar{3}23$	80.35
1.1916	5	$\bar{2}33$	80.54
1.1825	5	233	81.29
1.1586	5	400,040	83.34
1.1334	6	$\bar{2}26,\bar{3}24$	85.62

Reference

Byström, A., Hök, B. and Mason, B. (1941). The crystal structure of zinc metantimonate and similar compounds, Arkiv Kemi, Mineral. Geol. 15B, No. 4, 1-8.

Copper Antimony Oxide, $CuSb_2O_6$ (monoclinic)—continued

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.1179	5	226	87.10
1.0924	6	330	89.68
1.0747	4	$\bar{3}16$	91.57
1.0680	4	$\bar{1}36$	92.31
1.0629	5	$\bar{2}35$	92.88
1.0614	5	136	93.05
1.0585	6	$\bar{1}43$	93.38
1.0551	8	316	93.78
1.0502	5	413	94.35
1.0363	8	420,044	96.02

Erbium Vanadate, $ErVO_4$ (tetragonal)

Powder Diffraction File cards. None.

Additional published patterns. Milligan, Watt, and Rachford (1949).

NBS sample. The sample of erbium vanadate was prepared at NBS. A mixture of erbium oxalate and vanadium pentoxide was heated at 1100°C for 30 minutes.

Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, magnesium, and silicon.

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

$I/I_{corundum} = 3.1$.

Structural data. Milligan, Watt, and Rachford (1949) determined that erbium vanadate has the zircon structure with the space group D_{4h}^{19}-$I4_1/amd$ (No. 141) and $4(ErVO_4)$ per unit cell.

Lattice constants

	a(Å)	*c*(Å)
Milligan, Watt, and Rachford (1949)	7.06*	6.24
NBS, sample at 25°C	7.0975	6.2723

*contains 25% yttrium

The density of erbium vanadate calculated from the NBS lattice constants is 5.932 g/cm^3 at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
4.704	38	101	18.85
3.549	100	200	25.07
2.832	12	211	31.56
2.660	70	112	33.67
2.510	22	220	35.74
2.3504	5	202	38.26
2.2134	18	301	40.73
2.0060	12	103	45.16
1.8783	12	321	48.42
1.8250	58	312	49.93
1.7746	18	400	51.45
1.7461	4	213	52.35
1.6600	4	411	55.29
1.5868	12	420	58.08
1.5676	6	004	58.86
1.4758	15	332	62.92
1.4339	14	204	64.98
1.3842	5	501	67.62
1.3295	12	224	70.81
1.2720	12	512	74.53
1.2546	3	440	75.75
1.1825	5	600	81.29
1.1746	7	404,503	81.95
1.1664	3	215	82.65
1.1471	2	611	84.36
1.1345	8	532	85.52
1.1221	5	620	86.70
1.1154	10	424	87.35
1.0580	2	325	93.44
1.0434	1	631	95.16
1.0234	4	116	97.63
1.0190	2	613	98.21
1.0136	2	415	98.91
0.9841	3	640	103.01
.9797	4	444,543	103.66
.9634	1	721	106.17
.9560	6	712	107.35
.9478	5	316	108.71
.9443	4	604,633	109.31
.9398	2	505	110.08
.9126	6	624,703	115.14
.8933	5	732	119.15
.8870	3	800	120.55
.8718	1	811	124.13
.8623	1	217	126.57
.8605	2	820	127.05
.8450	<1	714	131.45
.8359	7	660,516	134.27
.8335	8	644,653	135.06
.7979	5	752	149.75
.7931	6	840,536	152.45

Reference

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X ray diffraction studies of heavy metal orthovanadates, J. Phys. & Colloid Chem. 53, 227-234.

Gadolinium Vanadate, $GdVO_4$ (tetragonal)

Powder Diffraction File cards. None.

Additional published patterns. Milligan, Watt, and Rachford (1949), and Nautov (1962).

NBS sample. The sample of gadolinium vanadate was prepared at NBS. A mixture of gadolinium oxalate and vanadium pentoxide was heated at 800°C for 15 minutes.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, copper, and iron.

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

$I/I_{corundum} = 3.1$.

Structural data. Milligan, Watt, and Rachford (1949) determined that gadolinium vanadate has the zircon structure with the space group D_{4h}^{19}-$I4_1/amd$ (No. 141) and $4(GdVO_4)$ per unit cell.

Lattice constants

	a(Å)	*c(Å)*
Milligan, Watt, and Rachford (1949)	7.19	6.33
Nautov (1962)	7.196	6.345
NBS, sample at 25°C	7.2126	6.3483

The density of gadolinium vanadate calculated from the NBS lattice constants is 5.474 g/cm³ at 25°C.

References

Milligan, W.O., Watt, L.M., and Rachford, H.H., Jr. (1949). X-ray diffraction studies of heavy metal orthovanadates, J. Phys. & Colloid Chem. 53, 227-234.

Nautov, V.A. (1962). X-ray study of scandium, yttrium, cerium, neodymium, and gadolinium orthovanadates, Zh. Strukt. Khim. 3, 608-611.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
4.766	28	101	18.60
3.606	100	200	24.67
2.874	12	211	31.09
2.694	76	112	33.22
2.551	23	220	35.15
2.383	4	202	37.71
2.2482	12	301	40.07
2.0303	10	103	44.59
1.9083	12	321	47.61
1.8520	56	312	49.15
1.8030	16	400	50.58
1.7694	5	213	51.61
1.6865	4	411	54.35
1.6127	12	420	57.06
1.5876	5	004	58.05
1.4986	16	332	61.86
1.4527	14	204	64.04
1.4067	6	501	66.40
1.3476	10	224	69.72
1.2922	12	512	73.18
1.2750	2	440	74.33
1.2020	6	600	79.70
1.1915	8	404,503	80.55
1.1813	4	215	81.39
1.1656	3	611	82.73
1.1527	10	532	83.86
1.1404	6	620	84.97
1.1313	10	424,523	85.82
1.0602	4	631	93.19
1.0361	8	116	96.04
1.0004	5	640	100.70
0.9942	6	543,444	101.57
.9711	8	712	104.97
.9599	4	316	106.72
.9531	4	505	107.83
.9261	6	703,624	112.55
.9077	6	732	116.12
.8472	8	516	130.78
.8107	6	752	143.65
.8040	10	536	146.66
.7840	6	833,804	158.54

Iron(II,III) Oxide (magnetite), Fe_3O_4(cubic)

Powder diffraction card. No. 11-614, Basta (1957).

Additional published patterns. Holgersson (1927), Jung and Köhler (1930), and Hanawalt, Rinn, and Frevel (1938).

NBS sample. The sample of iron(II,III) oxide was obtained from the Columbian Carbon Co., New York 17, N.Y.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent cobalt and 0.001 to 0.01 percent each of silver, aluminum, magnesium, manganese, molybdenum, nickel, silicon, titanium, and zinc.

The sample was a black opaque powder.

$I/I_{corundum} = 4.9$.

Structural data. Bragg (1915) determined that iron(II,III) oxide has the spinel structure, the space group O_h^7-Fd3m (No. 227) and 8(Fe_3O_4) per unit cell.

Lattice constants

	a(Å)
Goldschmidt (1942)	8.43
Lindroth (1946)	8.416
Mason (1947)	8.398
Pouillard (1950)	8.413
Tombs and Rooksby (1951), sample at 22°C	8.3940
Abrahams and Calhoun (1953) sample at 22°C	8.3940
Yearian et al. (1954) metal rich	8.396
Yearian et al. (1954) oxygen rich	8.390
Radavich (1955)	8.394
Basta (1957), sample at 18°C	8.3963
NBS, sample at 25°C	8.396

The density of iron(II,III) oxide calculated from the NBS lattice constant is 5.197 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C				
d (Å)	I	hkl	2θ(°)	a (Å)
4.852	8	111	18.27	8.40
2.967	28	220	30.09	8.393
2.532	100	311	35.42	8.398
2.4243	7	222	37.05	8.398
2.0993	21	400	43.05	8.397
1.7146	10	422	53.39	8.400
1.6158	27	511	56.94	8.396
1.4845	41	440	62.51	8.398
1.4192	2	531	65.74	8.396
1.3277	4	620	70.92	8.397
1.2807	9	533	73.95	8.398
1.2659	4	622	74.96	8.397
1.2119	2	444	78.93	8.396
1.1221	3	642	86.70	8.397
1.0930	12	731	89.61	8.396
1.0496	5	800	94.42	8.397
0.9896	2	822	102.21	8.397
.9695	6	751	105.21	8.396
.9632	3	662	106.20	8.397
.9388	3	840	110.27	8.397
.8952	2	664	118.73	8.398
.8802	5	931	122.09	8.397
.8569	7	844	128.03	8.396
.8233	3	10.2.0	138.63	8.396
.8117	6	951	143.23	8.396
.8080	4	10.2.2	144.82	8.397

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Lead Oxybromide, $Pb_3O_2Br_2$ (orthorhombic)

Powder Diffraction File cards. No. 6-0330, Lamb and Niebylski (1953), and No. 6-0412, Thornton Research Centre, The Shell Petroleum Co., Ltd. (1954).

Additional published patterns. None.

NBS sample. The sample of lead oxybromide was prepared at NBS from red lead monoxide and lead bromide. A stoichiometric mixture was placed on gold leaf, sealed in an evacuated tube, and heated 3/4 hr. at 350°C.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of bismuth, molybdenum, silicon, and strontium, and 0.001 to 0.01 percent each of alumunim, barium, calcium, chromium, copper, iron, sodium, nickel, titanium, and vanadium.

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

$I/I_{corundum} = 1.3$.

Structural data. Davies (1957) determined that lead oxybromide has the space group D_{2h}^{16}-Pbnm (No. 62), and $4(Pb_3O_2Br_2)$ per unit cell.

Lattice constants

	a(Å)	*b(Å)*	*c(Å)*
Thornton Research Centre (1954)	9.7	12.1	5.88
Davies (1957)	9.81	12.25	5.88
NBS, sample at 25°C	9.8162	12.253	5.8754

The density of lead oxybromide calculated from the NBS lattice constants is 7.645 g/cm³ at 25°C.

Internal standard Ag, a = 4.08625 Å
CuKα₁ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
7.67	54	110	11.53
5.20	23	120	17.03
4.91	7	200	18.06
4.66	2	111	19.04
4.241	6	021	20.93
3.895	39	121	22.81
3.771	3	130	23.57
3.600	48	211	24.71
3.172	75	131	28.11
3.139	64	230	28.41
2.937	95	002	30.41
2.857	92	301	31.28
2.783	40	311	32.14
2.715	100	041	32.96
2.597	9	240	34.50
2.591	9	321	34.59
2.554	13	330	35.11
2.522	3	202	35.57
2.454	4	400	36.59
2.376	11	241	37,84
2,317	2	132	38.83
2.278	7	420	39.53
2.236	28	340	40.29
2.145	43	232	42.09
2.124	7	421	42.53
2.058	4	322	43.95
2.042	6	060	44.32
2.000	4	160	45,31
1.962	5	350	46.24
1.938	10	510	46.83
1.927	9	332	47.11
1.861	7	412,351	48,90
1.842	5	511	49.44
1.833	6	123	49.69
1.822	3	441	50.03
1.800	12	422,213	50.67
1.779	29	342	51.30
1,738	9	133	52.61
1.724	9	170	53.08
1.694	16	531	54.08
1.680	18	303	54.57
1.663	14	451	55.19
1.650	20	043	55.65
1.631	7	352	56.36
1.621	8	610,323	56.73

References

Davies, P.T. (1957), An x-ray study of lead dioxybromide, Acta Cryst. **10**, 791.

Lamb, F.W. and Niebylski, L.M. (1953), Phase study of the PbO-$PbBr_2$ system by x-ray diffraction, J. Am. Chem. Soc. **75**, 511-518.

Thornton Research Centre, The Shell Petroleum Co., Ltd. (1954), **X-ray Diffraction Patterns of Lead Compounds**, 34-35.

Lead Oxybromide, $Pb_3O_2Br_2$ (orthorhombic)—continued

<table>
<tr><th colspan="4">Internal standard Ag, a = 4.08625 Å
CuKα$_1$ λ = 1.5405 Å; temp. 25 °C</th></tr>
<tr><th>d (Å)</th><th>I</th><th>hkl</th><th>2θ(°)</th></tr>
<tr><td>1.6182</td><td>9</td><td>512</td><td>56.85</td></tr>
<tr><td>1.5878</td><td>16</td><td>271</td><td>58.04</td></tr>
<tr><td>1.5637</td><td>3</td><td>243,611</td><td>59.02</td></tr>
<tr><td>1.5314</td><td>4</td><td>080</td><td>60.39</td></tr>
<tr><td>1.5265</td><td>3</td><td>621</td><td>60.61</td></tr>
<tr><td>1.5167</td><td>5</td><td>461</td><td>61.04</td></tr>
<tr><td>1.4921</td><td>3</td><td>371,362</td><td>62.16</td></tr>
<tr><td>1.4865</td><td>5</td><td>172</td><td>62.42</td></tr>
<tr><td>1.4694</td><td>11</td><td>004</td><td>63.23</td></tr>
<tr><td>1.4200</td><td>5</td><td>612</td><td>65.70</td></tr>
</table>

Lead Tungstate (stolzite), $PbWO_4$ tetragonal (revised)

Powder Diffraction File cards. No. 8-108 (natural), Claringbull and No. 8-476 (1957) National Bureau of Standards. These new NBS data are essentially the same as reported by us on card No. 8-476. However, the x-ray pattern was rerun to pick up additional weak lines which slower diffractometer scanning brought out.

NBS sample. This sample was also prepared by precipitation of solutions of lead nitrate and sodium tungstate.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, chromium, iron, and molybdenum.

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

$I/I_{corundum} = 8.3$.

Structural data. Vegard and Refsum (1928) determined that stolzite has the calcium tungstate structure, the space group C_{4h}^{6}-$I4_1/a$ (No. 88) and $4(PbWO_4)$ per unit cell. Shaw and Claringbull (1955) reported that the monoclinic lead tungstate, raspite, transforms irreversibly to stolzite at about 400°C.

