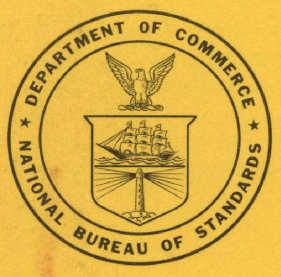
NBS MONOGRAPH 25—SECTION 6

Standard X-ray Diffraction Powder Patterns



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Standard X-ray Diffraction Powder Patterns

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

National Bureau of Standards Monograph 25—Section 6

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Contents

*A mineral name in parentheses indicates a synthetic sample.

Errata

Monograph 25, Section 6

Circular 539

Vol. 2, p. 32; The space group should be Pbma, from the reference: Byström, Arkiv Kemi Mineral. Geol. 25A, 1-26 (1947).
Vol. 9, p. 3: The corrected *hkl* values are: 214(d = 1.404), 131(d = 1.1382), 042(d = 1.0175), and 2·1·10(d = 0.9976).

Monograph 25

Sec. 1, p. 35; The space group should be $P2_13$, from the reference Bokiĭ and Tsinober, Tr. Inst. Kristallogr. Akad. Nauk SSSR *9*, 239-250 (1954).
Sec. 3, p. 5; Insert a new line of data:

242,341	1.7427	<2

Sec. 3, p. 45; Line 21 of the table should have the indices 201, $\bar{2}\bar{2}2$.
Sec. 5, p. 19; The title should be $CsCdCl_3$. Also, the line at d = 1.4200 should have the index 1·1·12.
Sec. 5, p. 20; The title should be $CsCdCl_3$.

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).
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NBS Circular 539, Volume 4, Standard X-ray Diffraction Powder Patterns (Data for 42 substances).
NBS Circular 539, Volume 5, Standard X-ray Diffraction Powder Patterns (Data for 45 substances).
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).
NBS Circular 539, Volume 9, Standard X-ray Diffraction Powder Patterns (Data for 43 substances).
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NBS Monograph 25, Section 4, Standard X-ray Diffraction Powder Patterns (Data for 103 substances) 55 cents.
NBS Monograph 25, Section 5, Standard X-ray Diffraction Powder Patterns (Data for 60 substances) 55 cents.

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 6.—Data for 60 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 60 substances. Fifty-four of these patterns represent experimental data and 6 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 weight percent mixture are given for 98 materials.

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

INTRODUCTION

The X-ray Powder Diffraction File (1967)[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 Standards.[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 60 compounds, 54 experimental and 6 calculated patterns. This compilation is the sixteenth 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 1966 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 weight 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. The assignment of *hkl's* and the refinement of lattice constants were obtained by using a computer program developed by Evans, Appleman and Handwerker (1963). Cell refinement was based only upon 2θ-values which could be indexed without ambiguity. The number of significant figures reported for d-values varies slightly with the symmetry and crystallinity of each sample. Lattice constant errors 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 Powder Diffraction Standards.

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

[3] This committee is sponsored jointly by the American Society for Testing and Materials, the American Crystalographic Association, The (British) Institute of Physics, and The National Association of Corrosion Engineers. 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.

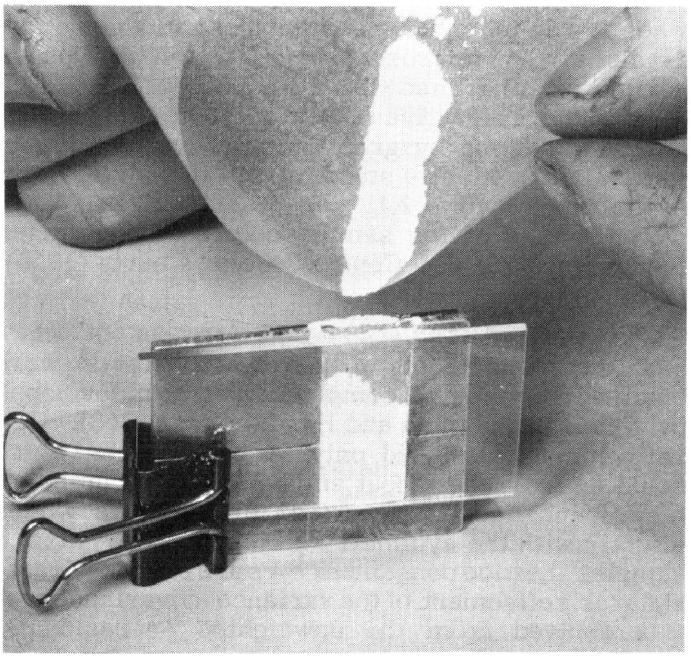

Figure 1

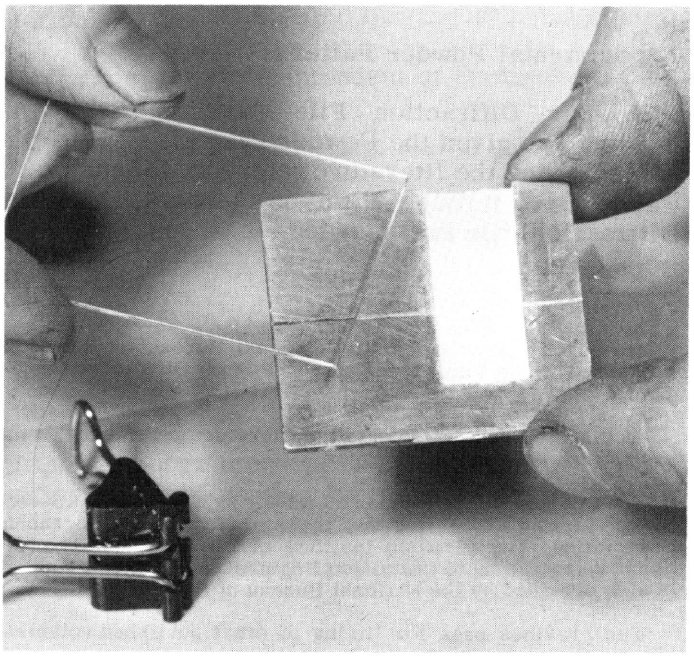

Figure 2

Calculated Powder Patterns

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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Ibid. (1962a). **III** 202-209.
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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.

Swanson, H. E., Morris, M. C., and Evans, E. H. (1966). Standard X-ray Diffraction Powder Patterns, Natl. Bur. Std. U.S. Monograph **25**, Sec. **4**, 3.

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. However this original attempt to establish absolute values started by the Dow Chemical Co. 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 of its chemical stability and freedom from shape orientation in sample preparation and partly because of its availability in approximately one micron particle size (Linde "A", Union Carbide Corp., East Chicago, Ind.).

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 38 $I/I_{corundum}$ 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 Powder Diffraction File.

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

Ammonium Bromide, NH_4Br (cubic)	6.0
Ammonium Chloride, NH_4Cl (cubic)	5.8
Ammonium Iodide, NH_4I (cubic)	6.1
Ammonium Nitrate, NH_4NO_3 (orthorhombic)	1.5
Ammonium Sulfate, $(NH_4)_2SO_4$ (orthorhomibc)	1.8
Barium Carbonate, $BaCO_3$ (orthorhombic)	4.2
Barium Sulfate, $BaSO_4$ (orthorhombic)	2.6
Cadmium, Cd (hexagonal)	2.0
Cadmium Carbonate, $CdCO_3$ (trigonal)	4.7
Cadmium Chloride, $CdCl_2$ (trigonal)	4.2
Cadmium Oxide, CdO (cubic)	8.6
Calcium Fluoride, CaF_2 (cubic)	2.4
Cesium Bromide, CsBr (cubic)	8.7
Chromium Oxide, Cr_2O_3 (trigonal)	1.8
Copper Chloride, CuCl (cubic)	2.0
Copper Carbonate, basic, $Cu_2(OH)_2CO_3$ (monoclinic)	0.6
Copper Oxide, CuO (monoclinic)	1.9
Iron Oxide, alpha, Fe_2O_3 (trigonal)	2.6
Lead Bromide, $PbBr_2$ (orthorhombic)	2.1
Lead Fluoride, alpha, PbF_2 (orthorhombic)	4.2
Lead Iodide, PbI_2 (trigonal)	4.2
Lead Oxide, yellow, PbO (orthorhombic)	6.6
Lead Sulfate, $PbSO_4$ (orthorhombic)	3.5
Lithium Fluoride, LiF (cubic)	1.3
Magnesium Oxide, MgO (cubic)	2.4
Magnesium Fluoride, MgF_3 (tetragonal)	0.4
Molybdenum Oxide, MoO_3 (orthorhombic)	3.0
Potassium Bromide, KBr (cubic)	5.5
Potassium Chloride, KCl (cubic)	3.9
Potassium Iodide, KI (cubic)	4.2
Potassium Nitrate, KNO_3 (orthorhombic)	1.4
Silver Bromide, AgBr (cubic)	5.6
Silver Oxide, Ag_2O (cubic)	5.6
Sodium Chloride, NaCl (cubic)	3.8
Sodium Sulfate, Na_2SO_4 (orthorhombic)	1.5
Strontium Nitrate, $SrNO_3$ (cubic)	3.2
Strontium Sulfate, $SrSO_4$ (orthorhombic)	1.8
Zinc Oxide, ZnO (hexagonal)	4.5

Sample

The sample was prepared at NBS by partial evaporation at 90° C of a water solution of $(NH_4)_2SO_4$ and $CdSO_4$, in a 2:1 weight ratio. The resulting double salt was washed with water and alcohol.

Major impurities

0.001-0.01% each: Ca, Mg, and Mn

Color

Colorless

Optical data

Isotropic, N=1.603

Structure

Cubic, $P2_13$ (198) Z=4, langbeinite type, [Gattow and Zemann,1958].

Lattice constants

	a(Å)
Jona and Pepinsky [1956]--------	10.35 ±.005
Gattow and Zemann [1958]--------	10.350 ±.003
NBS, sample at 25 °C----------	10.3511 ±.0001

Density

(calculated) 3.288 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.8$

Polymorphism

Inverts below -186° C to a ferroelectric form [Jona and Pepinsky, 1956].

References

Gattow, G.and J.Zemann(1958). Über Doppelsulfate vom Langbeinit-Typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. 293, 233-240.

Jona, F. and R. Pepinsky (1956). Ferroelectricity in the langbeinite system, Phy. Rev. 103, 1126.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.973	50	111	14.82
4.628	63	210	19.16
4.225	11	211	21.01
3.449	20	221	25.81
3.271	100	310	27.24
3.121	11	311	28.58
2.870	9	320	31.14
2.765	65	321	32.35
2.587	1	400	34.65
2.511	9	410	35.73
2.441	1	411	36.79
2.375	5	331	37.85
2.259	6	421	39.88
2.207	1	332	40.86
2.113	20	422	42.76
2.071	10	430	43.68
2.030	20	510	44.59
1.993	13	511	45.48
1.922	18	520	47.26
1.890	1	521	48.10
1.831	1	440	49.77
1.801	10	522	50.64
1.774	6	530	51.46
1.750	1	531	52.22
1.703	1	610	53.80
1.6788	17	611	54.62
1.6364	7	620	56.16
1.6166	8	621	56.91
1.5974	6	541	57.66
1.5786	2	533	58.41
1.5606	1	622	59.15
1.5433	3	630	59.88
1.5260	7	631	60.63
1.4938	2	444	62.08
1.4784	5	632	62.80
1.4640	5	710	63.49
1.4497	3	711	64.19
1.4360	1	640	64.88
1.4219	5	720	65.60
1.4086	3	721	66.30

Ammonium Nickel(II) Trichloride, NH_4NiCl_3 (hexagonal)

Sample source
The sample was made at NBS by heating $NiCl_2$ and NH_4Cl together at 300°C for 72 hours in a sealed glass tube. The $NiCl_2$ had been obtained by dehydrating $NiCl_2 \cdot 2H_2O$ in a stream of dry HCl at 150°C. NH_4NiCl_3 is hygroscopic.

Major impurities
0.001-0.01% each: Fe

0.01 -0.1 % each: Cu

Color
Pale orange yellow.

Optical data
Uniaxial (+) N_O=1.720, N_e=1.89 Pleochroism with the stronger absorption perpendicular to c.