Lattice constants

	a(Å)	*c(Å)*
NBS (1957), sample at 25°C	5.4616	12.046
NBS, sample at 25°C	5.4619	12.049

The density of stolzite calculated from the NBS lattice constants is 8.408 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å
CuKα₁ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
3.248	100	112	27.44
3.012	22	004	29.63
2.732	32	200	32.75
2.489	<1	202	36.05
2.395	1	211	37.52
2.376	2	114	37.83
2.205	1	105	40.89
2.087	2	213	43.31
2.024	35	204	44.73
1.931	16	220	47.01
1.838	<1	222	49.55
1.7997	<1	301	50.68
1.7820	21	116	51.22
1.6606	33	312	55.27
1.6258	16	224	56.56
1.5065	3	008	61.50
1.4175	<1	323	65.83
1.3656	4	400	68.67
1.3187	7	208	71.48
1.3093	11	316	72.07
1.2588	6	332	75.45
1.2436	5	404	76.54
1.2213	5	420	78.20
1.1876	5	228	80.87
1.1501	4	1·1·10	84.09
1.1318	7	424	85.77
1.0838	4	336	90.58
1.0547	6	512	93.82
1.0115	3	408	99.19
1.0039	1	0·0·12	100.21
0.9881	6	3·1·10	102.43
.9655	1	440	105.83
.9486	3	428	108.58
.9451	5	516	109.17
.9424	2	2·0·12	109.63
.9256	4	532	112.65
.9194	2	444	113.81
.9105	1	600	115.55
.8908	3	2·2·12	119.69
.8796	3	3·3·10	122.24
.8714	3	604	124.24
.8636	3	620	126.23
.8489	5	536	130.29
.8400	3	1·1·14	132.97
.8301	5	624	136.21
.8128	2	448	142.75
.8089	3	4·0·12	144.44
.8005	5	5·1·10	148.38
.7790	3	608	162.78

References

Swanson, H. E., Gilfrich, N. T., and Cook, M. I. (1957). Standard X-ray Diffraction Powder Patterns, Natl. Bur. Standards (U.S.) Circ. 539, No. 7, 24.

Shaw, R. and Claringbull, G. F. (1955). X ray study of raspite (monoclinic $PbWO_4$), Am. Mineralogist **40**, Nos. 9 and 10, 933.

Vegard, L. and Refsum, A. (1927). Further investigations on the structure of crystals belonging to the scheelite group, Neues Jahrb. Mineral. Geol. **1928**, Part I, 207-208.

Lithium Barium Trifluoride, $LiBaF_3$ (cubic)

Powder diffraction cards. None.

Additional published patterns. None.

NBS sample. The sample of lithium barium trifluoride was made at NBS by fusing stoichiometric amounts of anhydrous lithium and barium fluorides at approximately 800°C, and annealing at 500°C for several hours to react with the small percent of BaF_2 which formed because of the incongruent crystallization of $LiBaF_3$.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent strontium; 0.01 to 0.1 percent aluminum; and 0.001 to 0.01 percent each of iron, sodium, rubidium, silicon, and titanium.

The sample was almost colorless. The index of refraction was 1.544.

$I/I_{corundum}$ = 0.8.

Structural data. Ludekens and Welch (1952) reported that lithium barium trifluoride has an undistorted "inverted" perovskite structure with the space group O_h^1-Pm3m (No. 221) and 1 ($LiBaF_3$) per unit cell.

Lattice constants

	a(Å)
Ludekens and Welch (1952)------	3.996
NBS, sample at 25°C------------	3.9950

The density of lithium barium trifluoride calculated from the NBS lattice constant is 5.242 g/cm³ at 25°C.

Reference

Ludekens, W.L.W. and Welch, A.J.E. (1952). Reactions between metal oxides and fluorides: some new double-fluoride structures of type ABF_3, Acta Cryst 5, 841.

Internal standard W, a = 3.16504 Å
CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)	a (Å)
3.994	100	100	22.24	3.994
2.823	85	110	31.67	3.992
2.307	83	111	39.01	3.996
1.997	47	200	45.38	3.994
1.7868	34	210	51.07	3.9956
1.6307	30	211	56.37	3.9944
1.4123	20	220	66.10	3.9946
1.3318	15	300	70.67	3.9954
1.2633	11	310	75.14	3.9949
1.2044	17	311	79.51	3.9945
1.1531	6	222	83.82	3.9945
1.1080	5	320	88.08	3.9949
1.0676	10	321	92.35	3.9946
0.9986	5	400	100.95	3.9943
.9689	8	410	105.30	3.9950
.9417	7	411	109.74	3.9952
.9165	8	331	114.37	3.9949
.8934	6	420	119.13	3.9952
.8718	5	421	124.15	3.9949
.8516	6	332	129.50	3.9946
.8155	8	422	141.63	3.9953
.7990	5	500	149.15	3.9951
.7835	13	510	158.88	3.9951

Lutetium Arsenate, $LuAsO_4$ (tetragonal)

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of lutetium arsenate was prepared at NBS from lutetium oxide and arsenic trioxide. The mixture was heated 1 hr. at 1050°C. Later it was heated again for 1 hr. at 1250°C.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon; 0.01 to 0.1 percent each of aluminum and calcium; and 0.001 to 0.01 percent each of copper, iron, magnesium, nickel, lead, antimony, and titanium.

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

$I/I_{corundum} = 6.4$.

Structural data. No reference to the structure of lutetium arsenate was found, but it is apparently isostructural with yttrium arsenate with the space group D_{4h}^{19}-$I4_1/amd$ (No. 141) and 4($LuAsO_4$) per unit cell.

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25°C	6.9509	6.2321

The density of lutetium arsenate calculated from the NBS lattice constants is 6.924 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.643	22	101	19.10
3.477	100	200	25.60
2.783	6	211	32.14
2.632	73	112	34.03
2.458	25	220	36.53
2.321	3	202	38.77
2.172	10	301	41.54
1.991	6	103	45.52
1.8422	8	321	49.43
1.7964	57	312	50.78
1.7375	16	400	52.63
1.7275	2	213	52.96
1.6271	2	411	56.51
1.5578	6	004	59.27
1.5541	15	420	59.42
1.4499	15	332	64.18
1.4215	12	204	65.62
1.4131	<1	323	66.06
1.3568	3	501	69.18
1.3158	9	224	71.66
1.3092	1	413	72.08
1.2489	13	512	76.16
1.2287	3	440	77.64
1.1598	5	404	83.23
1.1584	3	600	83.35
1.1239	<1	611	86.52
1.1135	9	532	87.54
1.1002	11	424	88.87
1.0468	<1	325	94.75
1.0221	<1	631	97.81
1.0162	4	116	98.57
1.0017	<1	415,613	100.52
0.9806	<1	701	103.53
.9643	5	444,640	106.02
.9621	4	543	106.38
.9438	<1	721	109.40
.9390	7	316	110.22
.9374	10	712	110.51
.9296	3	604	111.90
.8981	6	624	118.11
.8771	3	336	122.84
.8758	6	732	123.15
.8689	1	800	124.87
.8559	<1	217	128.29
.8540	1	741	128.83
.8428	3	820	132.10
.8262	7	516	137.60
.8197	6	644	140.00
.8082	<1	327	144.72
.8065	<1	831	145.53
.7964	<1	743	150.57
.7873	<1	417	156.13
.7831	7	536	159.25

Lutetium Vanadate, $LuVO_4$ (tetragonal)

Powder Diffraction File cards. None.

Additional published patterns. Milligan, Watt, and Rachford (1949).

NBS sample. The sample of lutetium vanadate was prepared at NBS by precipitation from a solution of sodium vanadate and lutetium sulfate. It was annealed 15 hours at 1300°C.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium and silicon and 0.001 to 0.01 percent each of aluminum, cobalt, iron, magnesium, and tin.

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

$I/I_{corundum} = 3.7$.

Structural data. Milligan, Watt, and Rachford (1949) determined that lutetium vanadate has the zircon structure, with the space group D^{19}_{4h}-$I4_1/amd$ (No. 141) and $4(LuVO_4)$ per unit cell.

Lattice constants

	a(Å)	c(Å)
Milligan, Watt, and Rachford (1949)	7.00	6.21
NBS, sample at 25°C	7.0243	6.2316

The density of lutetium vanadate calculated from the NBS lattice constants is 6.262 g/cm³ at 25°C.

Reference

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X-ray diffraction studies of heavy metal orthovanadates, J. Phys. & Colloid Chem. 53, 227-234.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.660	41	101	19.03
3.510	100	200	25.35
2.805	12	211	31.88
2.640	65	112	33.92
2.483	17	220	36.15
2.330	3	202	38.60
2.191	14	301	41.16
1.9918	9	103	45.50
1.8592	9	321	48.95
1.8090	43	312	50.40
1.7558	13	400	52.04
1.7323	3	213	52.80
1.6434	4	411	55.90
1.5702	10	420	58.75
1.5580	3	004	59.26
1.5544		303	59.41
1.4621	11	332	63.58
1.4240	9	204	65.49
1.3703	12	501	68.40
1.3194	7	224	71.43
1.3171		413	71.58
1.2763	3	521	74.24
1.2598	10	512	75.38
1.2417	2	440	76.68
1.1708	3	600	82.28
1.1638	5	503	82.88
1.1354	<1	611	85.44
1.1238	6	532	86.53
1.1106	3	620	87.82
1.1061	6	424	88.27
1.0806	2	541	90.93
1.0499	<1	325	94.38
1.0326	<1	631	96.47
1.0167	2	116	98.50
1.0093	1	613	99.48
1.0058	1	415	99.95
0.9908	<1	701	102.05
.9742	1	640	104.49
.9712	1	444	104.95
.9535	1	721	107.76
.9465	4	712	108.93
.9409	3	316	109.89
.9360	1	604	110.76
.9326	<1	505	111.36
.9044	3	624	116.79
.8844	2	732	121.13
.8800	1	336	122.16
.8780	<1	800	122.64
.8750	<1	723	123.36
.8630	<1	811	126.39
.8567	1	217	128.08
.8519	2	820	129.41
.8294	2	516	136.46
.8259	3	644	137.68
.8151	<1	831	141.81
.8097	<1	327	144.07
.8034	<1	813	146.95
.7897	5	752	154.50
.7868	3	536	156.46
.7853	3	840	157.51

Potassium Cadmium Trichloride, $KCdCl_3$ (orthorhombic)

Powder diffraction cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium cadmium trichloride was prepared at NBS by melting potassium chloride and cadmium chloride (2 1/2 hydrate) at 550°C. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, barium, chromium, iron, manganese, sodium, rubidium, and strontium. The sample was colorless and optically positive with a small 2V. The refractive indices were $N_\alpha = 1.700$, $N_\beta = 1.708$, and $N_\gamma = 1.742$.

$I/I_{\text{corundum}} = 1.8$.

Structural data. Brandenberger (1947) reported that potassium cadmium trichloride is isostructural with ammonium cadmium trichloride, with the space group D_{2h}^{16}-Pnam (No. 62) and 4($KCdCl_3$) per unit cell.

Lattice constants

	a(Å)	*b(Å)*	*c(Å)*
Brandenberger (1947)-------	8.78	14.56	3.99
NBS, sample at 25°C--------	8.785 ±0.001	14.584 ±0.001	3.9969 ±0.0004

The density of potassium cadmium trichloride calculated from the NBS lattice constants is 3.345 g/cm³ at 25°C.

Reference

Brandenberger, E. (1947). Die Kristallstruktur von $K(CdCl_3)$, Experientia 3, 149.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
7.52	62	110	11.75
7.28	79	020	12.14
5.615	60	120	15.77
4.396	16	200	20.18
4.253	17	130	20.87
4.209	17	210	21.09
3.760	15	220	23.64
3.648	6	040	24.38
3.531	64	111	25.20
3.368	27	140	26.44
3.259	34	230,121	27.34
3.086	9	031	28.91
2.956	24	201	30.21
2.897	52	211	30.84
2.871	7	310	31.12
2.806	19	240	31.87
2.768	29	150	32.31
2.740	100	221	32.65
2.718	20	320	32.92
2.526	15	231	35.51
2.509	7	330	35.76
2.429	13	060,250	36.97
2.356	40	051	38.17
2.343	26	160	38.39
2.295	5	241	39.22
2.283	4	340	39.44
2.125	3	331	42.51
2.103	3	420	42.98
2.076	7	251	43.55
2.068	7	350	43.74
2.026	9	170	44.68
2.021	11	161	44.81
1.998	36	002	45.34
1.982	32	341	45.73
1.925	13	401	47.17
1.882	13	122,270,+	48.32
1.879	11	261	48.41
1.870	10	360	48.65
1.860	13	421	48.92
1.8478	6	071	49.27
1.8232	5	080	49.98
1.8077	23	132,171	50.44
1.7892	5	431	51.00
1.7650	4	222	51.75
1.7546	8	450	52.08

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
1.7446	4	510	52.40
1.7187	6	142	53.25
1.7077	8	520	53.62
1.7030	10	232,271,+	53.78
1.6975	7	370	53.97
1.6940	3	361	54.09
1.6839	2	280	54.44
1.6404	3	312	56.01
1.6292	7	460,181	56.43
1.6205	5	152	56.76
1.5825	2	540	58.25
1.5625	2	332,371	59.07
1.5438	4	062,252	59.86
1.5271	5	531	60.58
1.5205	7	290,162	60.87
1.5056	3	550	61.54
1.5034	4	342	61.64
1.4805	4	191	62.70
1.4719	4	541	63.11
1.4644	2	600	63.47
1.4383	6	1·10·0	64.76
1.4355	8	620	64.90
1.4240	6	560	65.49
1.4180	10	390	65.80

Praseodymium Vanadate, $PrVO_4$ (tetragonal)

Powder Diffraction File cards. None.

Additional published patterns. Milligan, Watt, and Rachford (1949).

NBS sample. The sample of praseodymium vanadate was prepared at NBS. A mixture of praseodymium oxalate and vanadium pentoxide was heated at 850°C for 30 minutes.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum and silicon, and 0.001 to 0.01 percent each of silver, iron, and magnesium.

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

$I/I_{corundum} = 3.2$.

Structural data. Milligan, Watt, and Rachford (1949) determined that praseodymium vanadate has the zircon structure with the space group D_{4h}^{19}-$I4_1/amd$ (No. 141) and 4($PrVO_4$) per unit cell.

Lattice constants

	a(Å)	c(Å)
Milligan, Watt, and Rachford (1949)	7.29	6.41
Vickery and Klann (1957)	7.31	6.45
Schwarz (1963)	7.367	6.468
NBS, sample at 25°C	7.3633	6.4652

The density of praseodymium vanadate calculated from the NBS lattice constants is 4.848 g/cm³ at 25°C.

References

Milligan, W. O., Watt, L. M. and Rachford, H. H., Jr. (1949). X-ray diffraction studies of heavy metal orthovanadates, J. Phys. & Colloid Chem. 53, 227-234.

Schwarz, H. (1963). Uber die Chromate(V) der Seltenen Erden, II. Praseodymchromat(V) $PrCrO_4$, Z. anorg. u allgem. Chem. 322, 15-24.

Vickery, R. C. and Klann, A. (1957). Magnetic susceptibilities of vanadates of neodymium and praseodymium, J. Chem. Phys. 27, 1219.

Internal standard W, a = 3.16504 Å
CuKα₁ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.862	28	101	18.23
3.682	100	200	24.15
2.936	10	211	30.42
2.747	68	112	32.57
2.604	22	220	34.41
2.430	4	202	36.96
2.295	16	301	39.22
2.069	10	103	43.71
1.947	10	321	46.60
1.889	53	312	48.11
1.841	16	400	49.47
1.803	4	213	50.58
1.721	3	411	53.17
1.647	12	420	55.78
1.620	5	303	56.78
1.617	5	004	56.91
1.529	12	332	60.49
1.480	12	204	62.70
1.435	5	501	64.92
1.373	9	224	68.23
1.318	12	512	71.50
1.3011	3	440	72.60
1.2272	35	600	77.75
1.2150	8	404	78.69
1.2036	3	215	79.58
1.1901	2	611	80.66
1.1763	7	532	81.81
1.1644	5	620	82.83
1.1535	8	424	83.79
1.0929	2	325	89.62
1.0822	2	631	90.75
1.0553	6	613,116	93.75
1.0475	1	415	94.67
1.0214	2	640	97.90
1.0140	2	444	98.85
0.9912	6	712	101.99
.9779	6	633,316	103.94
.9448	4	624	109.23
.9264	4	732	112.49
.9157	3	336,723	114.52
.8931	3	820	119.19
.8636	10	653,516	126.24
.8412	2	327,813	132.61
.8275	2	752	137.14
.8198	3	536	139.96
.7999	3	833,804	148.72
.7893	4	208	154.76
.7887	3	912	155.19

Rubidium Cadmium Trichloride, low form, $RbCdCl_3$ (orthorhombic)

Powder diffraction cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium cadmium trichloride was precipitated at NBS from solutions of rubidium chloride and cadmium chloride.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of cesium and potassium; 0.01 to 0.1 percent sodium; and 0.001 to 0.01 percent each of aluminum, barium, calcium, chromium, copper, iron, nickel, silicon, and strontium.

The sample was colorless and optically positive with a very small 2V. The refractive indices were $N_\alpha = 1.694$, $N_\beta = 1.696$, and $N_\gamma = 1.736$. $I/I_{corundum} = 2.2$.

Structural data. MacGillavry, Nijveld, Dierdorp, and Karsten (1939) determined that orthorhombic rubidium cadmium trichloride is isostructural with ammonium cadmium trichloride, with the space group D_{2h}^{16}-Pnam (No. 62) and $4(RbCdCl_3)$ per unit cell. In recent work here, two high temperature forms were also observed for rubidium cadmium trichloride. Between 135°C and 190°C a tetragonal phase exists which persists at room temperature for a day or two. Above 190°C a cubic form was noted on the hot stage of a microscope. This cubic form reverts to tetragonal again below 190°C.

Lattice constants

	a(Å)	b(Å)	c(Å)
MacGillavry, et al. (1939)----	9.03	14.96	4.02
NBS, sample at 25°C---------	8.959 ±0.001	14.976 ±0.002	4.0346 ±0.0004

The density of orthorhombic rubidium cadmium trichloride calculated from the NBS lattice constants is 3.733 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.67	28	110	11.52
7.47	34	020	11.83
5.741	25	120	15.42
4.480	5	200	19.80
4.358	45	130	20.36
4.289	32	210	20.69
3.840	14	220	23.14
3.740	4	040	23.77
3.570	57	111	24.92
3.452	31	140	25.79
3.332	25	230	26.73
3.300	20	121	27.00
3.138	7	031	28.42
2.996	11	201	29.79
2.960	10	131	30.17
2.934	64	211	30.40
2.930		310	30.48
2.871	18	240	31.12
2.839	31	150	31.48
2.782	100	221	32.15
2.775		320	32.23
2.623	4	141	34.15
2.570	10	231	34.88
2.563		330	34.98
2.491	4	250	36.03
2.404	48	051,160	37.38
2.371	6	311	37.91
2.336	15	340	38.51
2.287	11	321	39.37
2.214	2	410	40.71
2.181	2	260	41.37
2.164	6	331	41.71
2.146	2	420	42.06
2.115	3	350	42.71
2.081	3	170	43.44
2.066	8	161	43.77
2.044	12	430	44.28
2.021	48	341	44.80
2.017		002	44.90
1.9580	13	401	46.33
1.9305	10	270	47.03
1.9178	9	261	47.36
1.9148	9	360	47.44
1.8941	5	421	47.99
1.8900		071	48.10

Rubidium Cadmium Trichloride, low form, $RbCdCl_3$ (orthorhombic)—Con.

Internal standard W, a = 3.16504 Å

CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
1.8721	5	080,351	48.59
1.8496	14	171	49.22
1.8308	14	132	49.76
1.8235	16	431	49.97
1.7937	9	450	50.86
1.7790	2	510	51.31
1.7418	14	142,271,+	52.49
1.7387		370	52.59
1.7296	6	361	52.89
1.7259	5	232	53.01
1.6684	4	181	54.99
1.6512	6	242	55.61
1.6455		152	55.84
1.6395	4	451	56.04
1.6313	5	322	56.35
1.6163	2	540	56.92
1.6004	1	521	57.54
1.5679	1	252	58.85
1.5560	6	531	59.34
1.5454	5	162	59.79
1.5412	3	461	59.97
1.5264	3	342	60.61
1.5160	5	191	61.07
1.5005	5	541	61.77
1.4936	2	600	62.09
1.4642	5	620	63.48
1.4535	6	390	64.00
1.4363	7	480,551,+	64.86
1.3948	5	272,611	67.04
1.3871	3	1·10·1,640	67.46
1.3762	4	621	68.07
1.3726	4	082	68.27
1.3679	3	391	68.54
1.3534	3	481	69.38
1.3460	1	1·11·0	69.81
1.3402	5	452,2·10·1	70.16

Reference

MacGillavry, C. H., Nijveld, H., Dierdorp, S., and Karsten, J. (1939). Die Krystallstruktur von NH_4CdCl_3 und $RbCdCl_3$, Rec. trav. chim., 58, 193-200.

Rubidium Cadmium Trichloride, high form, $RbCdCl_3$ (tetragonal)

Powder diffraction cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium cadmium trichloride was prepared at NBS by fusing rubidium chloride with anhydrous cadmium chloride at approximately 500° C.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of cesium and potassium, and 0.01 to 0.1 percent of sodium.

The sample was colorless. The crystals were optically uniaxial negative with very low double refraction, both indices being near 1.662.

$I/I_{corundum}$ = 4.5.

Structural data. There is no published data on this form of rubidium cadmium trichloride. Its x-ray pattern is, however, very similar to cesium lead trichloride which has a tetragonal distorted perovskite structure. Rubidium cadmium trichloride has a superstructure requiring a double cell with 8 ($RbCdCl_3$) per cell.

This form is unstable at room temperature and inverts in a few days to the orthorhombic (low) form described by MacGillavry, Nijveld, Dierdorf, and Karsten (1939). Observations on a hot stage petrographic microscope show that the low form changes to the high form between 135° and 140° C. At about 190° C this form is seen to lose its double refraction, evidently changing to another high form, an undistorted cubic perovskite. This last change is rapidly reversible.

Lattice constants

	a(Å)	*c(Å)*
NBS, sample at 25°C------	10.304 ± .001	10.399 ± .001

The density of rubidium cadmium trichloride, high form, calculated from the NBS lattice constants is 3.661 g/cm³ at 25° C.

Reference

MacGillavry, C.H., Nijveld, H., Dierdorf, S., and Karsten, J. (1939). Die Krystallstruktur von NH_4CdCl_3 und $RbCdCl_3$, Rec. Trav. Chim. 58, 193.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
5.196	14	002	17.05
5.152	18	200	17.20
3.655	100	202	24.33
3.262	4	301,310	27.32
3.111	2	311	28.67
2.985	10	222	29.91
2.761	2	312	32.40
2.599	28	004	34.48
2.550	46	400	34.81
2.321	6	204	38.77
2.305	9	420	39.05
2.116	24	224	42.69
2.107	35	422	42.88
1.830	25	404	49.79
1.822	8	440	50.01
1.724	5	424	53.07
1.720	2	442	53.22
1.6428	6	206	55.92
1.6295	8	602	56.42
1.4921	8	444	62.16
1.3850	8	426	67.59
1.3805	10	624	67.84
1.3778	4	642	68.00
1.2519	3	644	75.94
1.2496	2	802	76.11
1.2243	3	228	77.97
1.2203	3	606	78.28
1.2147	5	660,822	78.71
1.1603	3	408	83.19
1.1535	4	418	83.79
1.1513	3	840	83.98
1.1023	2	646	88.66
1.1004	3	664	88.85
1.0579	3	448	93.45
1.0531	2	844	94.01
1.0194	2	2·0·10	98.16
1.0161	3	628	98.59
1.0135	3	826	98.92
1.0107	4	862	99.30
0.9478	2	4·2·10	108.70

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium manganese trifluoride was prepared at NBS by D. E. Roberts by heating rubidium fluoride and manganese difluoride to 1100°C.

Spectrographic analysis showed the following major impurities: <0.5 percent each of aluminum and silicon; 0.01 to 0.1 percent each of calcium, cesium, potassium, strontium, and vanadium.

The color of the sample was pale pink. The index of refraction is 1.483.

$I/I_{corundum} = 3.4$.

Structural data. Simanov, Batsanova, and Kovba (1957) determined that rubidium manganese trifluoride has the perovskite structure, the space group O_h^1-Pm3m (No. 221) and 1($RbMnF_3$) per unit cell.

Lattice constants

	a(Å)
Simanova, Batsanova, and Kovba (1957)	4.243
Hoppe, Liebe, and Dähne (1961)	4.25
NBS, sample at 25°C	4.2400

The density of rubidium manganese trifluoride calculated from the NBS lattice constant is 4.300 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å
CuKα$_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.235	2	100	20.96
2.998	100	110	29.78
2.447	20	111	36.70
2.119	50	200	42.63
1.895	2	210	47.97
1.731	32	211	52.85
1.499	21	220	61.85
1.413	2	300	66.05
1.341	19	310	70.13
1.278	9	311	74.11
1.2239	6	222	78.00
1.1759	2	320	81.84
1.1331	24	321	85.65
1.0599	4	400	93.22
1.0284	3	410	97.00
0.9993	7	411	100.85
.9726	4	331	104.73
.9481	17	420	108.67
.9252	3	421	112.72
.9040	4	332	116.86
.8655	6	422	125.74
.8315	14	510	135.74
.8160	2	511	141.44

References

Hoppe, R., Liebe, W., and Dähne, W. (1961). Über Fluoromanganate der Alkalimetalle, Z. anorg. u allgem Chem. 307, 276-289.

Simanov, Yu. P., Batsanova, L. P., and Kovba, L. M. (1957). X ray investigation of the binary fluorides of bivalent manganese, Russ. J. Inorg. Chem. 2, 207. (Translated from Zh. Neorgan. Khim. II, No. 10, 2410-2415.)

Powder Diffraction File cards. No. 14-38, Brown and McLaren (1962). Nos. 14-34 (cubic), 14-36 (cubic), and 14-37 (tetragonal) are for other forms of rubidium nitrate.

Additional published patterns. None.

NBS sample. The sample of rubidium nitrate was obtained from A.D. Mackay, Inc., New York, N.Y. The sample was recrystallized from aqueous solution at room temperature.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of potassium and sodium; 0.01 to 0.1 percent each of cesium and silicon.

The sample was colorless and optically positive with indices of refraction $N_e = 1.526$ and $N_o = 1.524$. A very slight 2V was noted.

Structural data. Pauling and Sherman (1933) proposed trigonal symmetry for rubidium nitrate, the probable space group C_{3v}^2-P31m (No. 157) and 9($RbNO_3$) per unit cell. Brown and McLaren (1962) reported that the space group was either D_3^4-P3$_1$12 or D_3^5-P3$_2$12.

Lattice constants

	a(Å)	*c*(Å)
Pauling and Sherman (1933)	10.47	7.39
Brown and McLaren (1962)	10.48	7.45
NBS, sample at 25°C	10.479	7.452

The density of rubidium nitrate calculated from the NBS lattice constants is 3.109 g/cm^3 at 25°C.

Internal standard Ag, a = 4.08625 Å

CuKα$_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.244	<1	110	16.89
4.285	30	111	20.71
3.877	<1	201	22.92
3.445	2	102	25.84
3.116	1	211	28.62
3.032	100	112	29.43
3.023	100	300	29.52
2.879	3	202	31.04
2.801	1	301	31.92
2.620	1	220	34.19
2.522	2	212,310	35.57
2.484	13	003	36.13
2.471	23	221	36.33
2.385	2	311	37.69
2.349	2	302	38.28
2.245	1	113	40.13
2.178	1	203	41.42
2.171	2	401	41.56
2.142	19	222	42.14
2.086	1	312	43.34
2.013	1	213	44.99
2.007	1	321	45.14
1.919	14	303	47.33
1.914	16	411	47.47
1.825	1	105	49.92
1.817	1	322	50.16
1.755	5	114	52.06
1.749	13	412	52.27
1.724	<1	204	53.09
1.715	1	420	53.38
1.674	1	403	54.79
1.672	1	421	54.88
1.636	1	214	56.17
1.631	1	502,510	56.36
1.596	1	323	57.69
1.518	3	224	60.97
1.513	4	600	61.22
1.498	1	314	61.91
1.494	1	431	63.51
1.434	3	115	65.00

References

Brown, R. N., and McLaren, A.C. (1962). The thermal transformation on solid rubidium nitrate, Acta Cryst. 15, 974-976.

Pauling, L., and Sherman, J. (1933). Note on the crystal structure of rubidium nitrate, Z. Krist. 84, 213-216.

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
1.428	7	333	65.27
1.426		521	65.37
1.416	1	205	65.88
1.412	1	423	66.11
1.3677	1	215	68.55
1.3570	5	414	69.17
1.3540	8	522	69.34
1.2955	2	225	72.96
1.2919	4	603	73.20
1.2770	1	701	74.19
1.2620	1	424	75.25
1.2356	1	442	77.13
1.1983	1	206	80.00
1.1909	1	415	80.60
1.1869	1	711	80.93
1.1676	1	216	82.55
1.1649	1	434	82.79
1.1491	2	703,306	84.18
1.1452	4	524	84.53
1.1436		712	84.68
1.1226	1	623,226	86.65
1.1141	1	316	87.48
1.1113	1	614	87.75
1.0716	1	444	91.91

Samarium Vanadate, $SmVO_4$ (tetragonal)

Powder Diffraction File cards. None.

Additional published pattern. Milligan, Watt, and Rachford (1949).

NBS sample. The sample of samarium vanadate was prepared at NBS. A mixture of samarium oxalate and vanadium pentoxide was heated at 850°C for 45 minutes.

Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, iron, magnesium, antimony, and silicon.

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

$I/I_{corundum} = 2.2.$

Structural data. Milligan, Watt, and Rachford (1949) determined that samarium vanadate has the zircon structure with the space group D_{4h}^{19}-$I4_1/amd$ (No. 141) and 4 ($SmVO_4$) per unit cell.