Structure
Isostructural with $RbCoCl_3$ and other similar ABX_3 compounds.

Space group
D_{6h}^4-$P6_3/mmc$ (194) Z=2. By comparison of the powder pattern with that of $RbCoCl_3$.

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25° C-----	6.9216 ±.0004	5.915 ±.001

Density
(calculated) 2.478 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 3.7

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

d (Å)	I	hkl	2θ(°)
5.98	100	100	14.80
4.211	6	101	21.08
3.459	9	110	25.73
2.998	2	200	29.77
2.957	6	002	30.20
2.675	43	201	33.47
2.266	8	210	39.74
2.249	11	112	40.05
2.104	17	202	42.94
1.998	2	300	45.34
1.894	1	301	47.98
1.799	5	212	50.70
1.731	10	220	52.84
1.663	7	310	55.19
1.656	7	302	55.44
1.601	1	311	57.51
1.4931	3	222	62.11
1.4790	2	004	62.77
1.4527	2	401	64.04
1.4495	3	312	64.20
1.4353	3	104	64.91
1.3753	2	320	68.12
1.3366	1	402	70.38
1.3081	1	410	72.15
1.2774	1	411	74.17
1.1961	2	412	80.18
1.1933	2	403	80.40
1.1752	1	501	81.90
1.1239	2	224	86.52
1.1124	2	421	87.64
1.0763	1	510	91.39
1.0745	1	332	91.59
1.0578	1	422	93.46

Bis (o-dodecacarborane), $C_4B_{20}H_{22}$ (monoclinic)

Sample source

The sample was obtained from Rohm and Haas Chemical Division of the Redstone Arsenal, Huntsville, Alabama. Treating the sample by the usual methods failed to improve the quality of the pattern.

Color

Colorless

Optical data

Biaxial (-), N_α=1.646, N_β=1.681, N_γ=1.683
2V is small.

Structure

Determined by Hall et al.[1965].

Space group

C_{2h}^5-$P2_1/n$ (14), Z=2 [Hall et al., 1965]

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Hall et al. [1965]—	7.014 ±.001	9.862 ±.001	12.360 ±.002	90°31′ ±2′
NBS, sample at 25°C--	7.016 ±.002	9.867 ±.003	12.376 ±.004	90°29′ ±2′

Density

(calculated) 1.110 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.5 (based upon double peak 012,111)

References

Hall, L.H., A. Perloff, F.A. Mauer, and S. Block, (1965). Crystal and molecular structure of $C_4B_{20}H_{22}$, Bis (o-dodecacarborane), J. Chem. Phys. **43**, No. 11, 3911-3917.

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

d (Å)	I	hkl	2θ(°)
7.71	71	011	11.47
6.12	90	$\bar{1}01$	14.46
6.08	90	101	14.56
5.72	36	110	15.49
5.23	100	012	16.93
5.19	100	111	17.08
4.94	8	020	17.95
4.58	13	021	19.36
3.85	2	022, $\bar{1}21$	23.08
3.810	1	013	23.33
3.509	1	200	25.36
3.177	1	031	28.06
2.981	1	130	29.95
2.925	2	$\bar{2}12$	30.54
2.900	2	032, $\bar{1}31$	30.80
2.861	1	220	31.24
2.788	1	$\bar{2}21$	32.08
2.730	1	$\bar{1}14$	32.78
2.622	1	024	34.17
2.571	3	033, 213	34.86
2.449	1	124	36.66
2.418	1	041, $\bar{1}33$	37.15
2.398	2	230, 015	37.48
2.356	2	$\bar{2}31$, $\bar{2}23$	38.16
2.340	1	223, $\bar{1}05$	38.43
2.310	2	204	38.95
2.286	2	$\bar{1}41$, 141	39.38
2.278	2	$\bar{1}15$, 310	39.52
2.253	1	034	39.98
2.239	<1	$\bar{2}32$, $\bar{3}11$	40.24
2.212	1	025	40.76
2.176	1	142	41.47
2.151	<1	$\bar{1}34$	41.96
2.141	<1	134, $\bar{3}12$	42.17
2.117	<1	043, $\bar{1}25$	42.68
2.085	<1	$\bar{3}21$	43.37
2.042	<1	$\bar{3}03$	44.31
2.029	<1	$\bar{1}43$, 303	44.63

Cadmium Sulfate Hydrate, $3CdSO_4 \cdot 8H_2O$ (monoclinic)

Sample source
The sample was obtained from Johnson, Mathey & Co.Ltd. High humidity is necessary to prevent formation of the monohydrate.

Major impurities
None over 0.001%.

Color
Colorless

Optical data
Biaxial (-) 2V,large. N_α=1.552,N_β=1.561, $N\gamma$=1.569.

Structure
Determined by Lipson [1936].

Space group
C_{2h}^6-C2/c(15),Z=4,Egartner et al.[1932].

Additional patterns
1.PDF card 12-0458[Inst. Physics,Cardiff].
2.PDF card 13-0525 [Shrier].

Density
(calculated) 3.090 g/cm^3 at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.0

References

Egartner,L., F.Halla and E.Schwarz (1932). Das Raumgitter des Cadmiumsulfats,$CdSO_4 \cdot 8/3H_2O$, Z. Krist. 83,422-425.

Lipson,H. (1936). The crystal structure of $3CdSO_4 \cdot 8H_2O$, Proc.Roy.Soc.(London) Ser.A 156, 462-470.

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

d (Å)	*I*	*hkl*	2θ(°)
7.36	18	200	12.02
6.88	100	$\bar{1}11$	12.86
6.34	65	111	13.96
5.94	70	020	14.89
5.02	11	021	17.65
4.691	10	002	18.90
4.621	16	220	19.19
4.525	48	310	19.60
4.329	41	$\bar{1}12$	20.50
4.281	40	$\bar{2}21$,$\bar{3}11$	20.73
4.213	7	$\bar{2}02$	21.07
4.057	15	112	21.89
4.021	35	221	22.09
3.745	65	202	23.74
3.682	9	022	24.15
3.672	7	400	24.22
3.590	88	$\bar{1}31$	24.78
3.505	37	131	25.39
3.467	7	$\bar{3}12$	25.67
3.434	19	$\bar{2}22$	25.92
3.169	36	222	28.13
3.125	23	420	28.54
3.090	53	$\bar{4}02$	28.87
3.066	13	$\bar{4}21$	29.10
3.000	45	$\bar{3}31$	29.75
2.974	13	040	30.02
2.919	4	132	30.60
2.894	45	113	30.87
2.851	5	510	31.35
2.827	10	$\bar{5}11$	31.62

-continued

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)	β(°)
Egartner,* et al. [1932]	14.98	11.65	9.44	98°
Lipson* [1936]	14.78	11.87	9.44	97.31°
NBS, sample at 25 °C	14.808 ±.001	11.902 ±.001	9.468 ±.001	97°22′ ±1′

*Values as published

Cadmium Sulfate Hydrate, $3CdSO_4 \cdot 8H_2O$ (monoclinic) – continued

d (Å)	*I*	*hkl*	2θ(°)
2.757	26	240	32.45
2.743	24	$\bar{4}22$	32.62
2.729	23	$\bar{3}13$,402	32.79
2.696	5	$\bar{2}23$	33.20
2.680	3	$\bar{2}41$,$\bar{3}32$	33.41
2.641	8	511	33.92
2.614	16	241	34.27
2.585	3	$\bar{5}12$	34.67
2.514	10	042	35.69
2.480	6	422	36.19
2.465	2	$\bar{1}33$	36.41
2.447	2	600	36.69
2.429	10	$\bar{2}42$	36.97
2.385	23	133	37.69
2.349	23	150,004	38.29
2.329	15	242	38.63
2.325	16	$\bar{2}04$	38.70
2.313	20	512,440	38.91
2.289	14	$\bar{1}51$,$\bar{3}33$	39.32
2.263	26	620,$\bar{6}21$	39.80
2.234	23	531,114	40.33
2.202	3	441,$\bar{5}32$	40.95
2.194	4	$\bar{3}14$	41.11
2.185	4	024	41.29
2.165	7	$\bar{2}24$	41.69
2.140	14	$\bar{6}22$,350	42.19
2.120	15	$\bar{2}43$,$\bar{1}52$	42.60
2.099	23	423	43.05
2.084	3	152	43.38
2.065	3	710,602	43.80
1.985	63	$\bar{7}12$,$\bar{5}33$,+	45.67
1.947	4	$\bar{6}23$	46.60
1.935	7	$\bar{4}43$,$\bar{5}14$	46.91
1.889	16	$\bar{6}41$,$\bar{2}61$,+	48.12
1.871	2	404,$\bar{1}15$	48.62
1.860	6	153,$\bar{7}31$	48.92
1.843	4	044,$\bar{5}51$	49.41
1.835	7	800,$\bar{7}13$	49.63
1.828	8	062	49.85
1.813	13	$\bar{3}15$,115	50.29
1.791	14	443,$\bar{2}25$	50.94
1.763	3	$\bar{8}21$	51.80
1.753	6	820,262	52.13
1.747	13	244	52.33
1.734	2	$\bar{4}61$	52.76

d (Å)	*I*	*hkl*	2θ(°)
1.7178	6	$\bar{4}44$	53.28
1.6958	9	461,642	54.03
1.6874	7	821	54.32
1.6774	3	$\bar{1}54$	54.67
1.6695	5	$\bar{4}62$	54.95
1.6642	13	$\bar{3}35$,135	55.14
1.6578	14	$\bar{7}14$,171	55.37
1.6404	1	802	56.01
1.6281	4	$\bar{9}11$,$\bar{3}54$	56.47
1.6168	9	$\bar{8}23$,910	56.90
1.6055	5	370	57.34
1.5968	6	$\bar{1}72$	57.68
1.5948	7	604,$\bar{3}71$	57.76
1.5883	2	$\bar{2}45$,045	58.02
1.5838	1	534,444	58.20
1.5766	1	$\bar{7}51$	58.49
1.5642	2	006,$\bar{1}16$	59.00
1.5489	7	335,$\bar{6}44$,+	59.64
1.5452	7	$\bar{8}04$	59.80
1.5382	13	553,$\bar{6}25$,+	60.10
1.5210	9	733	60.85
1.5178	7	$\bar{9}31$,$\bar{9}13$,+	60.99
1.5109	5	$\bar{4}06$	61.30
1.5008	1	$\bar{6}62$,372,+	61.76
1.4964	1	$\bar{8}24$,$\bar{1}73$	61.96
1.4918	2	206	62.17
1.4818	2	$\bar{1}55$	62.64
1.4777	2	173	62.83
1.4681	2	10·0·0,$\bar{5}71$	63.29
1.4644	4	$\bar{4}26$,$\bar{7}53$	63.47
1.4543	5	$\bar{3}73$	63.96
1.4505	4	752,$\bar{5}16$	64.15
1.4473	3	226	64.31
1.4437	3	$\bar{4}64$,$\bar{3}36$	64.49
1.4399	2	571	64.68
1.4363	2	$\bar{1}0·2·1$,842	64.86
1.4324	1	136	65.06
1.4304	1	$\bar{5}72$,662	65.16
1.4273	2	316,$\bar{9}33$	65.32
1.4182	2	$\bar{9}14$,082	65.79
1.4146	2	$\bar{1}0·2·2$	65.98
1.4054	3	644,373	66.47
1.4026	5	$\bar{2}82$,$\bar{6}06$	66.62
1.3899	2	$\bar{2}46$,932	67.31
1.3790	1	572,480	67.91

Cadmium Sulfate Monohydrate, $CdSO_4 \cdot H_2O$ (monoclinic)

Sample source

The sample was crystallized at NBS from an aqueous solution at 95° C. The starting material ($3CaSO_4 \cdot 8H_2O$) was obtained from Johnson, Matthey & Co.,Ltd.
$CdSO_4 \cdot H_2O$ is also obtained from $CdSO_4$ or $3CdSO_4 \cdot 8H_2O$ with prolonged exposure to air of about 50% relative humidity.

Major impurities

none over 0.001%.

Color

Colorless.

Optical data

Biaxial(-) N_α=1.582, N_β=1.624, N_γ=1.642, 2V is medium large.