Lattice constants

	a(Å)	*c(Å)*
Milligan, Watt, and Rachford (1949)	7.22	6.35
NBS, sample at 25°C	7.2652	6.3894

The density of samarium vanadate calculated from the NBS lattice constants is 5.225 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
4.802	31	101	18.46
3.633	100	200	24.48
2.895	14	211	30.86
2.712	76	112	33.00
2.569	20	220	34.89
2.399	6	202	37.45
2.265	16	301	39.76
2.0438	9	103	44.28
1.9220	12	321	47.25
1.8653	56	312	48.78
1.8161	15	400	50.19
1.7810	6	213	51.25
1.6989	5	411	53.92
1.6244	11	420	56.61
1.5976	6	004	57.65
1.5096	14	332	61.36
1.4623	10	204	63.57
1.4171	4	501	65.85
1.3564	10	224	69.20
1.3011	11	512	72.60
1.2107	4	600	79.02
1.1996	6	404	79.89
1.1892	6	215	80.76
1.1607	7	532	83.15
1.1487	5	620	84.22
1.1389	11	424	85.11
1.0793	1	325	91.07
1.0425	7	116	95.27
1.0343	3	415	96.27
1.0074	3	640	99.74
0.9780	6	712	103.92
.9660	8	316	105.76
.9650	6	633,604	105.91
.9327	6	624,703	111.24
.9141	5	732	114.83
.9040	4	723,336	116.88
.8809	4	820	121.94
.8787	4	217	122.46
.8528	10	516,653	129.17
.8166	4	752	141.22
.8123	8	840	142.96
.8095	10	536	144.16

Reference

Milligan, W. O., Watt, L. M. and Rachford, H. H., Jr. (1949). X-ray & diffraction studies of heavy metal orthovanadates, J. Phys. & Colloid Chem. 53, 227-234.

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of cubic silver antimony sulfide was prepared at NBS by heating miargyrite, $AgSbS_2$, in a closed tube at 600°C. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon, and 0.01 to 0.1 percent each of aluminum, arsenic, bismuth, calcium, iron, germanium, magnesium, manganese, nickel, lead, and tungsten.

The sample was an opaque metallic gray powder.

$I/I_{corundum} = 3.5$.

Structural data. Geller and Wernick (1959) reported that high temperature silver antimony sulfide has the sodium chloride structure, the space group O_h^5-Fm3m (No. 225) and $2(AgSbS_2)$ per unit cell. Silver antimony sulfide also occurs as a natural mineral miargyrite which is monoclinic if formed below melting temperature of 450°C.

Lattice constants

	a(Å)
Graham (1951)	5.653
Geller and Wernick (1959), sample at 25°C	5.647
NBS, sample at 25°C	5.652

The density of cubic silver antimony sulfide calculated from the NBS lattice constant is 5.403 g/cm³ at 25°C.

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
3.263	63	111	27.31
2.826	100	200	31.63
1.998	41	220	45.35
1.7039	21	311	53.75
1.6316	15	222	56.34
1.4131	7	400	66.06
1.2966	5	331	72.89
1.2635	7	420	75.12
1.1537	3	422	83.77
1.0877	3	511	90.17
0.9991	5	440	100.87
.9553	2	531	107.47
.9420	2	600	109.70
.8936	1	620	119.08
.8619	1	533	126.67
.8520	1	622	129.39
.8156	<1	444	141.60
.7913	2	711	153.53

References

Geller, S. and Wernick, J. H. (1951). Ternary semiconducting compounds with sodium chloride-like structure: $AgSbSe_2$, $AgSbTe_2$, $AgBiS_2$, $AgBiSe_2$, Acta Cryst. 12, 46-54.
Graham, A. R. (1959). Matildite, aramayoite, miargyrite, Am. Mineralogist 36, 436-449.

Powder Diffraction File cards. No. 4-0675, Graham (1951).

Additional published patterns. Hofmann (1938).

NBS sample. The sample of miargyrite was obtained from Tem-pres Research Inc., State College, Pa.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon, and 0.01 to 0.1 percent each of aluminum, arsenic, bismuth, calcium, iron, germanium, magnesium, manganese, nickel, lead, and tungsten.

The color of the sample was blackish red. The indices of refraction are very high and the sample was very fine-grained.

$I/I_{corundum} = 2.0$.

Structural data. Hofmann (1938) determined that miargyrite has the space group C^6_{2h}-A2/a (No. 15) and 8($AgSbS_2$) per unit cell. An irreversible cubic form is obtained at the melting point.

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
Hofmann (1938)	13.20	4.40	12.86	98.06°
NBS, sample at 25°C	13.224	4.410	12.881	98.48°

The density of miargyrite calculated from the NBS lattice constants is 5.252 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
4.259	4	202	20.84
3.440	81	211	25.88
3.186	31	004	27.98
3.101	30	$\bar{4}02$	28.76
3.051	14	$\bar{1}13$	29.25
2.892	100	$\bar{2}13$	30.89
2.748	70	402	32.55
2.639	8	$\bar{3}13$	33.94
2.265	<1	$\bar{5}11$	39.76
2.206	9	020	40.88
2.174	7	120	41.51
2.131	2	115	42.37
2.043	3	122	44.30
2.013	38	$\bar{2}22$,215	44.99
1.971	27	$\bar{6}11$	46.00
1.914	22	$\bar{4}06$	47.45
1.875	5	315	48.51
1.871	4	$\bar{6}13$	48.62
1.846	2	322	49.32
1.813	18	024	50.29
1.797	20	$\bar{4}22$	50.77
1.737	4	$\bar{7}11$	52.66
1.720	8	422	53.20
1.699	1	$\bar{1}17$	53.93
1.693	12	613	54.14
1.686	14	520,$\bar{2}17$	54.38
1.672	7	406	54.88
1.660	8	$\bar{6}15$	55.30
1.635	5	800	56.22
1.593	10	522,008	57.84
1.5504	9	$\bar{8}04$,620	59.58
1.5301	<1	802	60.45
1.5256	<1	$\bar{2}26$,$\bar{7}15$	60.65
1.4938	2	$\bar{3}26$	62.08
1.4455	4	$\bar{4}26$	64.40
1.4200	5	231,606	65.70
1.3990	1	$\bar{8}06$	66.81
1.3873	2	$\bar{6}08$	67.45
1.3860	2	$\bar{5}26$	67.52
1.3747	6	804	68.15
1.3321	6	426	70.65
1.3135	5	820	71.81
1.2850	5	219	73.65
1.2731	<1	$\bar{5}19$	74.46
1.2683	4	$\bar{8}24$	74.79

References

Graham, A. R. (1951). Matildite, aramayoite, miargyrite, Am. Mineralogist 36, 436-449.

Hofmann, W. (1938). Die Struktur von Miargyrit, $AgSbS_2$, Sitzber. preuss. Akad Wiss. Physik. Math. Kl. Berlin 7, 111-119.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.2583	1	135	75.49
1.2520	6	$\bar{5}33,\overline{10}\cdot1\cdot3$	75.93
1.2314	5	10·1·1	77.44
1.2261	5	$\bar{6}19$	77.84
1.1833	1	$\bar{9}24$	81.22
1.1734	1	717	82.05
1.1663	2	824	82.66
1.1462	3	633	84.44
1.1446	3	$\bar{2}37$	84.59
1.1361	1	$\bar{6}35$	85.37
1.1316	4	$4\cdot0\cdot10,\bar{2}\cdot1\cdot11$	85.79
1.1084	2	$\overline{10}\cdot1\cdot7$	88.04
1.1016	1	$\overline{12}\cdot0\cdot2$	88.73
1.0894	2	733	89.99
1.0877	3	$1\cdot2\cdot10,\bar{5}\cdot1\cdot11$	90.17
1.0784	1	2·1·11	91.16
1.0777	2	$\bar{8}28$	91.24
1.0669	2	$10\cdot1\cdot5,\overline{12}\cdot1\cdot1$	92.43
1.0648	<1	808	92.67
1.0619	<1	826,0·0·12	93.00
1.0491	1	437,3·1·11,+	94.48
1.0466	1	10·0·6,11·2·0	94.77
1.0421	2	$\bar{8}35,\bar{1}44,12\cdot1\cdot1$	95.32
1.0392	2	$\bar{6}\cdot2\cdot10$	95.67
1.0355	1	6·0·10	96.12
1.0239	<1	$\bar{2}39,2\cdot0\cdot12$	97.57
1.0135	2	537	98.92
1.0077	2	$\bar{7}\cdot2\cdot10$	99.71
0.9917	<1	239	101.91
.9855	1	$\overline{12}\cdot2\cdot2$	102.81
.9801	<1	5·1·11	103.60
.9762	2	$\overline{10}\cdot3\cdot3,637$	104.19
.9748	<1	819	104.40
.9708	1	$\overline{12}\cdot2\cdot4,146$	105.02
.9661	<1	$10\cdot3\cdot1,\overline{13}\cdot0\cdot6$	105.74
.9637	1	$\bar{3}\cdot1\cdot13,\bar{6}39$	106.11
.9590	1	828	106.86
.9570	2	$\bar{8}\cdot0\cdot12$	107.20
.9475	<1	$\overline{10}\cdot3\cdot5,12\cdot2\cdot2$	108.76
.9452	<1	10·2·6,439	109.16
.9435	2	$\bar{5}\cdot1\cdot13,6\cdot1\cdot11$	109.45

Silver Antimony Sulfide (pyrargyrite) Ag_3SbS_3(trigonal)

Powder Diffraction File cards. No. 14-280, Toulmin (1963).

Additional published patterns. None.

NBS sample. The sample of pyrargyrite was obtained from Tem-pres Research Inc., State College, Pa. It was annealed at 350°C over night in order to sharpen the diffraction pattern.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, arsenic, iron, germanium, molybdenum, lead, silicon, strontium, and tungsten.

The color of the sample was gray reddish brown. The indices of refraction are very high and the sample was very fine-grained.

$I/I_{\text{corundum}} = 1.1.$

Structural data. Grossner and Mussgnug (1928) determined that pyrargyrite is isostructural with proustite with the space group C_{3v}^{6}-R3c (No. 161), and 6(Ag_3SbS_3) per unit cell.

The unit cell measurements reported by Grossner and Mussgnug were converted from rhombohedral kX units to hexagonal angstrom units.

Lattice constants

	a(Å)	c(Å)
Grossner and Mussgnug (1928)	11.14	8.79
Hocart (1937)	11.05	8.74
Toulmin (1963)	11.052	8.7177
NBS, sample at 25°C	11.047	8.719

The density of pyrargyrite calculated from the NBS lattice constants is 5.855 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
3.962	15	012	22.42
3.338	53	211	26.68
3.220	67	202	27.68
3.185	57	300	27.99
2.780	100	122	32.17
2.761	9	220	32.40
2.571	60	113	34.86
2.538	60	131	35.34
2.267	19	312	39.73
2.128	20	321	42.43
2.096	7	042	43.11
2.088	10	410	43.30
2.002	3	223	45.26
1.983	5	024	45.72
1.961	29	232	46.26
1.867	22	214	48.73
1.842	8	330	49.44
1.771	8	241	51.56
1.7521	16	502	52.16
1.6957	8	413	54.03
1.6842	19	134	54.43
1.6703	14	422	54.92
1.6111	9	404	57.12
1.5983	11	152	57.62
1.5943		600	57.78
1.5703	4	125	58.75
1.5553	3	333	59.37
1.5480	4	431	59.68
1.5322	10	520	60.36
1.4796	2	342	62.74
1.4576	8	315	63.80
1.4535		006	64.00
1.4389	2	161	64.73
1.4052	5	116	66.48
1.3915	8	244	67.22
1.3835	4	612	67.66
1.3654	2	235	68.68
1.3554	5	523	69.26
1.3495	6	514	69.61
1.3225	1	306	71.24
1.3114	1	621	71.94
1.3040	1	532	72.41
1.2861	3	226	73.58
1.2752	1	434	74.32
1.2693	<1	262	74.72

References

Grossner, B. and Mussgnug, F. (1928). Original-Mitteilungen an die Redaktion. Über die Kristallstruktur von Pyrargyrit, Centr. Mineral., Geol. 65-73.

Hocart, R. (1937). Schéma structurale de la proustite et de la pyrargyrite, Compt. rend. **205**, 68-70.

Toulmin, P., 3rd. (1963). Proustite-pyrargyrite solid solutions, Am. Mineralogist **48**, Nos. 7 & 8, 725-736.

Internal standard W, a = 3.16504 Å CuKα$_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
1.2672	2	710	74.87
1.2551	<1	425	75.71
1.2128	4	164	78.88
1.2053	<1	630,027	79.43
1.1926	4	416	80.46
1.1793	4	452	81.56
1.1682	<1	345	82.50
1.1614	2	713	83.09
1.1580	4	271,704	83.39
1.1533	1	802	83.81
1.1406	3	336	84.95
1.1334	3	624	85.62
1.1275	1	137	86.18
1.1046	2	550,407	88.42
1.0849	1	182	90.47
1.0831	2	327,018	90.66
1.0758	1	535	91.45
1.0742	2	606	91.62
1.0681	3	731,544	92.30
1.0633	1	900	92.83
1.0451	2	372	94.96
1.0439	1	820,057	95.10
1.0302	1	274	96.77
1.0088	<1	517	99.55
0.9962	2	191	101.28
.9764	3	437	104.16
.9652	1	381,734	105.88
.9552	4	716	107.48
.9485	1	832	108.60
.9474	1	167	108.77

Silver Subfluoride, Ag_2F (hexagonal)

Powder Diffraction File cards. No. 3-0707, Terrey and Diamond (1928).

Additional published patterns. None.

NBS sample. The sample of silver subfluoride was supplied by L. D. Calvert of the Division of Applied Chemistry, National Research Council, Canada. It was prepared in that Division by P. Tymchuk by reacting pure silver with hydrogen fluoride and 30% hydrogen peroxide. A uniform precipitate was obtained when the sample was washed with alcohol and ether.

Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, copper, iron, magnesium, silicon, and tin.

The sample has a metallic luster and it was a light olive opaque powder.

$I/I_{corundum} = 3.2$.

Structural data. Ott and Seyfarth (1928) determined that silver subfluoride has the cadmium iodide structure, the space group D^3_{3d}-$P\bar{3}m1$ (No. 164) and $1(Ag_2F)$ per unit cell.

Lattice constants

	a(Å)	c(Å)
Terrey and Diamond (1928)	2.995	5.722
Ott and Seyfarth (1928)	3.0	5.75
NBS, sample at 25°C	3.0016	5.7014

The density of silver subfluoride calculated from the NBS lattice constants is 8.762 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

CuKα_1 λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.701	16	001	15.53
2.849	28	002	31.37
2.600	16	100	34.47
2.365	100	101	38.01
1.921	27	102	47.27
1.9000	16	003	47.83
1.5340	8	103	60.28
1.5010	11	110	61.75
1.4515	4	111	64.10
1.4248	4	004	65.45
1.3280	5	112	70.90
1.2999	2	200	72.67
1.2673	7	201	74.86
1.2499	8	104	76.09
1.1825	4	202	81.29
1.1777	6	113	81.69
1.1403	2	005	84.98
1.0729	1	203	91.77
1.0444	4	105	95.04
1.0334	2	114	96.38
0.9824	2	210	103.26
.9682	5	211	105.41
.9605	3	204	106.63
.9502	1	006	108.31
.9290	2	212	112.02
.9080	4	115	116.05
.8926	4	106	119.30
.8727	1	213	123.91
.8665	2	300	125.47
.8572	1	205,301	127.94
.8289	2	302	136.62
.8148	3	007	141.92
.8089	2	214	144.42
.8029	1	116	147.21
.7884	1	303	155.38

References

Ott, H. and Seyfarth, H. (1928). Die Struktur des Silbersubfluoride, Z. Krist. 67, 430-433.
Terrey, H. and Diamond, H. (1928). The crystal structure of silver subfluoride, J. Chem. Soc. (London), 2820-2824.

Sodium Hexametaphosphate Hexahydrate, $Na_6P_6O_{18}\cdot 6H_2O$ (orthorhombic)

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of sodium hexametaphosphate hexahydrate was prepared by E. J. Griffith (1965) of the Inorganic Chemicals Division, Monsanto Co., St. Louis, Mo.

Spectrographic analysis showed the following major impurities: 0.001 to 0.1 percent each of aluminum and silicon.

The sample is colorless and optically positive. The indices of refraction are $N_\alpha = 1.458 \pm .001$, $N_\beta = 1.453 \pm .001$, and $N_\gamma = 1.459 \pm .001$. 2V is large.

$I/I_{\text{corundum}} = 0.8$.

Structural data. Jost (1965) determined that sodium hexametaphosphate hexahydrate has the space group D_{2h}^{18}-Ccmb (No. 64) or C_{2v}^{17}-Cc2b (No. 41) and $4(Na_6P_6O_{18}\cdot 6H_2O)$ per unit cell.

Lattice constants

	a(Å)	b(Å)	c(Å)
Jost (1965)	11.58	18.54	10.48
NBS, sample at 25°C	11.547	18.492	10.495

The density of sodium hexametaphosphate hexahydrate calculated from the NBS lattice constants is 2.134 g/cm³ at 25°C.

Internal standard Ag, a = 4.08625 Å
CuKα₁ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
9.24	18	020	9.56
7.17	100	111	12.34
5.245	42	002	16.89
5.058	77	201	17.52
4.900	76	220	18.09
4.831	47	131	18.35
4.626	28	112,040	19.17
4.567	24	022	19.42
3.885	3	202	22.87
3.776	3	132	23.54
3.583	88	222	24.83
3.546	28	311	25.09
3.467	14	042	25.67
3.338	15	151	26.68
3.292	73	113	27.06
3.117	30	331	28.61
3.083	15	060	28.94
3.060	4	312	29.16
2.974	11	242	30.02
2.942	15	133	30.36
2.926	13	152	30.53
2.888	2	400	30.94
2.783	4	401	32.14
2.755	6	420	32.47
2.719	18	260	32.91
2.664	19	421	33.61
2.632	14	261	34.04
2.623	6	004	34.15
2.584	26	351	34.68
2.529	5	402	35.46
2.482	<2	153	36.16
2.440	5	422	36.81
2.414	18	262	37.21
2.386	27	441,333	37.67
2.312	15	224,172,080	38.92
2.238	4	511	40.26
2.227	3	403	40.47
2.164	5	423	41.70
2.147	14	263	42.05
2.121	11	353	42.59
2.104	18	154	42.94
2.073	7	173	43.63
2.067	5	461	43.76
2.012	8	372	45.02
2.006	6	443	45.15
1.972	2	205	45.98
1.955	4	462	46.41
1.925	4	551,600	47.17
1.917	2	513	47.38
1.893	11	601	48.02

References

Griffth, E. J. and Buxton, R. L. (1965). The preparation and properties of the twelve-membered ring hexametaphosphate anion, Inorg. Chem. 4, 549.

Jost, K-H. (1965). Die Struktur des Natrium-hexametaphosphates $Na_6(P_6O_{18}).6H_2O$. Acta Cryst. 19, 555-560.

Sodium Hexametaphosphate Hexahydrate, $Na_6P_6O_{18}\cdot 6H_2O$ (orthorhombic)—continued

Internal standard Ag, a = 4.08625 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
1.888	9	264,192	48.16
1.871	6	354	48.63
1.850	4	0·10·0,373	49.22
1.835	3	552	49.64
1.829	2	283	49.81
1.806	4	602,463	50.50
1.765	2	335	51.74
1.748	4	006	52.28
1.734	<2	084	52.74
1.726	3	514	53.02
1.715	4	571	53.38
1.707	3	482	53.66
1.686	3	603	54.36
1.669	2	425,2·10·2,534	54.97
1.661	2	265,284	55.24
1.649	4	355	55.71
1.632	<2	660	56.31
1.613	<2	661	57.05
1.609	<2	393	57.20
1.601	<2	194	57.50
1.587	<2	316,1·11·2	58.08
1.567	4	712,156	58.87
1.5568	3	4·10·0,573	59.31
1.5520	4	604	59.51
1.5475	4	515	59.70
1.5414	4	336,0·12·0	59.96
1.5192	2	591	60.93
1.5109	3	0·10·4,375	61.30
1.5065	4	750,535	61.50
1.5025	4	1·11·3	61.68
1.4869	<2	465,713,484	62.40
1.4794	3	663,680,027	62.75
1.4744	3	2·12·1	62.99
1.4706	<2	266,644	63.17
1.4560	2	195	63.88
1.4330	<2	227,2·12·2	65.03
1.4256	<2	820	65.41
1.4234	<2	682,446	65.52
1.4131	<2	821	66.06
1.4058	<2	593	66.45
1.4024	<2	625	66.63
1.3944	2	086	67.06
1.3919	2	802	67.20
1.3837	2	753	67.65
1.3799	<2	157	67.86
1.3760	<2	822	68.08
1.3561	<2	645,286	69.22
1.3483	<2	4·12·1,5·11·1	69.68
1.3303	3	407	70.76
1.3238	<2	3·13·1	71.16

Terbium Vanadate, $TbVO_4$ (tetragonal)

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of terbium vanadate was prepared at NBS. A mixture of terbium oxalate and vanadium pentoxide was heated 1 hr. at 1400°C.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, iron, and lead.

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

$I/I_{corundum} = 2.6$.

Structural data. Milligan, Watt, and Rachford (1949) determined that terbium vanadate is isostructural with zircon with the space group D_{4h}^{19} - $I4_1/amd$ (No. 141) and $4(TbVO_4)$ per unit cell.

Lattice constants

	a(Å)	c(Å)
Milligan and Vernon (1952)	7.15	6.31
NBS, sample at 25°C	7.1772	6.3289

The density of terbium vanadate calculated from the NBS lattice constants is 5.579 g/cm³ at 25°C.

References

Milligan, W. O., and Vernon, L. W. (1952). Crystal structure of heavy metal orthovanadates, J. Phys. Chem. 56, 145.

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X-ray diffraction studies on heavy metal orthovanadates, J. Phys. and Colloid Chem. 53, 227-234.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.75	33	101	18.66
3.587	100	200	24.80
2.862	12	211	31.22
2.684	76	112	33.35
2.537	22	220	35.35
2.374	4	202	37.87
2.238	17	301	40.26
2.024	11	103	44.73
1.899	11	321	47.86
1.844	60	312	49.38
1.794	16	400	50.85
1.763	6	213	51.81
1.679	5	411	54.61
1.606	12	420	57.34
1.5823	7	303,004	58.26
1.4914	18	332	62.19
1.4471	14	323,204	64.32
1.3996	6	501	66.78
1.3422	11	413,224	70.04
1.2858	10	512	73.60
1.2686	4	440	74.77
1.1960	4	600	80.19
1.1862	8	404,503	80.98
1.1770	3	215	81.75
1.1597	2	611	83.24
1.1470	8	532	84.37
1.1345	5	620	85.52
1.1262	10	424,523	86.30
1.1034	2	541	88.54
1.0681	4	325,622	92.30
1.0322	5	116	96.53
1.0296	4	613	96.85
1.0234	2	415	97.64
0.9956	4	640	101.36
.9898	4	543,444	102.19
.9666	8	712	105.67
.9562	4	316	107.32
.9540	6	633,604	107.69
.9220	6	703,624	113.31
.9031	6	732	117.05
.8971	3	800,107	118.31
.8948	4	336	118.81
.8702	4	820,217	124.54
.8438	6	516	131.81
.8067	6	752	145.43
.8007	6	536	148.31

Thulium Vanadate, $TmVO_4$ (tetragonal)

Powder Diffraction File cards. None.

Additional published patterns. Milligan, Watt, and Rachford (1949).

NBS sample. The sample of thulium vanadate was prepared at NBS. A mixture of thulium oxalate and vanadium pentoxide was heated at 1400°C for 1 hr.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum and silicon, and 0.001 to 0.01 percent magnesium.

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

$I/I_{corundum} = 3.6$.

Structural data. Milligan, Watt, and Rachford (1949) determined that thulium vanadate has the zircon structure with the space group $D_{4h}^{19}-I4_1/amd$ (No. 141) and $4(TmVO_4)$ per unit cell.

Lattice constants

	a(Å)	*c(Å)*
Milligan, Watt, and Rachford (1949)	7.00	6.21
NBS, sample at 25°C	7.0712	6.2606

The density of thulium vanadate calculated from the NBS lattice constants is 6.023 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
4.686	33	101	18.92
3.535	100	200	25.17
2.824	12	211	31.66
2.654	68	112	33.74
2.500	19	220	35.89
2.344	3	202	38.36
2.2061	16	301	40.87
2.0014	2	103	45.27
1.8714	11	321	48.61
1.8192	52	312	50.10
1.7678	22	400	51.66
1.7421	5	213	52.48
1.6543	3	411	55.50
1.5816	10	420	58.29
1.5652	5	004	58.96
1.5626	4	303	59.07
1.4710	12	332	63.15
1.4310	10	204	65.13
1.3790	4	501	67.91
1.3261	8	224	71.02
1.2850	<1	521	73.65
1.2678	10	512	74.83
1.2498	4	440	76.09
1.1784	4	600	81.63
1.1716	5	404	82.21
1.1643	2	215	82.84
1.1428	2	611	84.75
1.1306	6	532	85.89
1.1181	4	620	87.08
1.1121	8	424	87.67
1.0550	2	325	93.79
1.0392	2	631	95.67
1.0214	3	116	97.89
1.0156	2	613	98.65
0.9805	4	640	103.54
.9765	4	444,543	104.15
.9524	8	712	107.95
.9454	6	316	109.13
.9412	4	604,633	109.84
.9097	5	624,703	115.72
.9063	4	525	116.39
.8901	4	732	119.85
.8841	3	336,800	121.20
.8685	2	811	124.96
.8606	2	217	127.03
.8574	3	820	127.88
.8337	8	660,516	135.00
.8309	6	644	135.94
.8307	4	653	136.00
.8084	1	813	144.65
.7949	4	752	151.38
.7908	4	536,840	153.82

Reference

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X-ray diffraction studies of heavy metal orthovanadates, J. Phys. and Colloid Chem. 53, 227-234.

Powder Diffraction File cards. None.

Additional published patterns. Milligan, Watt, and Rachford (1949).

NBS sample. The sample of ytterbium vanadate was prepared at NBS. A mixture of ytterbium oxalate and vanadium pentoxide was heated at 1400°C for 1 hr.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum and silicon, and 0.001 to 0.01 percent each of calcium, iron, and magnesium.

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

$I/I_{corundum} = 3.7.$

Structural data. Milligan, Watt, and Rachford (1949) determined that ytterbium vanadate is isostructural with zircon with the space group D_{4h}^{19}-$I4_1/amd$ (No. 141) and $4(YbVO_4)$ per unit cell.

Lattice constants

	a(Å)	c(Å)
Milligan, Watt, and Rachford (1949)	7.02	6.23
NBS, sample at 25°C	7.0435	6.2470

The density of ytterbium vanadate calculated from the NBS lattice constants is 6.172 g/cm³ at 25°C.

Reference

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X-ray diffraction studies of heavy metal orthovanadates, J. Phys. and Colloid Chem. 53, 227-234.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.674	47	101	18.97
3.523	100	200	25.26
2.813	15	211	31.78
2.646	77	112	33.85
2.491	25	220	36.03
2.337	4	202	38.47
2.1979	20	301	41.03
1.9972	12	103	45.37
1.8649	16	321	48.79
1.8137	61	312	50.26
1.7609	18	400	51.88
1.7372	6	213	52.64
1.6477	6	411	55.74
1.5752	13	420	58.55
1.5620	6	004	59.09
1.5575	7	303	59.28
1.4662	16	332	63.38
1.4273	12	204	65.32
1.3739	6	501	68.20
1.3227	10	224	71.23
1.3203	4	413	71.38
1.2800	2	521	73.99
1.2632	11	512	75.15
1.2450	3	440	76.44
1.1736	4	600	82.04
1.1681	6	404	82.51
1.1612	3	215	83.11
1.1385	2	611	85.15
1.1265	10	532	86.28
1.1136	5	620	87.53
1.1088	11	424	88.00
1.0834	1	541	90.63
1.0524	2	325	94.09
1.0354	2	631	96.13
1.0191	4	116	98.19
1.0120	2	613	99.13
1.0085	1	415	99.59
0.9932	1	701	101.70
.9767	4	640	104.12
.9736	4	444	104.58
.9560	1	721	107.36
.9490	8	712	108.52
.9432	6	316	109.50
.9384	4	604	110.34
.9348	2	505	110.97
.9067	6	624	116.32
.9034	3	525	116.99
.8867	6	732	120.60
.8820	3	336	121.68
.8652	2	811	125.81
.8586	2	217	127.56
.8542	2	820	128.78
.8492	1	615	130.19
.8315	7	516	135.75
.8281	6	644	136.92
.8174	1	831	140.87
.8117	1	327	143.22
.8056	2	813	145.91
.8037	2	635	146.81
.7920	4	752	153.05

Yttrium Vanadate, YVO_4 (tetragonal)

Powder Diffraction File card. No. 4-0457, Broch (1933).

Additional published patterns. Milligan, Watt, and Rachford (1949) Nautov (1962), Schwarz (1963), and Gambino and Guare (1963).

NBS sample. The sample of yttrium vanadate was furnished by P. Lublin, General Telephone and Electronics Lab., Bayside, N. Y.

Analysis by that company showed no impurities greater than 0.005 percent.

The color of the sample was yellow white and it was optically positive with indices of refraction $N_e \sim 2.05$ and $N_o \sim 1.98$. Because of the fine particle size and extremely high indices, these values are approximate.