Space group

C_{2h}^5-$P2_1/n$ (14), Z=4 [Perloff, 1968].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Perloff [1968]--NBS, sample at 25 °C-	7.64	7.46	7.62	115°30′
	7.632 ±.002	7.459 ±.002	7.622 ±.001	115°26′ ±1′

Density

(calculated) 3.839 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.2

References

Perloff, A. [1968]. Private communication

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

d (Å)	I	hkl	2θ(°)
6.46	3	$\bar{1}01$	13.69
5.066	12	110,011	17.49
4.881	65	$\bar{1}11$	18.16
4.075	3	101	21.79
3.729	24	020	23.84
3.574	100	111	24.89
3.448	8	200,002	25.82
3.388	6	$\bar{2}11,\bar{1}12$	26.28
3.279	17	120,021	27.17
3.226	46	$\bar{1}21,\bar{2}02$	27.63
3.128	13	210,012	28.51
2.961	4	$\bar{2}12$	30.16
2.753	3	121	32.50
2.663	6	$\bar{2}21,\bar{1}22$	33.63
2.531	36	220,$\bar{3}01$,+	35.44
2.504	5	211,112	35.83
2.440	9	$\bar{2}22$	36.81
2.397	28	$\bar{3}11,\bar{1}13$	37.49
2.319	13	$\bar{1}31$	38.79
2.166	2	221,122	41.67
2.150	2	$\bar{3}03$	41.99
2.122	11	131	42.56
2.091	6	$\bar{1}23$	43.23
2.066	11	$\bar{3}13$	43.79
2.038	5	202	44.42
2.015	2	230,032	44.94
1.964	4	212	46.17
1.943	3	301,103	46.72
1.902	4	$\bar{4}02,\bar{2}04$	47.79
1.879	7	311,113	48.40
1.863	7	040,$\bar{3}23$	48.84
1.842	5	$\bar{4}12,\bar{2}14$	49.44
1.814	2	$\bar{4}11$,132,+	50.24
1.787	5	222	51.07
1.772	7	$\bar{3}31,\bar{1}33$	51.53
1.722	10	400,123,+	53.13
1.693	9	$\bar{4}22,\bar{2}24$,+	54.12
1.676	4	014	54.72
1.639	12	240,042	56.07
1.625	4	$\bar{3}33$	56.58
1.612	3	$\bar{4}04$	57.10
1.575	3	$\bar{4}14$,232	58.54
1.563	4	420,024	59.06
1.530	3	331,133	60.45
1.510	3	$\bar{4}32,\bar{2}34$	61.35

Cesium Cobalt(II) Trichloride, $CsCoCl_3$ (hexagonal)

Sample source
The sample was prepared at NBS by heating co-precipitated CsCl and $CoCl_2$ to about 500 °C in a sealed glass tube.

Major impurities

0.01 -0.1 % each: K, Na, Rb, and Si.

0.1 -1.0 % each: Ni.

Color
Unground - dark blue.
Ground - very light blue.

Optical data
Uniaxial (+) N_o=1.696, N_e=1.772

Structure
Isostructural with $RbCoCl_3$ [Seifert,1960] and other similar ABX_3 compounds.

Space group
D_{6h}^4 - $P6_3/mmc$ (194) Z=2 by analogy with $RbCoCl_3$.

Lattice constants

	a(Å)	c(Å)
Seifert (1960)----------	7.194	6.033
NBS, sample at 25 °C------	7.203 ±.001	6.032 ±.002

Density
(calculated) 3.654 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ =3.8

References
Seifert,H.J.(1960), Über die Systeme Alkalimetallchlorid/kobalt(II) - chlorid. Z. Anorg. Allgem. Chem. 307, 137-144.

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

d (Å)	I	hkl	2θ(°)
6.25	9	100	14.15
4.337	55	101	20.46
3.607	60	110	24.66
3.122	9	200	28.57
3.018	21	002	29.57
2.773	100	201	32.26
2.714	24	102	32.97
2.360	1	210	38.10
2.312	1	112	38.92
2.195	23	211	41.08
2.168	31	202	41.62
2.080	14	300	43.47
1.966	2	301	46.12
1.914	6	103	47.47
1.858	16	212	48.98
1.800	20	220	50.66
1.729	<1	310	52.90
1.712	<1	302	53.47
1.690	12	203	54.24
1.663	8	311	55.17
1.559	1	400	59.20
1.546	9	222	59.78
1.530	1	213	60.46
1.510	10	401	61.34
1.501	7	312	61.75
1.431	1	320	65.14
1.392	9	321,114	67.20
1.3857	4	402	67.54
1.3609	5	410	68.94
1.3282	<1	411	70.89
1.3118	1	313	71.91
1.2933	1	322	73.11
1.2321	1	403	77.37
1.2213	<1	501,304	78.20
1.2006	<1	330	79.81
1.1659	1	323	82.70
1.1570	10	421,224	83.48
1.1530	<1	502	83.83
1.1254	1	205	86.38
1.1016	1	511	88.73
1.0982	3	422	89.07
1.0505	2	512	94.32
1.0397	4	600	95.61
1.0171	3	423	98.45
1.0111	3	431	99.25

Cesium Nickel(II) Trichloride, $CsNiCl_3$ (hexagonal)

Sample source
The sample was prepared at NBS by heating co-precipitated CsCl and $NiCl_2$ at about 500 °C in a sealed glass tube. The material was hygroscopic.

Major impurities
0.01 -0.1 % each: Al, Rb, Si, and Sn.

0.1 -1.0 % each: K and Na.

Color
Unground - medium reddish brown.
Ground - medium orange.

Optical data
Uniaxial (+), N_o=1.711, N_e=1.812.

Structure
Isostructural with $RbCoCl_3$ [Seifert, 1960] Also isostructural with other similar ABX_3 compounds.

Space group
D_{6h}^4-$P6_3/mmc$ (194), Z=2 [Tishchenko, 1955].

Lattice constants

	a(Å)	c(Å)
Tishchenko [1955]--------	7.18	5.93
Asmussen and Soling [1956]----------	7.1695	11.87
NBS, sample at 25°C------	7.1700 ±.0003	5.941 ±.001

Density
(calculated) 3.741 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 4.0

References

Allamangy, P. (1960). Synthèses de fluorures de deux métaux par réactions entre le gaz HF et des chlorures cristallisés, Bull. Soc. Chim. France **1960**, 1099.

Asmussen, P. and H. Soling, (1956). Magneto chemische Untersuchungen an Nickel (II) Verbindungen vom Typus Me(I)-Hal, Ni(II)-Hal_3, Z. Anorg. Allgem. Chem. **283**, 1.

Tishchenko, G.N. (1955). Electron diffraction investigation of the structure of $CsNiCl_3$, Tr. Inst. Kristallogr., Akad. Nauk SSSR **1955**, 93.

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

d (Å)	I	hkl	2θ(°)
6.22	9	100	14.23
4.291	58	101	20.68
3.584	66	110	24.82
3.103	8	200	28.75
2.969	19	002	30.07
2.752	100	201	32.51
2.680	18	102	33.41
2.347	<1	210	38.31
2.287	1	112	39.36
2.183	12	211	41.32
2.147	29	202	42.05
2.070	11	300	43.68
1.955	1	301	46.40
1.8867	5	103	48.19
1.8415	13	212	49.45
1.7924	20	220	50.90
1.7222	<2	310	53.13
1.6982	2	302	53.95
1.6692	9	203	54.96
1.6543	6	311	55.50
1.5525	1	400	59.49
1.5347	5	222	60.25
1.5134	3	213	61.19
1.5021	8	401	61.70
1.4903	4	312	62.24
1.4244	<2	320	65.47
1.3857	4	321	67.54
1.3755	5	402	68.11
1.3551	3	410	69.28
1.3214	<3	411	71.31
1.2992	<3	313	72.72
1.2847	<3	322	73.67
1.2218	3	403	78.16
1.2066	<3	304	79.34
1.1953	<3	330	80.24
1.1512	4	421	83.99
1.1438	4	224	84.66
1.0958	<3	511	89.32
1.0915	3	422	89.77
1.0441	<3	512	95.08
1.0347	<3	600	96.22
1.0093	3	423	99.48

Additional patterns
PDF card 16-0109 [Allamangy, 1960].

Cesium Strontium Trichloride, $CsSrCl_3$ (tetragonal)

Sample source
The sample was prepared at NBS by melting a mixture of molar amounts of CsCl and $SrCl_2$ at about 900 °C. The material was hygroscopic.

Major impurities
0.001-0.01% each: Ba, Ca, Fe, Li, Mg, Ni, and Si

0.01 -0.1 % each: Al, Na, and Rb

0.1 -1.0 % each: K

Color
Colorless

Optical data
Almost isotropic, N≒1.572. The crystals showed polysynthetic twinning.

Structure
Tetragonal distorted perovskite. Isostructural with $CsPbCl_3$.

Space group
C_{4v}^1-P4mm (99) Z=1, by analogy with the $CsPbCl_3$ powder pattern.

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25°C------	5.593 ±0.001	5.628 ±0.001

Density
(calculated) 3.083 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 3.4$

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

d (Å)	I	hkl	2θ(°)
3.96	100	101,110	22.42
3.237	27	111	27.53
2.813	38	002	31.78
2.796	52	200	31.98
2.287	51	211,112	39.37
1.984	28	202	45.68
1.978	23	220	45.83
1.779	8	103	51.32
1.769	11	301,310	51.62
1.618	8	222	56.86
1.501	10	213	61.75
1.497	12	312,321	61.93
1.407	3	004	66.36
1.398	5	400	66.88
1.357	<2	401,410+	69.16
1.3253	4	114	71.07
1.3219	7	303	71.28
1.3180	8	411,330	71.52
1.2566	2	204	75.61
1.2519	<2	402,420	75.94
1.2213	<2	421	78.20
1.1957	3	323	80.21
1.1940	2	332	80.35
1.1464	<2	224	84.42
1.1429	3	422	84.74
1.1035	<2	105	88.53
1.1011	<2	314,413	88.78
1.0970	3	431,510	89.20

Chromium Iridium 3:1, Cr_3Ir (cubic)

Sample source
Sample was prepared by R. M. Waterstrat at NBS by arc-melting.

Major impurities
0.001-0.01% each:Au, Cu, Pd, and V.

0.01 -0.1 % each:Fe, Pb, Pt, and Rh.

Color
Metallic dark grey. Opaque.

Structure
A-15 "β-W"type [Knapton,1958-9].

Space group
O_h^3-Pm3n (223), Z=2 [Knapton,1958-9].

Lattice constants

	a(Å)
Knapton, [1958-9]----------	4.682
NBS, sample at 25°C----------	4.6810 ±.0001

Density
(calculated) 11.273 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.1$

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

d (Å)	*I*	*hkl*	*2θ(°)*
3.309	78	110	26.92
2.3404	54	200	38.43
2.0937	37	210	43.17
1.9106	100	211	47.55
1.6554	10	220	55.46
1.4805	12	310	62.70
1.2978	5	320	72.81
1.2506	44	321	76.03
1.1700	9	400	82.35
1.1031	7	411	88.58
1.0466	11	420	94.77
1.0216	4	421	97.87
0.9979	11	332	101.04
.9556	4	422	107.42
.9180	9	510	114.08
.8693	4	520	124.77
.8546	14	521	128.65
.8275	7	440	137.14
.8028	6	530	147.25

References
Knapton, A. G. (1958-9). An X-ray survey of certain transition - metal systems for sigma phases, J. Inst. Metals 87, 28-32.

Chromium Rhodium 3:1, Cr_3Rh (cubic)

Sample source
The sample was prepared at NBS by R. M. Waterstrat by arc-melting and it was annealed at 1200 °C for three days.

Major impurities
0.001-0.01% each: Au, Cu, Ni, Pb, and Sn.

0.01 -0.1 % each: Fe, Ir, Pt, and V.

Color
Metallic dark grey and opaque.

Structure
A15 type"β-W"[Greenfield and Beck,1956].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.].