$I/I_{corundum} = 3.6$.

Structural data. Broch (1933) determined that yttrium vanadate has the zircon structure, the space group D_{4h}^{19}-$I4_1/amd$ (No. 141), and 4(YVO_4) per unit cell.

Lattice constants

	a(Å)	c(Å)
Broch (1933)	7.140	6.191
Milligan, Watt, and Rachford (1949)	7.10	6.27
Nautov (1962)	7.114	6.258
Schwarz (1963)	7.123	6.291
NBS, sample at 25°C	7.1192	6.2898

The density of yttrium vanadate, calculated from the NBS lattice constants is 4.247 g/cm³ at 25°C.

References

Broch, E. (1933). Die Kristallstruktur von Yttriumvanadat, Z. physik. Chem. (B) 20, 345-350.

Gambino, J. R. and Guare, C. J. (1963). Yttrium and rare earth vanadates, Nature 198, (4885) 1084.

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X ray diffraction studies of heavy metal orthovanadates, J. Phys. and Colloid Chem. 53, 227-234.

Nautov, V. A. (1962). X ray study of scandium, yttrium, cerium, neodymium, and gadolinium orthovanadates, Zh. Strukt. Khim. 3, 608-611.

Schwarz, H. (1963). Über die chromate(V) der Seltenen Erden, IV. Yttriumchromat(V) $YCrO_4$, Z. anorg. u allgem. Chem. 322, 137-149.

Internal standard W, a = 3.16504 Å CuKα$_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	I	hkl	2θ(°)
4.711	8	101	18.82
3.559	100	200	25.00
2.831	1	211	31.58
2.668	46	112	33.56
2.518	12	220	35.63
2.357	6	202	38.15
2.220	12	301	40.60
2.012	5	103	45.03
1.884	6	321	48.26
1.830	46	312	49.78
1.780	13	400	51.28
1.751	1	213	52.19
1.666	1	411	55.09
1.5915	8	420	57.89
1.5722	4	004	58.67
1.5485	1	402	59.66
1.4805	11	332	62.70
1.4381	7	204	64.77
1.3884	3	501	67.39
1.3334	7	224	70.57
1.2894	<1	314	73.37
1.2761	7	512	74.25
1.2586	2	440	75.47
1.1865	5	600	80.96
1.1783	3	503,404	81.64
1.1699	1	215	82.35
1.1507	1	611	84.04
1.1383	7	532	85.17
1.1255	4	620	86.37
1.1189	5	424	87.01
1.0609	1	325	93.11
1.0466	1	631	94.78
1.0262	2	116	97.29
1.0218	2	613	97.84
1.0164	1	415	98.54
0.9873	2	640	102.55
.9826	2	444,543	103.24
.9662	1	721	105.73
.9643	1	534	106.03
.9589	5	712	106.88
.9503	2	316	108.30
.9472	3	604,633	108.81
.9427	1	505	109.59
.9153	3	624,703	114.61
.8960	4	732	118.56
.8897	2	800	119.93
.8890	2	336	120.09
.8745	1	811	123.47
.8648	2	217	125.91
.8633	2	820	126.31
.8383	6	516	133.51
.8362	5	644,653	134.19

Zirconium Dihydride, ZrH_2 (tetragonal)

Powder Diffraction File cards. None.

Additional published patterns. None.

NBS sample. The sample of zirconium hydride was obtained as grade "R" from Metal Hydrides Inc., Beverly, Mass.

The sample was dark gray and opaque.

$I/I_{corundum} = 8.8$.

Structural data. Rundle, Shull, and Wollan (1952) determined that zirconium dihydride has a body-centered tetragonal structure and $2(ZrH_2)$ per unit cell. The constants of Hägg have been converted to a body-centered cell.

Lattice constants

	a(Å)	*c(Å)*
Hägg (1930)	3.517	4.449
Rundle, Shull, and Wollan (1952)	3.520	4.449
NBS, sample at 25°C	3.5199	4.4500

The density of zirconium hydride calculated from the NBS lattice constants is 5.616 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
2.7608	100	101	32.40
2.4886	28	110	36.06
2.2248	11	002	40.51
1.7599	11	200	51.91
1.6587	17	112	55.34
1.4843	20	211	62.51
1.3804	8	202	67.83
1.3666	7	103	68.61
1.2443	2	220	76.51
1.1346	4	301	85.51
1.1128	4	310	87.60
1.0863	3	222	90.32
1.0797	6	213	91.02
1.0155	2	114	98.66
0.9955	5	312	101.38
.9537	3	321	107.73
.9403	2	204	110.00
.9204	2	303	113.63
.8801	1	400	122.14
.8628	2	105	126.45
.8386	3	411	133.42
.8294	3	330,224	136.46
.8184	2	402	140.48
.8156	4	323	141.63
.7869	6	420,314	156.41

References

Hägg, G. (1930). Röntgenuntersuchungen über die Hydride von Titan, Zirconium, Vanadin, und Tantal, Z. physik. Chem. B 11, 433.

Rundle, R. E., Shull, C. G., and Wollan, E. O. (1952). The crystal structure of thorium and zirconium dihydrides by x-ray and neutron diffraction, Acta Cryst. 5, 22-26.

Antimony Terbium, SbTb (cubic)

Additional published patterns. Olcese (1961).

Structural data. Brixner (1960) determined that antimony terbium is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(SbTb) per unit cell. The atoms occupy the special positions:

Sb: 0 0 0 ;F.C.
Tb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Brixner (1960)	6.178
Olcese (1961)	6.181
Iandelli (1961)	6.180

The lattice constant used in this calculated pattern is the average value a = 6.180 Å.

The calculated density is 7.898 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.57	3	111	24.93
3.09	100	200	28.87
2.18	69	220	41.28
1.863	1	311	48.81
1.784	23	222	51.16
1.545	10	400	59.81
1.418	<1	331	65.81
1.382	26	420	67.75
1.261	19	422	75.26
1.189	40	511	80.73
1.092	6	440	89.67
1.045	<1	531	95.01
1.030	12	600	96.80
0.977	9	620	104.0
.942	<1	533	109.6
.932	8	622	115.3
.892	3	444	119.4
.865	<1	711	125.8
.857	8	640	128.0
.826	16	642	137.7
.805	<1	731	146.4

Barium Selenide, BaSe (cubic)

Additional published pattern. Slattery (1925).

Structural data. Haase (1927) determined that barium selenide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(BaSe) per unit cell. The atoms occupy the special positions:

Ba: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

The lattice constant used in this calculated pattern is a = 6.600 Å as reported by Miller, Komarek, and Cadoff (1960).

The calculated density is 4.997 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.81	13	111	23.32
3.30	100	200	27.00
2.33	70	220	38.55
1.990	5	311	45.54
1.905	23	222	47.69
1.650	10	400	55.66
1.514	2	331	61.15
1.476	27	420	62.92
1.347	19	422	69.74
1.270	1	511	74.66
1.167	6	440	82.63
1.116	1	531	87.33
1.100	12	600	88.89
1.044	8	620	95.14
1.006	<1	533	99.86
0.995	7	622	101.4
.953	2	444	107.9
.924	<1	711	112.9
.915	6	640	114.6
.882	12	642	121.7
.859	1	731	127.4
.825	2	800	138.0
.806	<1	733	145.6
.800	13	820	148.5

Beryllium Cobalt, BeCo (cubic)

Structural data. Misch (1936) determined that beryllium cobalt is isostructural with cesium chloride with the space group O_h^1-Pm3m (No. 221) and 1(BeCo) per unit cell. The atoms occupy the special positions:

Be: 0 0 0
Co: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 2.611 Å as reported by Misch (1936).

The calculated density is 6.338 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
2.61	100	100	34.3
1.846	89	110	49.3
1.507	19	111	61.5
1.306	12	200	72.3
1.168	21	210	82.6
1.066	23	211	92.5
0.923	8	220	113.1
.870	12	300	124.5
.826	15	310	137.8
.787	11	311	156.2

Beryllium Palladium, BePd (cubic)

Structural data. Misch (1936) determined that beryllium palladium is isostructural with cesium chloride with the space group O_h^1-Pm3m (No. 221) and 1(BePd) per unit cell. The atoms occupy the special positions:

Be: 0 0 0
Pd: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 2.819 Å as reported by Misch (1936).

The calculated density is 8.554 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
2.82	100	100	31.7
1.993	82	110	45.5
1.628	21	111	56.5
1.410	11	200	66.2
1.261	23	210	75.3
1.151	21	211	84.0
0.997	7	220	101.22
.940	13	300	110.11
.891	13	310	119.55
.850	10	311	129.98
.814	4	222	142.35

Cadmium Cerium, CdCe (cubic)

Powder Diffraction File card. No. 2-1455, Iandelli and Botti (1937).

Structural data. Iandelli and Botti (1937) determined that cadmium cerium is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(CdCe) per unit cell. The atoms occupy the special positions:

Cd: 0 0 0
Ce: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.865 Å as reported by Iandelli and Botti (1937).

The calculated density is 7.262 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.86	1	100	23.0
2.73	100	110	32.7
2.23	<1	111	40.4
1.932	16	200	47.0
1.728	<1	210	52.9
1.578	31	211	58.4
1.366	9	220	68.6
1.288	<1	300	73.4
1.222	12	310	78.1
1.165	<1	311	82.8
1.116	3	222	87.3
1.072	<1	320	91.9
1.033	14	321	96.4
0.966	2	400	105.7
.937	<1	410	110.5
.911	9	411	115.4
.864	6	420	126.1
.843	<1	421	131.9
.824	6	332	138.4
.789	6	422	155.0

Cadmium Lanthanum, CdLa (cubic)

Powder Diffraction File card. No. 2-0855, Iandelli and Botti (1937).

Structural data. Iandelli and Botti (1937) determined that cadmium lanthanum is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(CdLa) per unit cell. The atoms occupy the special positions:

Cd: 0 0 0
La: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in the calculated pattern is a = 3.905 Å as reported by Iandelli and Botti (1937).

The calculated density is 7.008 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.90	1	100	22.8
2.76	100	110	32.4
2.25	<1	111	40.0
1.952	16	200	46.5
1.746	<1	210	52.3
1.594	31	211	57.8
1.381	9	220	67.8
1.302	<1	300	72.6
1.235	12	310	77.2
1.177	<1	311	81.7
1.127	3	222	86.2
1.044	14	321	95.1
0.976	2	400	104.2
.947	<1	410	108.8
.920	8	411	113.6
.873	5	420	123.8
.852	<1	421	129.4
.833	6	332	135.4
.797	6	422	150.2

Cadmium Praseodymium, CdPr (cubic)

Powder Diffraction File card. No. 2-1457, Iandelli and Botti (1937).

Structural data. Iandelli and Botti (1937) determined that cadmium praseodymium is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(CdPr) unit cell. The atoms occupy the special positions:

Cd: 0 0 0
Pr: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.830 Å as reported by Iandelli and Botti (1937).

The calculated density is 7.486 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.83	2	100	23.20
2.71	100	110	33.05
2.21	<1	111	40.77
1.915	16	200	47.43
1.713	<1	210	53.45
1.564	31	211	59.03
1.354	9	220	69.34
1.277	<1	300	74.22
1.211	12	310	78.98
1.155	<1	311	83.67
1.106	3	222	88.32
1.062	<1	320	92.96
1.024	14	321	97.61
0.958	2	400	107.1
.929	<1	410	112.0
.903	9	411	117.1
.856	6	420	128.2
.836	<1	421	134.3
.817	6	332	141.2

Calcium Selenide, CaSe (cubic)

Additional published pattern. Oftedal (1927).

Structural data. Oftedal (1927) determined that calcium selenide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(CaSe) per unit cell. The atoms occupy the special positions:

Ca: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Oftedal (1927)	5.924
Senff and Klemm (1939)	5.924

The lattice constant used in this calculated pattern is a = 5.924 Å.

The calculated density is 3.803 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.42	18	111	26.03
2.96	100	200	30.15
2.09	65	220	43.15
1.786	8	311	51.09
1.710	20	222	53.54
1.481	9	400	62.68
1.359	3	331	69.05
1.325	23	420	71.11
1.209	16	422	79.13
1.140	2	511	85.00
1.047	5	440	94.70
1.001	2	531	100.6
0.987	11	600	102.6
.937	8	620	110.6
.903	<1	533	117.0
.893	8	622	119.2
.855	2	444	128.5
.830	2	711	136.4
.822	8	640	139.3
.792	17	642	153.3

Cerium Magnesium, CeMg (cubic)

Powder Diffraction File card. No. 9-61, Rossi (1934).

Additional published pattern. Nowotny (1942).

Structural data. Nowotny (1942) determined that cerium magnesium is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(CeMg) per unit cell. The atoms occupy the special positions:

Ce: 0 0 0
Mg: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

Lattice constants

	a(Å)
Rossi (1934)	3.892
Nowotny (1942)	3.906

The calculations are based on the average value, a = 3.899 Å.

The calculated density is 4.606 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.90	62	100	22.8
2.76	100	110	32.4
2.25	17	111	40.0
1.950	16	200	46.5
1.744	21	210	52.4
1.592	31	211	57.9
1.378	9	220	67.9
1.300	9	300	72.7
1.233	12	310	77.3
1.176	5	311	81.9
1.126	3	222	86.4
1.081	4	320	90.8
1.042	14	321	95.3
0.975	1	400	104.4
.946	6	410	109.1
.919	8	411	113.9
.894	3	331	118.9
.872	5	420	124.1
.851	6	421	129.7
.831	5	332	135.8
.796	6	422	150.8

Cerium Zinc, CeZn (cubic)

Powder Diffraction File card. No. 2-0974, Iandelli and Botti (1937).

Structural data. Iandelli and Botti (1937) determined that cerium zinc is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(CeZn) per unit cell. The atoms occupy the special positions:

Ce: 0 0 0
Zn: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.704 Å as reported by Iandelli and Botti (1937).

The calculated density is 6.714 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.70	15	100	24.0
2.62	100	110	34.2
2.14	4	111	42.2
1.852	16	200	49.2
1.656	5	210	55.4
1.512	29	211	61.2
1.310	8	220	72.1
1.235	2	300	77.2
1.171	11	310	82.2
1.117	1	311	87.2
1.069	3	222	92.2
1.027	1	320	97.1
0.990	14	321	102.2
.926	2	400	112.6
.898	2	410	118.0
.873	9	411	123.8
.850	<1	331	130.0
.828	6	420	136.9
.808	2	421	144.7
.790	7	332	154.5

Dysprosium Gold, DyAu (cubic)

Structural data: Chao, Luo, and Duwez (1963) reported that dysprosium gold is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1 (DyAu) per unit cell. The atoms occupy the special positions:

Dy: 0 0 0
Au: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.555 Å as reported by Chao, Luo, and Duwez (1963).