Lattice constants

	a(Å)
Greenfield and Beck, [1956]-----	4.656
NBS, sample at 25 °C----------	4.6731 ±.0001

Density
(calculated) 8.425 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 1.4$

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

d (Å)	*I*	*hkl*	*2θ(°)*
3.304	23	110	26.96
2.337	57	200	38.49
2.090	82	210	43.25
1.909	100	211	47.60
1.652	4	220	55.60
1.4775	4	310	62.84
1.3491	3	222	69.63
1.2960	17	320	72.93
1.2489	38	321	76.16
1.1683	13	400	82.49
1.1016	<1	411	88.73
1.0450	10	420	94.97
1.0197	10	421	98.11
0.9963	9	332	101.27
.9538	<1	422	107.72
.9166	<1	510	114.36
.8677	11	520	125.16
.8532	14	521	129.05
.8261	10	440	137.62
.8015	<1	530	147.88

Additional patterns
1.Greenfield and Beck [1956].

References
Greenfield,P. and P.A.Beck (1956). Intermediate phases in binary systems of certain transition elements, Trans. AIME 206, 265-276.

Gold Niobium 1:3, $AuNb_3$ (cubic)

Sample source
The sample was prepared at NBS by R. M. Waterstrat by arc-melting and it was annealed at 800 °C for one hour.

Major impurities
0.001-0.01% each: Cu, Ir, Mo, Os, Pd, Rh, Si, V.

0.01 -0.1 % each: Cr and Fe.

0.1 -1.0 % each: Pt.

Color
Metallic dark grey and opaque.

Structure
A15 type "β-W" [Wood and Matthias, 1956].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.]

Lattice constants

	a(Å)
Wood and Matthias [1956]--------	5.21
NBS, sample at 25 °C----------	5.2024 ±0.0001

Density
(calculated) 11.219 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.2$.

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

d (Å)	*I*	*hkl*	*2θ(°)*
3.678	18	110	24.18
2.601	50	200	34.45
2.327	73	210	38.66
2.125	100	211	42.51
1.840	4	220	49.49
1.6455	5	310	55.82
1.5021	2	222	61.70
1.4429	12	320	64.53
1.3908	40	321	67.26
1.3005	12	400	72.64
1.2262	3	411	77.83
1.1632	9	420	82.93
1.1355	9	421	85.43
1.1093	7	332	87.95
1.0620	1	422	92.98
1.0202	2	510	98.05
0.9661	7	520	105.74
.9499	10	521	108.37
.9197	6	440	113.75
.8921	<1	530	119.40
.8670	5	600	125.36
.8552	3	610	128.48
.8438	12	611	131.80

Additional patterns
1. PDF card 11-19 [Wood and Matthias, 1956].

References
Wood, E. A. and B. T. Matthias (1956). The crystal structure of Nb_3Au and V_3Au, Acta Cryst. **9**, 534.

Gold Titanium 1:3, $AuTi_3$ (cubic)

Sample source
The sample was prepared at NBS by R. M. Waterstrat by arc-melting and it was annealed at 800 °C for one hour.

Major impurities
0.001-0.01% each: Al, Cu, In, Ni, Rh, and Si.

0.01 -0.1 % each: Fe, Pd, and Pt.

0.1 -1.0 % each: V

Color
Metallic dark grey and opaque.

Structure
A15 type "β-W" [Duwez and Jordan, 1952]

Space group
O_h^3-Pm3n (223), Z=2 [ibid.]

Lattice constants

	a(Å)
Duwez and Jordan [1952]---------	5.096
NBS, sample at 25 °C----------	5.0974 ±0.0001

Density
(calculated) 8.542 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 3.1$

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

d (Å)	I	hkl	2θ(°)
3.604	90	110	24.68
2.549	47	200	35.18
2.281	26	210	39.48
2.082	100	211	43.43
1.802	12	220	50.62
1.6117	16	310	57.10
1.4710	<1	222	63.15
1.4135	4	320	66.04
1.3625	43	321	68.85
1.2746	8	400	74.36
1.2015	8	411	79.74
1.1397	11	420	85.04
1.1123	4	421	87.65
1.0870	9	332	90.24
1.0406	3	422	95.50
0.9997	9	510	100.80
.9465	3	520	108.93
.9307	11	521	111.71
.9011	6	440	117.47
.8742	5	530	123.54
.8496	8	600	130.09
.8380	1	610	133.60
.8269	16	611	137.35
.8058	2	620	145.81
.7865	4	541	156.69

Additional patterns
1. PDF card 7-352 [Duwez and Jordan, 1952].

References
Duwez, P. and C.B. Jordan (1952). The crystal structure of Ti_3Au and Ti_3Pt, Acta Cryst. **5**, 213-214.

Gold Vanadium 1:3, AuV_3 (cubic)

Sample source
The sample was prepared at NBS by R. M. Waterstrat by arc-melting and it was annealed at 800 °C for one hour.

Major impurities
0.001-0.01% each: Ag, Cu, Ni, Si, Sn, Ti.

0.01 -0.1 % each: Cr, Fe, and Pt.

0.1 -1.0 % each: Pd.

Color
Metallic dark grey and opaque.

Structure
A15 type "β-W" [Wood and Matthias,1956].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.]

Lattice constants

	a(Å)
Wood and Matthias [1956]--------	4.88 ±0.01
Köster and Nordskog [1960]------	4.88
NBS, sample at 25 °C----------	4.8813 ±0.0001

Density
(calculated) 9.987 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.1$

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

d (Å)	I	hkl	2θ(°)
3.4515	85	110	25.79
2.4402	53	200	36.80
2.1831	31	210	41.32
1.9930	100	211	45.47
1.7260	10	220	53.01
1.5435	11	310	59.87
1.3535	4	320	69.37
1.3046	33	321	72.37
1.2204	12	400	78.27
1.1506	6	411	84.05
1.0916	8	420	89.76
1.0652	2	421	92.62
1.0407	6	332	95.48
0.9966	3	422	101.23
.9575	6	510	107.12
.9065	5	520	116.35
.8912	9	521	119.60
.8629	5	440	126.41
.8371	3	530	133.90
.8136	5	600	142.42
.7918	8	611	153.20

Additional patterns
1. PDF card 11-20 [Wood and Matthias,1956].

References

Köster,W. and H.Nordskog (1960). Das Zweistoffsystem Gold-Vanadium,Z.Metallk. **51**, 501-502.

Wood,E. A. and B. T. Matthias (1956). The crystal structures of Nb_3Au and V_3Au, Acta Cryst. **9**, 534.

Iridium Niobium 1:3, $IrNb_3$ (cubic)

Sample source

The sample was prepared by R. M. Waterstrat at NBS by arc-melting and it was annealed at 2000 °C for three hours.

Major impurities

0.001-0.01% each: Al, Cr, Cu, Pd, Rd, Si and V.

0.01 -0.1 % each: Fe and Pt.

Color

Metallic dark grey and opaque.

Structure

A15 "β-W" type [Geller, Matthias and Goldstein, 1955]. Solid solution range found from 21.5 to 28.5 At. % Ir [Giesson and Grant, 1964].

Space group

O_h^3-Pm3n (223), Z=2 [Geller, Matthias and Goldstein, 1955].

Lattice constants

	a(Å)
Geller et al. [1955]	5.131
Knapton [1958-9]	5.139
Giesson and Grant [1964]	5.138
NBS, sample at 25°C	5.1333 ±.0001

Density

(calculated) 11.561 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 2.8$.

Internal standard W, a = 3.16504 Å

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

d (Å)	*I*	*hkl*	*2θ(°)*
3.632	18	110	24.49
2.566	46	200	34.93
2.296	68	210	39.20
2.096	100	211	43.11
1.8147	4	220	50.23
1.6236	5	310	56.64
1.4820	2	222	62.63
1.4238	13	320	65.50
1.3716	49	321	68.33
1.2832	13	400	73.78
1.2097	3	411	79.10
1.1478	3	420	84.31
1.1198	11	421	86.92
1.0943	10	332	89.48
1.0478	<1	422	94.63
1.0067	3	510	99.83
0.9532	12	520	107.82
.9370	17	521	110.57
.9075	9	440	116.16
.8804	2	530	122.07
.8556	8	600	128.39
.8439	4	610	131.76
.8327	21	611	135.33
.8117	<1	620	143.23
.7921	2	541	153.03

References

Geller, S., B. T. Matthias and R. Goldstein (1955). Some new intermetallic compounds with the "β-Wolfram" structure, J. Am. Chem. Soc. **77**, 1502-4.

Knapton, A. G. (1958-9). An X-ray survey of certain transition - metal systems for sigma phases, J. Inst. Metals **87**, 28-32.

Giessen, B.C., and N.J. Grant (1964). Constitution diagrams Nb-Rh and Nb-Ir. Technical Report No. WADD TR 60-132, **Part III**, 223-279.

Iridium Titanium 1:3, $IrTi_3$ (cubic)

Sample source
The sample was prepared at NBS by R. M. Waterstrat by arc-melting.

Major impurities
0.001-0.01% each:Al, Cr, Cu, Pd, Si, V.

0.01 -0.1 % each:Au, Fe, Mo, Pt, and Rh.

Color
Metallic dark grey and opaque.

Structure
A15 type "β-W" [Geller, 1956].

Space group
O_h^3-Pm3n (223), Z=2 [Geller, 1956].

Lattice constants

	a(Å)
Nevitt, [1958]----------	5.0101 ±.0004
Matthias et al., [1961]---------	5.009
NBS, sample at 25 °C----------	5.0087 ±.0001

Density
(calculated) 8.877g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.1$

Additional patterns
1. PDF card 10-298 [Nevitt, 1958].

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

d (Å)	I	hkl	2θ(°)
3.542	87	110	25.12
2.504	47	200	35.83
2.240	27	210	40.22
2.046	100	211	44.24
1.7713	10	220	51.55
1.5840	13	310	58.19
1.3891	4	320	67.35
1.3387	35	321	70.25
1.2524	6	400	75.91
1.1806	6	411	81.45
1.1200	8	420	86.90
1.0931	1	421	89.60
1.0680	8	332	92.31
1.0222	3	422	97.79
0.9822	8	510	103.29
.9301	2	520	111.82
.9143	8	521	114.79
.8854	8	440	120.91
.8590	5	530	127.46
.8348	4	600	134.63
.8126	12	611	142.85
.7919	1	620	153.13

References

Geller, S.(1956). A set of effective coordination number (12)radii for the β-Wolfram structure elements, Acta Cryst. **9**, 885-889.

Matthias,B.T.,V.B.Compton and E. Corenzwit (1961). Some new superconducting compounds, J.Phys. Chem. Solids **19**,Nos.1-2, 130-133.

Nevitt,M.V.(1958). Atomic size effects in Cr_3O-type structure,Trans. AIME **212**,350.

Iridium Vanadium 1:3, IrV_3 (cubic)

Sample source
The sample was prepared by R. M. Waterstrat at NBS by arc-melting.

Major impurities
0.001-0.01% each:Ag,Au,Cr,Cu,Rh,Si,Sn,Ti.

0.01 -0.1 % each:Fe,Pd,and Pt.

0.1 -1.0 % each:

Color
Metallic dark grey. Opaque.

Structure
A15 type "β-W" [Nevitt, 1958].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.]

Lattice constants

	a(Å)
Nevitt, [1958]----------	4.7854
Matthias et al., [1961]---------	4.795
NBS, sample at 25 °C----------	4.7876 ±.0001

Density
(calculated) 10.441g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.5$.

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

d (Å)	I	hkl	2θ(°)
3.386	78	110	26.30
2.395	50	200	37.52
2.142	31	210	42.16
1.956	100	211	46.39
1.6929	12	220	54.13
1.5143	15	310	61.15
1.3819	1	222	67.75
1.3277	5	320	70.92
1.2793	44	321	74.04
1.1971	8	400	80.10
1.1285	8	411	86.09
1.0705	11	420	92.03
1.0448	4	421	94.99
1.0208	10	332	97.97
0.9772	4	422	104.04
.9390	10	510	110.23
.8890	4	520	120.09
.8741	20	521	123.58
.8463	9	440	131.04
.8210	6	530	139.49
.7979	14	600	149.73
.7871	2	610	156.24

Additional patterns
1. PDF card 10-295 [Nevitt, 1958].

References

Matthias,B.T., V.B.Compton and E.Corenzwit (1961). Some new superconducting compounds, J.Phys. Chem. Solids.**19**,Nos.1-2, 130-133.

Nevitt, M. V. (1958). Atomic size effects in Cr_3O-type structures, Trans.AIME **212**, 350-355.