The calculated density is 13.28 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I (Peak height)	hkl	2θ(°)
3.56	1	100	25.03
2.51	100	110	35.69
2.05	<1	111	44.08
1.778	16	200	51.36
1.590	<1	210	57.96
1.451	30	211	64.11
1.257	9	220	75.59
1.185	<1	300	81.08
1.124	12	310	86.50
1.072	<1	311	91.88
1.026	3	222	97.28
0.986	<1	320	102.7
.950	17	321	108.3
.889	2	400	120.2
.862	<1	410	126.6
.838	8	411	133.6
.816	<1	331	141.6
.795	9	420	151.4

Dysprosium Silver, DyAg (cubic)

Structural data. Baenziger and Moriarty (1961) determined that dysprosium silver is isostructural with cesium chloride with the space group O_h^1-Pm3m (No. 221) and 1(DyAg) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Dy: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.608 Å as reported by Baenziger and Moriarty (1961).

The calculated density is 9.558 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I (Peak height)	hkl	2θ(°)
3.61	4	100	24.65
2.55	100	110	35.14
2.08	1	111	43.40
1.804	15	200	50.55
1.614	2	210	57.03
1.473	29	211	63.06
1.276	8	220	74.29
1.203	<1	300	79.65
1.141	11	310	84.92
1.088	<1	311	90.15
1.042	3	222	95.38
1.001	<1	320	100.66
0.964	15	321	106.03
.902	2	400	117.28
.875	<1	410	123.34
.850	10	411	129.8
.828	<1	331	137.0
.807	7	420	145.4
.787	<1	421	156.1

Erbium Silver, ErAg (cubic)

Structural data: Chao, Luo, and Duwez (1963) reported that erbium silver is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(ErAg) per unit cell. The atoms occupy the special positions:

Er: 0 0 0
Ag: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

Lattice constants

	a(Å)
Dwight (1959a)	3.58
Chao, et al. (1963)	3.574

The lattice constant used in this calculated pattern is the average value a = 3.577 Å.

The calculated density is 9.98 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.57	5	100	24.9
2.53	100	110	35.5
2.06	1	111	43.8
1.787	15	200	51.1
1.598	2	210	57.6
1.459	28	211	63.7
1.264	8	220	75.1
1.191	<1	300	80.6
1.130	11	310	85.9
1.078	<1	311	91.2
1.032	3	222	96.6
0.991	<1	320	102.0
.955	15	321	107.5
.894	2	400	119.1
.867	<1	410	125.4
.842	11	411	132.2
.820	<1	331	139.9
.799	8	420	149.1

Gadolinium Indium, GdIn (cubic)

Structural data: Baenziger and Moriarty (1961) reported that gadolinium indium is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(GdIn) per unit cell. The atoms occupy the special positions:

Gd: 0 0 0
In : $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.830 Å as reported by Baenziger and Moriarty (1961).

The calculated density is 8.041 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.83	3	100	23.20
2.71	100	110	33.05
2.21	<1	111	40.77
1.915	16	200	47.43
1.713	<1	210	53.45
1.564	31	211	59.03
1.354	9	220	69.34
1.277	<1	300	74.22
1.211	12	310	78.98
1.155	<1	311	83.67
1.106	3	222	88.32
1.062	<1	320	92.96
1.024	15	321	97.61
0.958	2	400	107.1
.929	<1	410	112.0
.903	9	411	117.1
.879	<1	331	122.5
.856	6	420	128.2
.836	<1	421	134.3
.817	6	332	141.2

Gold Holmium, AuHo (cubic)

Structural data. Dwight (1961) reported that gold holmium is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1 (AuHo) per unit cell. The atoms occupy the special positions:

Au: 0 0 0
Ho: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

Lattice constants

	a(Å)
Dwight (1961)	3.549
Chao, et al. (1963)	3.541

The lattice constant used in this calculated pattern is the average value a = 3.545 Å.

The calculated density is 13.49 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.54	1	100	25.1
2.50	100	110	35.8
2.04	<1	111	44.3
1.770	16	200	51.6
1.584	<1	210	58.2
1.446	30	211	64.4
1.252	9	220	75.9
1.180	<1	300	81.5
1.120	12	310	86.9
1.068	<1	311	92.4
1.022	3	222	97.8
0.946	17	321	109.0
.885	2	400	120.9
.859	<1	410	127.5
.835	12	411	134.7
.792	9	420	153.2

Holmium Silver, HoAg (cubic)

Structural data. Walline and Wallace (1964) determined that holmium silver is isostructural with cesium chloride with the space group O_h^1-Pm3m (No. 221) and 1(HoAg) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Ho: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is the average value a = 3.593 Å.

The calculated density is 9.765 g/cm^3.

Lattice constants

	a(Å)
Dwight (1959a)	3.594
Chao, et al. (1963)	3.592

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.59	4	100	24.76
2.54	100	110	35.31
2.07	1	111	43.61
1.79	15	200	50.79
1.606	2	210	57.30
1.466	29	211	63.37
1.270	8	220	74.68
1.197	<1	300	80.08
1.136	11	310	85.39
1.083	<1	311	90.67
1.037	3	222	95.95
0.996	<1	320	101.3
.960	15	321	106.7
.898	2	400	118.1
.871	<1	410	124.3
.847	11	411	131.0
.824	<1	331	138.4
.803	8	420	147.1
.784	<1	421	158.6

Lanthanum Magnesium, LaMg (cubic)

Powder Diffraction File card. No. 9-241, Rossi (1934).

Additional published pattern. Nowotny (1942).

Structural data. Nowotny (1942) determined that lanthanum magnesium is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(LaMg) per unit cell. The atoms occupy the special positions:

La: 0 0 0
Mg: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$

Lattice constants

	a(Å)
Rossi (1934)	3.960
Nowotny (1942)	3.973

The calculations are based on the average value, a = 3.966 Å.

The calculated density is 4.345 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.97	62	100	22.40
2.80	100	110	31.88
2.29	16	111	39.31
1.983	16	200	45.71
1.774	20	210	51.48
1.619	31	211	56.81
1.402	9	220	66.64
1.322	9	300	71.27
1.254	12	310	75.78
1.196	5	311	80.20
1.145	3	222	84.56
1.100	4	320	88.89
1.060	14	321	93.22
0.992	1	400	102.0
.962	6	410	106.4
.935	8	411	111.0
.910	3	331	115.7
.887	5	420	120.6
.865	5	421	125.8
.846	5	332	131.3
.810	5	422	144.2
.793	4	500	152.4

Lanthanum Phosphide, LaP (cubic)

Additional published pattern. landelli and Botti (1936).

Structural data. Iandelli and Botti (1936) determined that lanthanum phosphide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(LaP) per unit cell. The atoms occupy the special positions:

La: 0 0 0 ;F.C.
P: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$;F.C.

The lattice constant used in this calculated pattern is a = 6.025 Å as reported by landelli and Botti (1936).

The calculated density is 5.159 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.48	78	111	25.6
3.01	100	200	29.6
2.13	66	220	42.4
1.817	32	311	50.2
1.739	22	222	52.6
1.506	10	400	61.5
1.382	12	331	67.7
1.347	25	420	69.7
1.230	18	422	77.6
1.160	8	511	83.3
1.065	6	440	92.6
1.018	9	531	98.3
1.004	12	600	100.2
0.953	9	620	107.9
.919	4	533	113.9
.908	9	622	116.0
.870	3	444	124.7
.844	7	711	131.8
.836	8	640	134.4
.805	17	642	146.2
.784	13	731	158.2

Lanthanum Zinc, LaZn (cubic)

Powder Diffraction File card. No. 2-1460, Iandelli and Botti (1937).

Structural data. Iandelli and Botti (1937) determined that lanthanum zinc is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(LaZn) per unit cell. The atoms occupy the special positions:

La: 0 0 0
Zn: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.760 Å as reported by Iandelli and Botti (1937).

The calculated density is 6.381 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.76	14	100	23.64
2.66	100	110	33.68
2.17	4	111	41.56
1.880	16	200	48.37
1.682	5	210	54.52
1.535	30	211	60.24
1.329	9	220	70.82
1.253	2	300	75.84
1.189	11	310	80.75
1.134	1	311	85.60
1.085	3	222	90.41
1.043	1	320	95.23
1.005	14	321	100.1
0.940	2	400	110.0
.912	2	410	115.3
.886	9	411	120.7
.863	<1	331	126.5
.841	6	420	132.7
.820	2	421	139.7
.802	6	332	147.8

Magnesium Selenide, MgSe (cubic)

Additional published pattern. Broch (1927).

Structural data. Broch (1927) determined that magnesium selenide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(MgSe) per unit cell. The atoms occupy the special positions:

Mg: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

The lattice constant used in this calculated pattern is a = 5.462 Å as reported by Broch (1927).

The calculated density is 4.209 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.15	54	111	28.3
2.73	100	200	32.8
1.931	64	220	47.0
1.647	19	311	55.8
1.577	20	222	58.5
1.366	9	400	68.7
1.253	7	331	75.9
1.221	22	420	78.2
1.115	16	422	87.4
1.051	6	511	94.2
0.966	5	440	105.8
.923	7	531	113.1
.910	13	600	115.6
.864	10	620	126.2
.833	3	533	135.2
.823	9	622	138.6
.788	4	444	155.4

Neodymium Selenide, NdSe (cubic)

Structural data. Iandelli (1955) determined that neodymium selenide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(NdSe) per unit cell. The atoms occupy the special positions:

Nd: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Iandelli (1955)	5.909
Guittard and Benecerraf (1959)	5.891

The lattice constant used in this calculated pattern is the average value a = 5.900 Å.

The calculated density is 7.218 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.41	16	111	26.1
2.95	100	200	30.3
2.09	67	220	43.3
1.779	7	311	51.3
1.703	22	222	53.8
1.475	9	400	63.0
1.354	2	331	69.4
1.319	25	420	71.4
1.204	18	422	79.5
1.135	2	511	85.4
1.043	6	440	95.2
0.997	2	531	101.1
.983	13	600	103.1
.933	9	620	111.3
.900	<1	533	117.8
.889	9	622	120.0
.852	3	444	129.5
.826	2	711	137.6
.818	9	640	140.6
.788	20	642	155.4

Neodymium Silver, NdAg (cubic)

Structural data. Iandelli (1960) reported that neodymium silver is isostructural with cesium chloride with the space group O_h^1-Pm3m (No. 221) and 1(NdAg) per unit cell. The atoms occupy the special positions:

Nd: 0 0 0
Ag: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

Lattice constants

	a(Å)
Dwight (1959a)	3.722
Iandelli (1960)	3.711
Ferro (1955)	3.714

The lattice constant used in this calculated pattern is the average value a = 3.716 Å.

The calculated density is 8.158 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.71	2	100	23.9
2.63	100	110	34.1
2.14	<1	111	42.1
1.857	16	200	49.0
1.661	<1	210	55.3
1.516	29	211	61.1
1.313	8	220	71.8
1.238	<1	300	77.0
1.174	11	310	82.0
1.120	<1	311	86.9
1.072	3	222	91.9
1.030	<1	320	96.8
0.993	14	321	101.8
.928	2	400	112.1
.901	<1	410	117.5
.875	9	411	123.3
.852	<1	331	129.4
.830	6	420	136.1
.810	<1	421	143.8
.792	7	332	153.2

Palladium Hydride, $PdH_{0.706}$ (cubic)

Structural data. Worsham, Wilkinson, and Shull (1957) determined that palladium hydride is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(PdH) per unit cell. The atoms occupy the special positions:

Pd: 0 0 0 ;F.C.
H: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$;F.C.

The lattice constant used in this calculated pattern is a = 4.02 Å as reported by Worsham, Wilkinson, and Shull (1957).

The calculated density is 11.0 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
2.32	100	111	38.8
2.01	49	200	45.1
1.42	26	220	65.6
1.21	29	311	78.9
1.16	8	222	83.2
1.00	4	400	100.1
0.922	15	331	113.3
.899	14	420	117.9
.821	14	422	139.7

Praseodymium Zinc, PrZn (cubic)

Powder Diffraction File card. No. 2-0994, Iandelli and Botti (1937).

Structural data. Iandelli and Botti (1937) determined that praseodymium zinc is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(PrZn) per unit cell. The atoms occupy the special positions:

Pr: 0 0 0
Zn: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.678 Å as reported by Iandelli and Botti (1937).

The calculated density is 6.884 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.68	16	100	24.2
2.60	100	110	34.4
2.12	4	111	42.5
1.839	16	200	49.5
1.645	5	210	55.8
1.501	29	211	61.7
1.300	8	220	72.6
1.226	2	300	77.8
1.163	11	310	82.9
1.109	1	311	88.0
1.062	3	222	93.0
1.020	1	320	98.1
0.983	15	321	103.2
.920	2	400	113.8
.892	2	410	119.4
.867	9	411	125.4
.844	1	331	131.8
.822	7	420	139.0
.803	2	421	147.4
.784	8	332	158.4

Rubidium Amide, $RbNH_2$ at 50°C (cubic)

Powder Diffraction File card. No. 12-748, Juza and Mehne (1959).

Structural data. Juza and Mehne (1959) determined that rubidium amide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4($RbNH_2$) per unit cell. The atoms occupy the special positions:

Rb: 0 0 0 ;F.C.
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.
H: Undetermined

The lattice constant used in this calculated pattern is a = 6.395 Å as reported by Juza and Mehne (1959).

The calculated density is 2.577 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.69	100	111	24.08
3.20	100	200	27.88
2.26	65	220	39.84
1.928	42	311	47.09
1.846	21	222	49.32
1.599	9	400	57.60
1.467	15	331	63.34
1.430	23	420	65.18
1.305	16	422	72.32
1.231	11	511	77.49
1.130	5	440	85.90
1.081	11	531	90.89
1.066	10	600	92.55
1.011	7	620	99.24
0.975	4	533	104.3
.964	6	622	106.1
.923	2	444	113.1
.895	7	711	118.7
.887	6	640	120.6
.855	11	642	128.7
.833	11	731	135.4
.799	2	800	149.0

Samarium Silver, SmAg (cubic)

Structural data: Walline and Wallace (1964) reported that samarium silver is isostructural with cesium chloride, with the space group O_h^1-Pm3m (No. 221) and 1(SmAg) per unit cell. The atoms occupy the special positions:

Sm: 0 0 0
Ag: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

Lattice constants

	a(Å)
Dwight (1959a)	3.678
Iandelli (1960)	3.684
Chao, et al. (1963)	3.673

The lattice constant used in this calculated pattern is the average value a = 3.678 Å.

The calculated density is 8.617 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.67	3	100	24.2
2.60	100	110	34.5
2.12	<1	111	42.6
1.836	16	200	49.6
1.643	1	210	55.9
1.500	29	211	61.8
1.299	8	220	72.8
1.224	<1	300	78.0
1.162	11	310	83.1
1.107	<1	311	88.1
1.060	3	222	93.2
1.019	<1	320	98.2
0.982	15	321	103.4
.918	2	400	114.0
.891	<1	410	119.7
.866	10	411	125.7
.843	<1	331	132.2
.821	7	420	139.4
.802	<1	421	147.9
.783	8	332	159.2

Silver Terbium, AgTb (cubic)

Structural data: Walline and Wallace (1964) reported that silver terbium is isostructural with cesium chloride, with the space group 0_h^1-Pm3m (No. 221) and 1(AgTb) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Tb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.625 Å as reported by Chao, Luo, and Duwez (1963).