Lithium Niobate, $LiNbO_3$ (trigonal)

Sample source
The $LiNbO_3$ was obtained from CIBA, Rare Metals Division, Summit, N.J. The sample was recrystallized at NBS by W.S. Brower. It was pulled from a melt and then annealed in oxygen at 1100° C for 10 hours.

Major impurities
0.001-0.01% each: Ba, Na, Mo.

Color
Colorless

Optical data
Uniaxial (-). N > 2.00.

Structure
Determined by Bailey [1952].

Space group
C_{3v}^6-R3 (161), Z=6, [ibid.].

Lattice constants

	a(Å)	c(Å)
Zachariasen [1928]-------	5.12*	13.84*
Bailey [1952]------------	5.147	13.856
Lapickij and Simanov [1955]-----------------	5.150*	13.816*
Abrahams et al.[1966] at 23° C------------------	5.14829 ±.00002	13.8631 ±.0004
NBS, sample at 25° C-----	5.1494 ±.0001	13.8620 ±.0005

* from kX

Density
(calculated) 4.627 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 8.0

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

d (Å)	I	hkl	2θ(°)
3.754	100	012	23.68
2.739	38	104	32.67
2.576	21	110	34.79
2.311	3	006	38.93
2.249	9	113	40.05
2.124	10	202	42.51
1.876	15	024	48.47
1.720	21	116	53.21
1.674	1	211	54.80
1.638	12	122	56.11
1.615	6	018	56.96
1.515	11	214	61.10
1.487	9	300	62.41
1.441	1	125	64.63
1.3682	4	208	68.52
1.3238	4	1·0·10	71.16
1.2872	2	220	73.51
1.2504	3	306	76.05
1.2403	1	223	76.78
1.2321	1	131	77.39
1.2178	4	312	78.47
1.2080	5	128	79.23
1.1775	1	0·2·10	81.71
1.1652	2	134	82.76
1.1553	1	0·0·12	83.63
1.1294	<1	315	86.00
1.1246	3	226	86.46
1.1008	2	042	88.81
1.0708	4	2·1·10	92.00
1.0615	1	404	93.04
1.0539	3	1·1·12	93.92
1.0123	2	232	99.09
1.0069	3	318	99.81
0.9879	1	229	102.46
.9814	3	324	103.42
.9734	2	410	104.62
.9667	1	0·1·14	105.65
.9523	<1	413	107.97
.9376	2	048	110.47
.9228	2	1·3·10	113.17

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
.9121	1	3•0•12	115.23
.9050	2	2•0•14	116.66
.8968	4	416	118.38
.8846	1	502	121.08
.8811	2	238	121.91
.8688	2	4•0•10	124.88
.8637	2	054	126.19
.8598	3	2•2•12	127.24
.8583	2	330	127.65
.8537	2	1•2•14	128.92
.8504	2	1•0•16	129.86
.8412	1	241	132.60
.8366	1	422	134.06
.8231	2	3•2•10	138.71
.8190	2	244	140.28
.8075	2	1•3•13,0•2•16	145.05
.8063	1	425	145.64
.8045	1	336	146.46
.7956	2	152	150.99
.7930	2	508	152.48
.7804	4	514	161.52

Additional patterns

1.PDF card 9-186. [Lapickij and Simanov, 1955].

References

Abrahams, S.C., J.M. Reddy, and J.L. Bernstein (1966). Ferroelectric lithium niobate. 3.Single crystal x-ray diffraction study at 24° C, J.Phys. Chem. Solids **27**, 997-1012.

Bailey, P., Thesis, Bristol (1952). Quoted by Megaw, H.D. (1954). Ferroelectricity and crystal structure. II, Acta Cryst.**7**, 187-194.

Lapickij, A. V. and Ju. P. Simanov (1955). Lithium metaniobate and metatantalate,Z. Fiz. Khim. SSSR **29**, 1201-1203.

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

Lithium Sodium Sulfate, $LiNaSO_4$ (trigonal)

Sample source
The sample was prepared by melting equal molecular amounts of Li_2SO_4 and Na_2SO_4 together and annealing at 500 °C overnight.

Major impurities
0.001-0.01% each: Fe,Mg,Ni

0.1 -1.0 % each: Al

Color
Colorless

Optical data
Uniaxial (+), N_o=1.491, N_e=1.495.

Structure
Determined by Morosin and Smith [1967].

Space group
C_{3v}^4-P31c (159), Z=6 [Hilmy,1953].

Lattice constants

	a(Å)	c(Å)
Cavalca and Nardelli (1952)----------	7.613 ±.004	9.80 ±.03
Hilmy (1953)----------	7.64	9.76
Morosin and Smith (1967)-	7.6270 ±.0007	9.8579 ±.0010
NBS, sample at 25 °C-----	7.6355 ±.0002	9.861 ±.001

Density
(calculated) 2.521 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.5

Internal standard Ag, a = 4.08625 Å
CuK_{α_1} λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.62	2	100	13.37
5.494	5	101	16.12
4.932	1	002	17.97
3.912	74	102	22.48
3.814	100	110	23.30
3.307	4	200	26.94
3.136	3	201	28.44
3.020	39	112	29.55
2.944	39	103	30.33
2.744	78	202	32.60
2.499	1	210	35.90
2.465	8	004	36.41
2.437	8	211	37.06
2.332	5	203	38.58
2.310	5	104	38.95
2.228	12	212	40.45
2.205	6	300	40.90
2.151	17	301	41.97
2.071	1	114	43.67
2.012	8	302	45.02
1.989	1	213	45.57
1.976	15	204	45.89
1.909	18	220	47.58
1.891	7	105	48.07
1.834	6	310	49.66
1.804	1	311	50.56
1.780	4	222	51.27
1.756	4	214	52.04
1.720	4	312	53.22
1.694	3	205	54.08
1.653	3	400	55.53
1.644	5	006,304	55.87
1.630	<1	401	56.39
1.602	3	313	57.48
1.568	3	402	58.83
1.549	4	215	59.64
1.5098	7	116,224	61.35
1.4999	<1	321	61.80
1.4769	<1	403	62.87
1.4721	9	206,314	63.10

Internal standard Ag, a = 4.08625 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
1.4499	5	322	64.18
1.4430	11	410	64.52
1.3846	5	412	67.60
1.3781	6	107,323	67.96
1.3735	7	216,404	68.22
1.3427	2	315	70.01
1.3222	1	500	71.26
1.3176	1	306	71.55
1.2960	2	207	72.93
1.2925	1	324	73.16
1.2775	1	502	74.16
1.2722	5	330	74.52
1.2494	2	420	76.12
1.2454	3	226,414	76.41
1.2323	3	008,332	77.37
1.2274	1	217,503	77.74
1.2245	1	316	77.99
1.2113	4	108,422	78.97
1.2023	1	325	79.68
1.1869	1	307	80.93
1.1790	<1	511	81.58
1.1656	3	406,504	82.72
1.1548	2	208,512	83.67
1.1306	1	334	85.89
1.1171	4	317,513	87.18
1.1146	1	326,424	87.43
1.1052	1	218	88.36
1.1025	1	600	88.64
1.0985	<1	505	89.04
1.0953	1	601	89.35
1.0845	1	416	90.51
1.0808	1	109,431	90.90
1.0720	1	407	91.86

Additional patterns

1.Hilmy [1953].

References

Cavalca, L. and M.Nardelli (1952). Sistema ternario: Na_2SO_4-Li_2SO_4-H_2O a 27.0° ed a 45.6°,Gazz.Chim.Ital.**82**,394-405.

Hilmy, M.E. (1953). Structural crystallographic relation between sodium sulfate and potassium sulfate and some other synthetic sulfate minerals, Am.Mineralogist **38**, 118-135.

Morosin,B.and D.L.Smith (1967).The crystal structure of lithium sodium sulfate,Acta Cryst. **22**, 906-910.

Lithium Sulfate, Li_2SO_4 (monoclinic)

Sample source

The sample was prepared by heating Fisher reagent $Li_2SO_4 \cdot H_2O$ for 24 hours at 600 °C.

Major impurities

0.1 -1.0 % each: Na

Color

Colorless

Optical data

Biaxial (-), N_α=1.468, N_β=1.472, N_γ=1.475, 2V is large.

Structure

Determined by Albright [1932].

Space group

C_{2h}^5-$P2_1/a$ (14). Z=4.

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Albright [1932]--NBS, sample at 25°C-	8.27*	4.96*	8.46*	107°54′
	8.2414 ±.0004	4.9533 ±.0003	8.474 ±.001	107°58.8′ ±0.3′

*from kX

Density

(calculated) 2.219 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.7

References

Albright, J.G. (1932). The crystal structure of lithium sulfate, Z. Krist. **84**, 150-158.

Forland, T., and J. Krogh-Moe, (1957). The structure of the high temperature modification of lithium sulfate, Acta Chem. Scand. **11**, 565-567.

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

Internal standard W, a = 3.16504 Å

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

d (Å)	I	hkl	2θ(°)
4.225	11	011	21.01
4.193	9	110	21.17
4.048	100	$\bar{2}01$	21.94
4.030		002	22.04
3.999	100	$\bar{1}11$	22.21
3.919	47	200	22.67
3.490	22	111	25.50
3.382	10	$\bar{2}02$	26.33
3.177	28	$\bar{1}12$	28.06
3.163	41	201	28.19
3.139	12	$\bar{2}11$	28.41
3.074	5	210	29.02
2.792	10	$\bar{2}12$	32.03
2.691	5	112	33.27
2.665	3	211	33.60
2.628	8	$\bar{2}03$	34.09
2.479	22	020	36.21
2.402	10	$\bar{3}11$	37.40
2.361	6	013,120	38.08
2.319	9	$\bar{2}13$	38.79
2.211	2	121	40.77
2.111	3	022,113	42.81
2.094	4	220	43.16
2.025	2	$\bar{4}02$	44.71
2.015	2	004	44.94
1.997	1	$\bar{2}22$	45.38
1.952	12	203	46.47
1.947	9	$\bar{1}14$	46.62
1.912	1	$\bar{2}14$	47.52
1.900	1	$\bar{4}11$	47.84
1.884	4	$\bar{4}03$	48.26
1.875	5	$\bar{4}12$	48.52
1.866	2	014	48.75
1.839	1	$\bar{3}21$	49.53
1.823	3	410,023	50.00
1.816	2	213	50.19
1.803	2	312,$\bar{2}23$	50.59
1.789	1	$\bar{3}22$	50.99
1.781	3	401	51.24
1.778	2	$\bar{3}14$	51.35
1.744	1	222	52.43
1.709	1	114	53.59
1.697	1	123	53.98
1.686	2	$\bar{2}05$	54.37
1.667	2	$\bar{3}23$	55.05

d (Å)	I	hkl	2θ(°)
1.617	1	031	56.88
1.616	1	130	56.94
1.603	3	$\bar{1}31$,204	57.44
1.595	2	$\bar{2}15$,$\bar{1}15$	57.74
1.582	1	$\bar{4}21$,402	58.29
1.565	2	$\bar{4}22$,131	58.96
1.553	1	313,$\bar{5}11$	59.45
1.533	3	$\bar{3}15$,015,+	60.32
1.529	4	$\bar{2}31$,032	60.52
1.525	3	322,214	60.66
1.510	1	$\bar{3}24$	61.33
1.507	1	412	61.48
1.499	1	$\bar{4}23$	61.83
1.4947	4	510	62.04
1.4910	4	$\bar{4}05$	62.21
1.4830	3	$\bar{2}32$	62.58
1.4677	1	132,124	63.31
1.4638	1	231	63.50
1.4463	1	421	64.36
1.4256	2	$\bar{1}33$	65.41
1.4160	2	$\bar{5}14$	65.91
1.4116	2	$\bar{2}06$	66.14
1.4067	2	033	66.40
1.3974	3	$\bar{2}33$,$\bar{5}11$	66.90
1.3921	2	403,$\bar{3}32$	67.19
1.3735	1	$\bar{6}02$	68.22
1.3653	1	323,$\bar{5}21$	68.69
1.3570	<1	$\bar{6}01$,$\bar{2}16$	69.17
1.3503	1	$\bar{6}03$	69.56
1.3432	2	006	69.98
1.3344	<1	$\bar{5}23$	70.51
1.3096	1	$\bar{6}11$	72.05
1.3067	2	600	72.24
1.2937	1	$\bar{6}04$	73.08
1.2913	<1	$\bar{2}34$	73.24
1.2836	1	$\bar{5}12$	73.75
1.2796	2	$\bar{4}32$	74.02
1.2771	2	125,034,+	74.19
1.2693	<1	$\bar{5}24$,$\bar{4}16$	74.72
1.2624	1	430	75.20
1.2553	<1	521	75.70
1.2479	1	$\bar{3}34$	76.23
1.2307	1	601	77.49
1.2229	1	140,134	78.08
1.2183	1	$\bar{1}41$	78.43
1.2147	1	$\bar{6}05$	78.71
1.2009	1	$\bar{6}22$,141	79.79
1.1947	1	611	80.29
1.1917	<1	414	80.53
1.1876	2	$\bar{5}16$	80.87
1.1861	1	$\bar{1}42$,225	80.99
1.1801	3	$\bar{6}15$,315	81.49
1.1652	1	$\bar{3}17$,206	82.76
1.1620	1	$\bar{5}31$,$\bar{4}07$	83.04
1.1605	1	$\bar{1}17$,$\bar{4}26$	83.17
1.1547	1	142	83.68
1.1535	1	035,241	83.79
1.1498	1	234	84.12
1.1421	<1	432	84.82
1.1383	1	$\bar{7}13$	85.17
1.1290	1	$\bar{3}41$,$\bar{7}11$	86.04
1.1266	1	$\bar{6}06$	86.27
1.1169	<1	342	87.20
1.1064	<1	$\bar{4}35$,135	88.24
1.1027	1	621	88.62
1.1012	<1	$\bar{5}34$	88.77
1.0982	<1	$\bar{6}16$	89.07
1.0922	1	531,710	89.69
1.0906	1	$\bar{6}25$,405	89.86
1.0853	1	$\bar{3}43$	90.42
1.0818	1	523	90.80
1.0685	1	$\bar{1}44$	92.25
1.0657	1	$\bar{7}15$,415	92.57
1.0631	1	$\bar{7}22$,$\bar{2}44$	92.86
1.0574	1	$\bar{7}23$,208	93.51
1.0545	1	226	93.85
1.0485	<1	$\bar{6}31$	94.55
1.0456	<1	243,235,+	94.89
1.0414	1	711	95.40
1.0355	1	$\bar{4}08$,532,+	96.12
1.0277	<1	$\bar{8}02$,$\bar{4}36$	97.09
1.0239	1	144	97.57
1.0183	<1	$\bar{1}18$,$\bar{6}34$	98.30
1.0128	<1	$\bar{8}04$	99.02
1.0088	<1	$\bar{7}16$,$\bar{5}27$	99.53
1.0071	<1	$\bar{8}13$	99.78
0.9889	<1	$\bar{5}42$	102.32
.9873	1	$\bar{5}41$,018	102.55
.9855	<1	434	102.81
.9822	1	712,$\bar{3}45$,+	103.30

Polymorphism

Above 575° Li_2SO_4 is cubic. [Forland and Krogh-Moe, 1957]

Additional patterns

1. PDF card 1-0443 [Hanawalt et al., 1938]

Molybdenum Osmium 3:1, Mo_3Os (cubic)

Sample source
The sample was prepared at NBS by R. M. Waterstrat by arc-melting and it was annealed at 2000 °C for two days.

Major impurities
0.001-0.01% each: Al, Au, Co, Cr, Cu, Nb, Si, Sn, V, and Zr.
0.01 -0.1 % each: Fe, Ir, and Rh.

Color
Metallic dark grey and opaque.

Structure
A15 type "β-W" [Raub, 1954].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.].

Lattice constants

	a(Å)
Raub, [1954]----------	4.973*
NBS, sample at 25 °C----------	4.9689 ±.0001

*from kX

Density
(calculated) 12.940 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 2.5

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

d (Å)	I	hkl	2θ(°)
3.513	14	110	25.33
2.483	50	200	36.14
2.222	81	210	40.56
2.028	100	211	44.64
1.758	3	220	51.98
1.5712	4	310	58.71
1.4342	3	222	64.97
1.3778	17	320	67.98
1.3277	49	321	70.92
1.2420	15	400	76.66
1.1711	2	411	82.25
1.1110	12	420	87.78
1.0844	14	421	90.52
1.0595	11	332	93.27
1.0142	1	422	98.83
0.9745	3	510	104.45
.9226	14	520	113.21
.9072	18	521	116.22
.8783	11	440	122.55
.8522	<1	530	129.34
.8282	11	600	136.87
.8169	4	610	141.10
.8061	22	611	145.71
.7856	<1	620	157.30

References
Raub E. (1954).Die Legierungen der Platinmetalle mit Molybdän, Z. Metallk. **45**,23.

2-Naphthylamine, N-phenyl-, $C_{16}H_{13}N$ (orthorhombic)

Sample source
The sample was supplied by F.J.Linnig at NBS.

Color
Colorless.

Optical data
Biaxial (-) N_α=1.636, N_β=1.82, N_γ=1.92
2v= 65° [McCrone, 1951]

Structure
Orthorhombic [ibid.].

Space group
Not determined. Z=8 [ibid.].

Lattice constants

	a(Å)	b(Å)	c(Å)
McCrone [1951]---	17.45	18.25	7.52
NBS, sample at 25°C--------	17.303 ±.002	18.183 ±.004	7.518 ±.002

Density
(calculated) 1.232 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.1

Additional patterns
1.PDF card 5-0254 [McCrone,1951].

References
McCrone, W.C.(1951). N-Phenyl-2-naphthylamine, Anal. Chem. **23**, 1884.

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

d (Å)	I	hkl	2θ(°)
12.49	<3	110	7.07
9.07	39	020	9.74
8.66	7	200	10.20
6.894	<3	101	12.83
6.449	12	111	13.72
6.267	9	220	14.12
5.497	28	310,121	16.11
4.815	100	221	18.41
4.572	7	301	19.40
4.544	11	131,040	19.52
4.327	58	400	20.51
4.143	72	231	21.43
3.907	15	420	22.74
3.797	24	141	23.41
3.669	30	102,411	24.24
3.556	5	150	25.02
3.475	11	022	25.61
3.459	10	500	25.73
3.401	4	510	26.18
3.218	15	151	27.70
3.193	14	032	27.92
3.140	16	501,132	28.40
3.098	20	511	28.79
2.971	9	521	30.05
2.883	9	600	30.99
2.855	4	142	31.30
2.790	<3	531	32.05
2.581	<3	621	34.73
2.431	<3	171	36.94
2.382	<3	352	37.74
2.359	<3	062,461	38.12
2.277	<3	262	39.54
2.272	<3	080,612+	39.64
2.139	<3	072	42.22
2.090	<3	660	43.26
2.006	<3	253,190	45.15
1.952	<3	840,091	46.47
1.944	<3	481,353	46.69
1.921	<3	163	47.28
1.881	<3	613,920+	48.34
1.859	<3	850,114	48.95
1.843	<3	382,581	49.41
1.825	<3	921	49.94
1.794	<3	034,173	50.84
1.733	<3	842,2·10·1	52.79

Niobium Osmium 3:1, Nb_3Os (cubic)

Sample source
The sample was prepared at NBS by R. M. Waterstrat by arc-melting and it was annealed at 1600 °C for five days.

Major impurities
0.001-0.01% each: Ag,Au,Cu,Ir,Pd,Si,Sn,V

0.01 -0.1 % each: Cr, and Pt.

Color
Metallic dark grey and opaque

Structure
A15 type "β-W" [Geller et al., 1955].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.].

Lattice constants

	a(Å)
Geller, et al., [1955]----------	5.121 ±.002
NBS, sample at 25 °C----------	5.1348 ±.0001

Density
(calculated) 11.502 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 4.7$

Internal standard Ag, a = 4.08625 Å
CuK_{α_1} λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
3.632	23	110	24.49
2.568	50	200	34.91
2.297	78	210	39.18
2.097	100	211	43.09
1.816	4	220	50.20
1.625	6	310	56.60
1.4826	2	222	62.60
1.4240	13	320	65.49
1.3721	40	321	68.30
1.2836	12	400	73.75
1.2104	2	411	79.04
1.1483	10	420	84.25
1.1206	9	421	86.84
1.0950	7	332	89.41
1.0479	1	422	94.62
1.0270	<1	430	97.18
1.0070	3	510	99.80
0.9534	9	520	107.78
.9374	13	521	110.50
.9077	7	440	116.11
.8807	2	530	122.00
.8679	<1	531	125.12
.8559	7	600	128.31
.8442	3	610	131.69
.8330	15	611	135.25
.8119	1	620	143.13
.7923	1	541	152.91

References
Geller,S., B.T. Matthias, and R. Goldstein (1955). Some new intermetallic compounds with the "β-Wolfram" structure, J. Am. Chem. Soc. **77**, 1502-1504.

Niobium Platinum 3:1, Nb_3Pt (cubic)

Sample source
The sample was prepared at NBS by R. M. Waterstrat by arc-melting and it was annealed at 1600 °C for five days.

Major impurities
0.001-0.01% each: Al, Cu, Ir, Pd, and Si.

0.01 -0.1 % each: Au, Cr, Fe, Os, Rh, and V.

Color
Metallic dark grey and opaque.

Structure
A15 type "β-W" [Geller et al., 1955].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.]

Lattice constants

	a(Å)
Geller et al., [1955]	5.153
Greenfield and Beck [1956]	5.11
NBS, sample at 25 °C	5.1524 ±0.0001

Density
(calculated) 11.503 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 4.9$

Additional patterns
1. PDF card 8-371[Greenfield and Beck,1956]

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

d (Å)	I	hkl	2θ(°)
3.642	14	110	24.42
2.575	42	200	34.81
2.304	64	210	39.07
2.102	100	211	42.99
1.823	5	220	50.00
1.629	6	310	56.42
1.488	3	222	62.35
1.4289	16	320	65.24
1.3765	55	321	68.05
1.2886	16	400	73.42
1.2144	4	411	78.73
1.1522	16	420	83.90
1.1244	14	421	86.48
1.0983	13	332	89.06
1.0518	2	422	94.16
1.0105	6	510	99.32
0.9568	16	520	107.22
.9408	23	521	109.91
.9110	14	440	115.26
.8838	3	530	121.26
.8588	13	600	127.50
.8470	7	610	130.84
.8358	31	611	134.30
.8146	1	620	142.01
.7950	3	541	151.33

References

Geller, S., B. T. Matthias, and R. Goldstein (1955). Some new intermetallic compounds with the "β-Wolfram" structure, J. Am. Chem. Soc. **77**, 1502-1504.

Greenfield, P. and P.A.Beck (1956). Intermediate phases in binary systems of certain transition elements, Trans. AIME **206**, 265-276.

Palladium Vanadium, 1:3, PdV_3 (cubic)

Sample source
The sample was prepared by R. M. Waterstrat at NBS by arc-melting and it was annealed at 1100 °C for two weeks.

Major impurities
0.001-0.01% each: Ni, Rh and Ru.

0.01 -0.1 % each: Cr, Fe, Mo, Pt, Si, and Ti.

Color
Metallic dark grey and opaque

Structure
A-15 type "β-W", isomorphous with CoV_3 and NiV_3 [Köster and Haehl, 1958].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.]

Lattice constants

	a(Å)
Köster and Haehl [1958]	4.81
NBS, sample at 25°C	4.8254 ±.0001

Density
(calculated) 7.662 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.2

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

d (Å)	I	hkl	2θ(°)
3.414	17	110	26.08
2.4124	45	200	37.24
2.1582	76	210	41.82
1.9697	100	211	46.04
1.7066	4	220	53.66
1.5255	4	310	60.65
1.3926	2	222	67.16
1.3384	14	320	70.27
1.2895	45	321	73.36
1.2065	15	400	79.35
1.1373	3	411	85.26
1.0790	13	420	91.10
1.0528	12	421	94.05
1.0288	12	332	96.96
0.9848	2	422	102.92
.9463	5	510	108.97
.8960	14	520	118.55
.8809	19	521	121.94
.8530	14	440	129.12
.8276	3	530	137.09
.8042	12	600	146.55
.7933	4	610	152.32
.7828	25	611	159.46

Additional patterns
1. Köster and Haehl [1958]

References
Köster, W. and W.-D. Haehl (1958). Das Zweistoffsystem Palladium-Vanadin, Z. Metallk. **49**, 647-649.