The calculated density is 9.300 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.62	4	100	24.54
2.56	100	110	34.97
2.09	1	111	43.19
1.812	15	200	50.30
1.621	1	210	56.74
1.480	29	211	62.73
1.282	8	220	73.88
1.208	<1	300	79.20
1.146	11	310	84.43
1.093	<1	311	89.61
1.046	3	222	94.79
1.005	<1	320	100.0
0.969	15	321	105.3
.906	2	400	116.4
.879	<1	410	122.4
.854	10	411	128.7
.832	<1	331	135.7
.811	7	420	143.7
.791	<1	421	153.7

Silver Thulium, AgTm (cubic)

Structural data: Chao, Luo, and Duwez (1963) reported that silver thulium is isostructural with cesium chloride, with the space group 0_h^1-Pm3m(No. 221) and 1(AgTm) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Tm: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.562 Å as reported by Chao, Luo, and Duwez (1963).

The calculated density is 10.17 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.56	5	100	24.98
2.52	100	110	35.61
2.06	2	111	43.99
1.781	16	200	51.25
1.593	2	210	57.83
1.454	29	211	63.97
1.259	8	220	75.41
1.187	1	300	80.89
1.126	11	310	86.28
1.074	<1	311	91.65
1.028	3	222	97.02
0.988	<1	320	102.5
.952	5	321	108.0
.890	2	400	119.8
.864	<1	410	126.2
.840	7	411	133.1
.817	<1	331	141.0
.796	8	420	150.5

Silver Yttrium, AgY (cubic)

Structural data. Moriarty et al. (1966) reported that silver yttrium is isostructural with cesium chloride with the space group O_h^1-Pm3m (No. 221) and 1(AgY) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Y: $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$

Lattice constants

	a(Å)
Dwight (1959b)	3.617
Bruzzone, et al. (1962)	3.619
Moriarty, et al. (1966)	3.6196

The lattice constant used in this calculated pattern is a = 3.6196 Å as reported by Moriarty et al. (1966).

The calculated density is 6.890 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I (Peak height)	hkl	2θ(°)
3.62	1	100	24.6
2.56	100	110	35.0
2.09	<1	111	43.3
1.808	15	200	50.4
1.618	<1	210	56.8
1.477	27	211	62.8
1.279	8	220	74.1
1.206	1	300	79.4
1.144	11	310	84.6
1.044	3	222	95.0
0.967	14	321	105.5
.904	2	400	116.7
.877	1	410	122.7
.853	9	411	129.1
.809	7	420	144.2
.789	<1	421	154.4

Terbium Arsenide, TbAs (cubic)

Additional published pattern. Olcese (1961).

Structural data. Brixner (1960) determined that terbium arsenide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(TbAs) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0 ;F.C.
As: $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Brixner (1960)	5.813
Olcese (1961)	5.827
Iandelli (1961)	5.827

The lattice constant used in this calculated pattern is the average value a = 5.822 Å.

The calculated density is 7.870 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I (Peak height)	hkl	2θ(°)
3.36	24	111	26.5
2.91	100	200	30.7
2.06	88	220	44.0
1.755	13	311	52.1
1.680	29	222	54.6
1.455	13	400	63.9
1.335	5	331	70.5
1.301	33	420	72.6
1.188	24	422	80.8
1.120	4	511	86.9
1.029	8	440	97.0
0.984	4	531	103.1
.970	17	600	105.1
.920	13	620	113.6
.888	2	533	120.4
.877	13	622	122.8
.840	4	444	133.0
.815	4	711	141.9
.807	13	640	145.2

Terbium Phosphide, TbP (cubic)

Additional published pattern. Olcese (1961).

Structural data. Olcese (1961) determined that terbium phosphide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(TbP) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0;F.C.
P: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Iandelli (1961)	5.686
Olcese (1961)	5.688

The lattice constant used in this calculated pattern is the average value a = 5.687 Å.

The calculated density is 6.857 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.28	89	111	27.1
2.84	100	200	31.4
2.01	66	220	45.0
1.715	35	311	53.4
1.642	21	222	56.0
1.422	9	400	65.6
1.305	13	331	72.4
1.272	24	420	74.6
1.161	18	422	83.1
1.095	9	511	89.5
1.006	6	440	100.0
0.961	11	531	106.5
.948	14	600	108.7
.899	10	620	117.9
.867	5	533	125.3
.858	10	622	127.9
.821	3	444	139.6
.796	11	711	150.6
.789	12	640	155.2

Terbium Selenide, TbSe (cubic)

Additional published pattern. Olcese (1961).

Structural data. Olcese (1961) determined that terbium selenide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(TbSe) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Iandelli (1961)	5.740
Olcese (1961)	5.741

The lattice constant used in this calculated pattern is a = 5.741 Å.

The calculated density is 8.350 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.31	22	111	26.87
2.87	100	200	31.13
2.03	66	220	44.60
1.731	9	311	52.84
1.657	22	222	55.39
1.435	9	400	64.91
1.317	3	331	71.58
1.284	25	420	73.74
1.172	18	422	82.19
1.105	2	511	88.40
1.015	6	440	98.75
0.970	3	531	105.1
.957	14	600	107.2
.908	10	620	116.1
.875	1	533	123.2
.865	10	622	125.7
.829	3	444	136.7
.804	3	711	146.7
.796	10	640	150.7

Terbium Sulfide, TbS (cubic)

Additional published pattern. Olcese (1961).

Structural data. Olcese (1961) determined that terbium sulfide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(TbS) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0 ;F.C.
S: $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Iandelli (1961)	5.517
Olcese (1961)	5.516

The lattice constant used in this calculated pattern is a = 5.516 Å.

The calculated density is 7.558 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I (Peak height)	hkl	2θ(°)
3.18	83	111	27.99
2.76	100	200	32.43
1.950	63	220	46.53
1.663	33	311	55.18
1.592	20	222	57.86
1.379	9	400	67.91
1.265	12	331	74.99
1.233	23	420	77.29
1.126	18	422	86.33
1.062	9	511	93.04
0.975	6	440	104.4
.932	11	531	111.4
.919	14	600	113.8
.872	11	620	124.0
.841	5	533	132.6
.832	11	622	135.7
.796	4	444	150.7

Terbium Telluride, TbTe (cubic)

Additional published pattern. Olcese (1961).

Structural data. Brixner (1960) determined that terbium telluride is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(TbTe) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0 ;F.C.
Te: $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Brixner (1960)	6.101
Iandelli (1961)	6.101
Olcese (1961)	6.102

The lattice constant used in this calculated pattern is a = 6.101 Å.

The calculated density is 8.380 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I (Peak height)	hkl	2θ(°)
3.52	3	111	25.26
3.05	100	200	29.25
2.16	68	220	41.84
1.840	1	311	49.50
1.762	22	222	51.86
1.526	10	400	60.65
1.400	<1	331	66.76
1.364	26	420	68.74
1.246	19	422	76.40
1.174	<1	511	81.98
1.079	6	440	91.13
1.031	<1	531	96.62
1.017	13	600	98.47
0.965	9	620	105.9
.931	<1	533	111.7
.920	8	622	113.7
.881	3	444	122.0
.854	<1	711	128.7
.846	8	640	131.1
.815	17	642	141.7
.794	<1	731	151.7

Uranium Oxide, UO (cubic)

Structural data. Rundle, Wilson, Baenziger, and Trevebaugh (1958) determined that uranium oxide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(UO) per unit cell. The atoms occupy the special positions:

U: 0 0 0 ;F.C.
O: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

The lattice constant used in this calculated pattern is a = 4.91 Å as reported by Rundle, Wilson, Baenziger, and Trevebaugh (1958).

The calculated density is 14.3 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
2.83	100	111	31.5
2.46	66	200	36.6
1.74	41	220	52.7
1.48	36	311	62.7
1.42	13	222	65.8
1.23	6	400	77.7
1.13	15	331	86.3
1.10	16	420	89.1
1.00	13	422	100.4
0.945	13	511	109.2
.868	5	440	125.1
.830	19	531	136.3
.818	15	600	140.5

Uranium Selenide, USe (cubic)

Structural data. Ferro (1954) determined that uranium selenide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(USe) per unit cell. The atoms occupy the special positions:

U: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

The lattice constant used in this calculated pattern is a = 5.751 Å as reported by Ferro (1954). Khodadad (1961) gives a = 5.66 Å.

The calculated density is 11.07 g/cm^3, based on the value a = 5.751 Å.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	*I(Peak height)*	*hkl*	*2θ(°)*
3.32	46	111	26.8
2.88	100	200	31.1
2.03	68	220	44.5
1.734	19	311	52.8
1.660	22	222	55.3
1.438	10	400	64.8
1.319	7	331	71.4
1.286	26	420	73.6
1.174	19	422	82.0
1.107	5	511	88.2
1.017	6	440	98.5
0.972	6	531	104.8
.958	14	600	107.0
.909	11	620	115.8
.877	3	533	122.9
.867	10	622	125.4
.830	4	444	136.2
.805	6	711	146.1
.798	12	640	150.0

Ytterbium Selenide, YbSe (cubic)

Additional published pattern. Senff and Klemm (1939).

Structural data. Senff and Klemm (1939) determined that ytterbium selenide is isostructural with sodium chloride with the space group O_h^5-Fm3m and 4(YbSe) per unit cell. The atoms occupy the special positions:

Yb: 0 0 0 ;F.C.
Se: $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Senff and Klemm (1939)	5.879
Iandelli (1961)	5.931
Miller, et al. (1962)	5.94

Senff and Klemm (1939) identified the presence of 0.9 weight percent of an impurity. The lattice constant a = 5.935 Å used to calculate this pattern is an average of the last two values above.

The calculated density is 8.006 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.43	26	111	26.0
2.97	100	200	30.1
2.10	68	220	43.1
1.789	11	311	51.0
1.713	22	222	53.4
1.484	10	400	62.6
1.362	4	331	68.9
1.327	25	420	71.0
1.211	18	422	79.0
1.142	3	511	84.8
1.049	6	440	94.5
1.003	3	531	100.3
0.989	13	600	102.3
.938	10	620	110.3
.905	1	533	116.7
.895	9	622	118.8
.857	3	444	128.1
.831	3	711	135.9
.823	9	640	138.7
.793	20	642	152.4

Ytterbium Telluride, YbTe (cubic)

Additional published pattern. Senff and Klemm (1939).

Structural data. Senff and Klemm (1939) determined that ytterbium telluride is isostructural with sodium chloride, with the space group O_h^5-Fm3m (No. 225) and 4(YbTe) per unit cell. The atoms occupy the special positions:

Yb: 0 0 0 ;F.C.
Te: $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$;F.C.

Lattice constants

	a(Å)
Senff and Klemm (1939)	6.353
Iandelli (1961)	6.361
Miller, et al. (1962)	6.37

Senff and Klemm (1939) identified the presence of 0.6 weight percent of an impurity. The lattice constant a = 6.365 Å used to calculate this pattern is an average of the last two values above.

The calculated density is 7.743 g/cm³.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.67	5	111	24.2
3.18	100	200	28.0
2.25	70	220	40.0
1.919	2	311	47.3
1.837	23	222	49.6
1.591	10	400	57.9
1.460	<1	331	63.7
1.423	27	420	65.5
1.299	19	422	72.7
1.225	<1	511	77.9
1.125	6	440	86.4
1.076	<1	531	91.4
1.061	12	600	93.1
1.006	9	620	99.9
0.971	<1	533	105.0
.960	8	622	106.8
.919	3	444	113.9
.891	<1	711	119.6
.883	7	640	121.5
.851	15	642	129.8
.829	<1	731	136.7
.796	2	800	151.0

Yttrium Sulfide, YS (cubic)

Structural data. Picon and Patrie (1956) determined that yttrium sulfide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(YS) per unit cell. The atoms occupy the special positions:

Y: 0 0 0 ;F.C.
S: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

The lattice constant used in this calculated pattern is a = 5.466 Å as reported by Flahaud and Guittard (1956). Iandelli (1961) reports a value a = 5.493 Å.

The calculated density is 4.920 g/cm^3, based on the value a = 5.466 Å.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.16	43	111	28.2
2.73	100	200	32.7
1.933	61	220	47.0
1.648	16	311	55.7
1.578	19	222	58.4
1.366	8	400	68.6
1.254	6	331	75.8
1.222	21	420	78.1
1.116	16	422	87.3
1.052	4	511	94.2
0.966	6	440	105.7
.924	5	531	113.0
.911	13	600	115.4
.864	10	620	126.1
.834	2	533	135.0
.824	10	622	138.4
.789	4	444	155.0

Zirconium Nitride, ZrN (cubic)

Powder diffraction file card. No. 2-0956, General Electric Co.

Additional published patterns. Becker and Ebert (1925) and van Arkel (1924).

Structural data. Becker and Ebert (1925) determined that zirconium nitride is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(ZrN) per unit cell. The atoms occupy the special positions:

Zr: 0 0 0 ;F.C.
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

The lattice constant used in this calculated pattern is a = 4.575 Å as reported by Baker (1958).

The calculated density is 7.298 g/cm^3.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
2.64	100	111	33.91
2.29	85	200	39.35
1.618	47	220	56.87
1.379	32	311	67.89
1.321	13	222	71.35
1.144	6	400	84.67
1.050	13	331	94.42
1.023	18	420	97.69
0.934	15	422	111.1
.880	13	511	122.0
.809	8	440	144.5

Zirconium Oxide, ZrO (cubic)

Structural data. Samsonov (1957) determined that zirconium oxide is isostructural with sodium chloride with the space group O_h^5-Fm3m (No. 225) and 4(ZrO) per unit cell. The atoms occupy the special positions:

Zr: 0 0 0 ;F.C.
O: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$;F.C.

The lattice constant used in this calculated pattern is a = 4.62 Å as reported by Schönberg (1954) The calculated density is 7.22 g/cm³.
Elliott (1965) describes the compound as unstable.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
2.67	100	111	33.6
2.31	98	200	39.0
1.63	55	220	56.3
1.39	33	311	67.1
1.33	15	222	70.6
1.16	7	400	83.6
1.06	13	331	93.2
1.03	20	420	96.4
0.943	17	422	109.5
.889	13	511	120.1
.817	8	440	141.2

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

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

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

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CUMULATIVE INDEX—Continued

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CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE MINERAL INDEX

*Natural mineral.

m—Monograph 25.

CUMULATIVE MINERAL INDEX—Continued

*Natural mineral.

M—Monagraph 25.

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