Platinum Titanium 1:3, $PtTi_3$ (cubic)

Sample source
The sample was prepared by R. M. Waterstrat at NBS by arc-melting.

Major impurities
0.001-0.01% each: Al, Cr, Cu and Si.

0.01 -0.1 % each: Fe and Pd.

Color
Metallic dark grey and opaque.

Structure
A15 type "β-W" [Duwez and Jordan, 1952].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.]

Lattice constants

	a(Å)
Duwez and Jordan [1952]---------	5.031
Nishimura and Hiramatsu [1957]--	5.024
NBS, sample at 25 °C----------	5.0327 ±0.0001

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

d (Å)	I	hkl	2θ(°)
3.559	90	110	25.04
2.516	46	200	35.65
2.250	27	210	40.03
2.055	100	211	44.02
1.7791	11	220	51.31
1.5910	15	310	57.91
1.4531	<1	222	64.02
1.3955	4	320	67.00
1.3449	42	321	69.88
1.2581	7	400	75.50
1.1861	8	411	80.99
1.1253	10	420	86.39
1.0981	3	421	89.09
1.0729	9	332	91.76
1.0272	2	422	97.15
0.9871	7	510	102.58
.9346	3	520	111.01
.9188	12	521	113.93
.8895	5	440	119.97
.8631	5	530	126.37
.8389	7	600	133.33
.8274	<1	610	137.15
.8164	16	611	141.27
.7957	2	620	150.92

Density
(calculated) 8.826 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.7$.

Additional patterns
1. PDF card 7-353 [Duwez and Jordan, 1952].

References

Duwez, P., and C.B. Jordan (1952). The crystal structure of Ti_3Au and Ti_3Pt, Acta Cryst. **5**, 213-214.

Nishimura, H. and T. Hiramatsu (1957). On the corrosion resistance of titanium alloys (2nd report) The equilibrium diagram of the titanium - platinum system, Nippon Kinzoku Gakkaishi **21**, 469-474.

Platinum Vanadium 1:3, PtV_3 (cubic)

Sample source
The sample was prepared at NBS by R. M. Waterstrat by arc-melting and it was annealed at 800 °C for one hour.

Major impurities
0.001-0.01% each:Ag,Au,Cr,Cu,Ir,Si,and Sn.

0.01 -0.1 % each:Fe, Pd, and Ti.

Color
Metallic dark grey and opaque.

Structure
A15 type"β-W"[Greenfield and Beck,1956].

Space group
O_h^3-Pm3n (223), Z=2 [ibid.]

Lattice constants

	a(Å)
Greenfield and Beck, [1956]-----	4.808
Matthias et al., [1961]---------	4.814
NBS, sample at 25 °C----------	4.8166 ±0.0001

Density
(calculated) 10.340 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.4$

Additional patterns
1·PDF card 8-434[Greenfield and Beck,1956]

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

d (Å)	I	hkl	2θ(°)
3.407	60	110	26.13
2.409	46	200	37.30
2.154	29	210	41.90
1.967	100	211	46.11
1.7027	10	220	53.79
1.5233	13	310	60.75
1.3359	5	320	70.42
1.2875	8	321	73.49
1.2043	8	400	79.52
1.1354	10	411	85.44
1.0771	4	420	91.31
1.0510	4	421	94.26
1.0271	13	332	97.17
0.9833	5	422	103.13
.9446	12	510	109.25
.8944	5	520	118.90
.8794	19	521	122.31
.8515	10	440	129.54
.8260	8	530	137.64
.8028	14	600	147.27
.7918	2	610	153.19
.7813	25	611	160.68

References

Greenfield,P. and P.A.Beck (1956). Intermediate phases in binary systems of certain transition elements, Trans. AIME **206**, 265-276.

Matthias,B.T.,V.B.Compton and E. Corenzwit (1961). Some new superconducting compounds, J.Phys. Chem. Solids **19**,Nos.1-2, 130-133.

Potassium Cobalt(II) Sulfate, $K_2Co_2(SO_4)_3$ (cubic)

Sample source
The sample was prepared at NBS by melting K_2SO_4 and $CoSO_4$ together at approximately 600° C.

Major impurities
0.001-0.01% each: Al, and Na.

Color
Deep purple

Optical data
Isotropic. N=1.608.

Structure
Isostructural with $K_2Mg_2(SO_4)_3$, langbeinite. [Gattow and Zemann, 1958]

Space group
T^4-$P2_13$ (198), Z=4 [ibid.]

Lattice constants

	a(Å)
Gattow and Zemann (1958)--------	9.929 ±.004
NBS, sample at 25 °C----------	9.9313 ±.0001

Density
(calculated) 3.283 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.0$

References
Gattow, G. and J. Zemann (1958). Über Doppelsulfate vom Langbeinit-Typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. 293, 233-40.

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

d (Å)	I	hkl	2θ(°)
5.74	14	111	15.42
4.442	14	210	19.97
4.057	16	211	21.89
3.312	6	221	26.90
3.142	100	310	28.38
2.996	24	311	29.80
2.756	10	320	32.46
2.654	58	321	33.74
2.409	6	410	37.30
2.278	3	331	39.52
2.222	1	420	40.57
2.167	2	421	41.65
2.118	4	332	42.65
2.027	17	422	44.67
1.987	5	430	45.62
1.948	18	510	46.58
1.912	4	511	47.50
1.845	10	520	49.34
1.814	2	521	50.25
1.756	1	440	52.04
1.728	12	522	52.95
1.703	3	530	53.78
1.678	1	531	54.64
1.656	1	600	55.45
1.633	3	610	56.30
1.611	21	611	57.12
1.571	6	620	58.73
1.551	6	621	59.54
1.533	5	541	60.33
1.515	<1	533	61.13
1.498	2	622	61.88
1.481	6	630	62.69
1.465	9	631	63.44
1.4334	4	444	65.01
1.4188	4	632	65.76
1.4046	2	710	66.51
1.3910	1	711	67.25
1.3772	1	640	68.01
1.3642	2	720	68.75
1.3515	6	721	69.49
1.3274	2	642	70.94
1.3155	2	722	71.68
1.3040	2	730	72.41
1.2931	7	731	73.12
1.2716	1	650	74.56

Potassium Cobalt(II) Sulfate, $K_3Co_2(SO_4)_3$ (cubic) – continued

d (Å)	I	hkl	2θ(°)
1.2614	3	651	75.27
1.2321	5	810	77.39
1.2228	2	811	78.09
1.2134	1	733	78.81
1.2044	1	820	79.51
1.1954	9	821	80.23
1.1869	1	653	80.93
1.1703	4	822	82.32
1.1627	2	830	82.98
1.1546	5	831	83.69
1.1468	5	751	84.39
1.1394	1	662	85.07
1.1318	3	832	85.77
1.1246	4	752	86.46
1.1102	1	840	87.86
1.1035	2	841	88.53
1.0966	2	910	89.24
1.0904	3	911	89.90
1.0840	2	842	90.58
1.0773	2	920	91.28
1.0710	2	921	91.98
1.0589	2	664	93.34
1.0528	7	922	94.05
1.0472	2	930	94.71
1.0412	5	931	95.43
1.0300	1	852	96.80
1.0243	1	932	97.52
1.0135	<1	844	98.93
1.0087	<1	940	99.57
1.0031	4	941	100.32
0.9984	1	933	100.98
.9933	1	10•0•0	101.69
.9883	3	10•1•0	102.40
.9835	3	10•1•1	103.10
.9739	2	10•2•0	104.54
.9692	2	10•2•1	105.26
.9647	5	950	105.96
.9602	2	951	106.67
.9555	1	10•2•2	107.44
.9512	2	10•3•0	108.14
.9470	2	10•3•1	108.85
.9344	2	10•3•2	111.04
.9302	1	871	111.79
.9263	<1	953	112.52
.9223	1	10•4•0	113.26
.9181	2	10•4•1	114.06
.9142	<1	10•3•3	114.81
.9067	2	10•4•2	116.32
.9028	1	962	117.11
.8992	1	11•1•0	117.88
.8954	1	11•1•1	118.68
.8884	3	11•2•0	120.23
.8847	2	11•2•1	121.06
.8779	<1	880	122.66
.8744	2	11•2•2	123.50
.8710	1	11•3•0	124.34
.8676	1	11•3•1	125.19
.8645	3	10•4•4	126.00
.8611	2	964	126.88
.8579	5	11•3•2	127.74
.8515	2	10•6•0	129.53
.8484	1	11•4•0	130.43
.8454	2	11•4•1	131.33
.8423	1	11•3•3	132.25
.8393	1	10•6•2	133.20
.8364	1	11•4•2	134.12
.8334	2	965	135.09
.8276	1	12•0•0	137.09
.8247	4	12•1•0	138.12
.8220	3	12•1•1	139.12
.8192	3	11•5•1	140.20
.8163	2	12•2•0	141.31
.8136	2	12•2•1	142.43
.8109	2	11•5•2	143.58
.8055	2	12•2•2	145.98
.8029	3	12•3•0	147.23
.8002	3	12•3•1	148.53
.7977	2	11•5•3	149.85
.7926	1	12•3•2	152.71
.7901	1	11•6•1	154.28
.7851	1	12•4•0	157.66
.7827	3	12•4•1	159.56

Potassium Cobalt(II) Trifluoride, $KCoF_3$ (cubic)

Sample source
The sample prepared at NBS was a washed precipitate obtained from a mixture of KF and $CoCl_2$ solutions.

Major impurities
0.001-0.01% each: Ca,Cs,Cu,Fe,Na,Pb,Rb, Si,and V.
0.01 -0.1 % each: Al,Mn,Ni,and Sr.

Color
Medium purplish pink.

Optical data
Isotropic N=1.468

Structure
Cubic perovskite [Rüdorff et al,1959]and [Okazaki et al, 1959].$KCoF_3$ has been reported to have a doubled cell [Martin et al. 1956]; however, we found no evidence for this.

Space group
O_h^1-Pm3m(221) Z=1. [Rüdorff et al.,1959]

Lattice constants

	a(Å)
Rüdorff et al. [1959]----------	4.062
Okazaki et al. [1959]----------	4.069 ±.001
Knox [1961]----------	4.071
NBS, sample at 25°C----------	4.0708 ±.0001

Density
(calculated) 3.816 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 3.4$

Polymorphism
Below 78°K. $KCoF_3$ is distorted to a tetragol cell.[Okazaki and Suemune, 1961].

Additional patterns
1. PDF card 1-949,[Dow Chemical Co.]

Internal standard W, a = 3.16504 Å
CuK_{α_1} λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.071	26	100	21.81
2.879	100	110	31.04
2.349	14	111	38.28
2.0351	72	200	44.48
1.8202	12	210	50.07
1.6623	36	211	55.21
1.4393	30	220	64.71
1.3564	4	300	69.20
1.2869	12	3$\bar{1}$0	73.53
1.2278	<1	311	77.71
1.1750	8	222	81.92
1.1290	<1	320	86.04
1.0879	11	321	90.15
1.0177	3	400	98.37
0.9874	2	410	102.53
.9596	5	411	106.77
.9340	<1	331	111.11
.9103	8	420	115.59
.8884	2	421	120.23
.8678	3	332	125.15
.8309	5	422	135.93
.8141	<1	500	142.20
.7983	7	510	149.54

References

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Okazaki, A., Y. Suemune and T. Fuchikami (1959). The crystal structures of $KMnF_3$, $KFeF_3$, $KCoF_3$, $KNiF_3$ and $KCuF_3$, J. Phys. Soc. Japan **14**, 1823.

Rüdorff, W., J. Kändler, G. Lincke and D. Babel (1959). Über Doppelfluoride von Nickel und Kobalt, Angew. Chem. **71**, 672.

Potassium Copper(II) Trifluoride, $KCuF_3$ (tetragonal)

Sample source
The sample was precipitated at NBS by adding $CuCl_2$ to an excess of KF in solution.

Major impurities
0.001-0.01% each: Ca,Co,Cs,Fe,Mg,Mn,Pb, Rb,Sn and Sr.
0.01 -0.1 % each: Al,Na,Si and V.

Color
Very pale blue.

Optical data
Crystals averaged 5μ in size and appeared almost isotropic; N= 1.516.

Structure
Tetragonal distorted perovskite type [Edward and Peacock,1959]. $KCuF_3$ is reported to have a superstructure [Okazaki and Suemune,1961], but Knox [1961] found no evidence detectable in a powder pattern and it was not seen in the present study. In the superstructure cell $a=\sqrt{2}a_o$ and $c=2c_o$, where a_o and c_o are the constants for the simple cell.

Space group
C_{4v}^1-P4mm (99) [Edward and Peacock, 1959]
Z=1.

Lattice constants

	a(Å)	c(Å)
Edward and Peacock [1959]	4.13	3.92
Hoppe [1959]	4.14	3.92
Okazaki et al. [1959]	4.14	3.926
Knox [1961]	4.140	3.922
NBS, sample at 25°C	4.1429	3.9260
	±.0004	±.0009

Density
(calculated) 3.934 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.8$

Internal standard W, a = 3.16504 Å
CuK_{α_1} λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.15	27	100	21.41
3.93	13	001	22.60
2.933	55	110	30.45
2.853	100	101	31.33
2.349	11	111	38.28
2.073	65	200	43.63
1.963	29	002	46.20
1.854	6	210	49.10
1.832	6	201	49.73
1.775	5	102	51.45
1.676	32	211	54.72
1.631	16	112	56.36
1.465	13	220	63.46
1.424	24	202	65.47
1.381	2	300	67.82
1.372	2	221	68.28
1.347	4	212	69.77
1.3101	8	310,003	72.02
1.3028	7	301	72.49
1.2477	5	103	76.26
1.1738	8	222	82.02
1.1066	1	203	88.22
1.1026	5	321	88.63
1.0896	5	312	89.97
1.0688	5	213	92.22
1.0357	3	400	96.09

References

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Knox,K. (1961). Perovskite-like fluorides. I.Structures of $KMnF_3$, $KFeF_3$, $KCoF_3$, $KNiF_3$ and $KZnF_3$. Crystal field effects in the series and in $KCrF_3$ and $KCuF_3$. Acta Cryst. 14, 583-585.

Okazaki,A. and Y. Suemune (1961).The crystal structure of $KCuF_3$, J. Phys. Soc. Japan. 16 176-183.

Okazaki, A., Y. Suemune and T.Fuchikami (1959). The crystal structures of $KMnF_3$, $KFeF_3$, $KCoF_3$, $KNiF_3$ and $KCuF_3$, J.Phys.Soc. Japan 14 1823-1824.

Potassium Iron(II) Trifluoride, $KFeF_3$ (cubic)

Sample source
The sample was precipitated at NBS by mixing solutions of $FeCl_2$ and KF. The material was washed, then heated to about 400 °C. in vacuum.

Major impurities
0.001-0.01% each: Al.

0.01 -0.1 % each: Na and Si.

Color
Light yellowish brown.

Optical data
Isotropic, N= 1.438.

Structure
Cubic perovskite [Okazaki and Suemune, 1961]. $KFeF_3$ has been reported to be only pseudo-cubic at room temperature [Martin et al., 1956]. It is reported as rhombohedral at 78 °K. [Okazaki et al., 1959]. We found no departure from cubic symmetry at 25 °C.

Space group
O_h^1-Pm3m (221) Z=1.

Lattice constants

	a(Å)
Okazaki et al. [1959]	4.122
Martin et al. [1960]	4.11
Hirakawa et al. [1960]	4.122
Okazaki et al. [1961]	4.121
Knox [1961]	4.120
NBS, sample at 25°C	4.1205 ±.0001

Density
(calculated) 3.606 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.7$.

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

d (Å)	I	hkl	2θ(°)
4.124	30	100	21.53
2.915	100	110	30.64
2.380	13	111	37.77
2.061	67	200	43.89
1.843	12	210	49.40
1.6822	32	211	54.50
1.4564	30	220	63.86
1.3733	6	300	68.23
1.3029	13	310	72.48
1.2426	<1	311	76.61
1.1894	6	222	80.72
1.1431	1	320	84.73
1.1015	9	321	88.74
1.0303	4	400	96.77
0.9995	1	410	100.82
.9713	5	411	104.94
.9454	<1	331	109.13
.9215	6	420	113.42
.8991	1	421	117.89
.8784	2	332	122.54
.8410	6	422	132.65
.8241	<1	500	138.33
.8081	8	510	144.80

References

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Okazaki, A., and Y. Suemune (1961). The crystal structures of $KMnF_3$, $KFeF_3$, $KCoF_3$, $KNiF_3$ and $KCuF_3$ above and below their Néel temperatures. J. Phys. Soc. Japan **16**, 671-675.

Potassium Magnesium Sulfate (langbeinite), $K_2Mg_2(SO_4)_3$ (cubic)

Sample source
The sample was prepared at NBS by melting K_2SO_4 and $MgSO_4$ together at about 1000 °C. The material was somewhat hygroscopic.

Major impurities
0.001-0.01% each: Cs, Rb, Si, and Sr.

0.01 -0.1 % each: Ca, Fe, and Na.

Color
Colorless.

Optical data
Isotropic; N=1.536.

Structure
Determined by Zemann and Zemann [1957]. There are many other double sulfates of the langbeinite-type [Gattow and Zemann 1958].

Space group
T^4-$P2_13$ (198), Z=4 [Gossner and Koch, 1931].

Lattice constants

	a(Å)
Gossner and Koch [1931]	9.98*
Gattow and Zemann [1958]	9.920
NBS, sample at 25°C	9.9211 ±.0001

*from kX

Density
(calculated) 2.823 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.5$.

Additional patterns
1. PDF card 17-740 [Morey et al., 1964].

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

d (Å)	I	hkl	2θ(°)
5.730	4	111	15.45
4.051	25	211	21.92
3.505	2	220	25.39
3.308	4	221	26.93
3.137	100	310	28.43
2.992	15	311	29.84
2.864	2	222	31.20
2.753	15	320	32.49
2.651	35	321	33.78
2.481	2	400	36.18
2.405	12	410	37.36
2.338	1	411	38.47
2.277	4	331	39.55
2.220	2	420	40.60
2.165	4	421	41.69
2.115	4	332	42.71
2.025	7	422	44.71
1.984	2	430	45.70
1.946	9	510	46.63
1.909	1	511	47.58
1.842	6	520	49.43
1.811	2	521	50.33
1.727	6	522	52.96
1.702	2	530	53.81
1.677	1	531	54.68
1.653	1	600	55.55
1.631	3	610	56.35
1.609	12	611	57.19
1.569	3	620	58.80
1.549	4	621	59.62
1.531	2	541	60.42
1.513	1	533	61.19
1.496	1	622	61.99
1.479	6	630	62.76
1.463	3	631	63.53
1.432	1	444	65.06
1.417	2	632	65.85
1.403	1	710	66.58
1.376	2	640	68.07
1.363	1	720	68.83
1.350	4	721	69.56
1.326	2	642	71.05
1.314	1	722	71.77
1.302	1	730	72.51
1.292	3	731	73.20

d (Å)	I	hkl	2θ(°)
1.271	2	650	74.62
1.2597	2	732	75.39
1.2303	1	810	77.52
1.2213	1	811	78.20
1.2121	1	733	78.91
1.2033	1	820	79.60
1.1943	2	821	80.32
1.1859	1	653	81.01
1.1695	1	822	82.39
1.1609	<1	830	83.13
1.1532	2	831	83.81
1.1458	1	751	84.48
1.1310	<1	832	85.85
1.1233	1	752	86.58
1.1094	<1	840	87.94
1.1024	1	841	88.65
1.0958	1	910	89.32
1.0890	2	911	90.03
1.0826	2	842	90.71
1.0760	1	920	91.43
1.0700	1	921	92.09
1.0577	1	664	93.48
1.0516	2	922	94.19
1.0458	1	930	94.87
1.0400	<1	931	95.57
1.0290	1	852	96.93
1.0232	1	932	97.67
1.0127	1	844	99.03
1.0073	1	940	99.76
1.0020	1	941	100.47
0.9971	1	933	101.15
.9921	1	10·0·0	101.86
.9872	1	10·1·0	102.57
.9824	1	10·1·1	103.27
.9728	1	10·2·0	104.71
.9682	2	10·2·1	105.41
.9637	1	950	106.12
.9591	1	951	106.86
.9546	1	10·2·2	107.58
.9503	1	10·3·0	108.30
.9458	1	10·3·1	109.05
.9333	<1	10·3·2	111.23
.9291	1	871	111.99
.9251	<1	953	112.73
.9211	1	10·4·0	113.48
.9172	1	10·4·1	114.24
.9131	<1	10·3·3	115.03
.9058	1	10·4·2	116.51
.9019	<1	962	117.31
.8981	1	11·1·0	118.10
.8947	<1	11·1·1	118.84
.8874	1	11·2·0	120.45
.8838	1	11·2·1	121.28
.8769	1	880	122.89
.8735	2	11·2·2	123.72
.8702	<1	11·3·0	124.55
.8668	1	11·3·1	125.40
.8635	<1	10·4·4	126.25
.8603	<1	964	127.09
.8570	2	11·3·2	127.99
.8507	<1	10·6·0	129.75
.8476	1	11·4·0	130.66
.8445	1	11·4·1	131.60
.8415	1	11·3·3	132.50
.8355	1	11·4·2	134.41
.8326	1	965	135.38
.8239	1	12·1·0	138.43
.8210	1	12·1·1	139.49
.8183	1	11·5·1	140.54
.8155	1	12·2·0	141.63
.8127	1	12·2·1	142.78
.8101	1	11·5·2	143.92
.8047	1	12·2·2	146.34
.8021	1	12·3·0	147.61
.7995	1	12·3·1	148.92
.7969	1	11·5·3	150.29
.7918	2	12·3·2	153.22
.7892	1	11·6·1	154.82
.7843	1	12·4·0	158.30
.7818	1	12·4·1	160.24
.7794	1	12·3·3	162.37

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Potassium Magnesium Trifluoride, $KMgF_3$ (cubic)

Sample source

The sample was made at NBS by adding HF to a slurry of K_2CO_3 and $MgCO_3$ and evaporating to dryness. The pattern was sharpened by heating the sample to the melting point.

Major impurities

0.001-0.01% each: Al, Ca, Pt, Rb and Sr.

0.01 -0.1 % each: Na, Pb and Si.

Color

Colorless

Optical data

Isotropic N = 1.404

Structure

Cubic perovskite [van Arkel,1925]. $KMgF_3$ has been reported to be monoclinic and to have a doubled cell. [Ludekens and Welch, 1952] and [Náray-Szabó, 1947]. We found no evidence to confirm the double cell.

Space group

O_h^1-Pm3m (221). Z=1.[van Arkel,1925].

Internal standard W, a = 3.16504 Å

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

d (Å)	*I*	*hkl*	2θ(°)
3.988	2	100	22.27
2.819	94	110	31.71
2.302	83	111	39.09
1.9943	100	200	45.44
1.7842	1	210	51.15
1.6284	24	211	56.46
1.4101	36	220	66.22
1.3298	<1	300	70.79
1.2614	6	310	75.27
1.2028	8	311	79.64
1.1516	8	222	83.96
1.0661	8	321	92.52
0.9972	2	400	101.14
.9403	2	330	110.00
.9150	2	331	114.66
.8920	10	420	119.43
.8505	1	332	129.83
.8142	3	422	142.16
.7823	4	510	159.89

Lattice constants

	a(Å)
van Arkel [1925]	4.01
Brisi [1952]	3.982
de Vries and Roy [1953]	3.98
Klasens et al. [1953]	4.00
Remy and Hansen [1956]	3.973
NBS, sample at 25°C	3.9889 ±.001

Density

(calculated) 3.150 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 0.9

Additional patterns

1. PDF card 3-1060 [Remy and Hansen, 1956];
2. Brisi (1952).

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Potassium Manganese(II) Sulfate (manganolangbeinite), $K_2Mn_2(SO_4)_3$ (cubic)

Sample source
Prepared at NBS by melting K_2SO_4 and $MnSO_4$ together and annealing at about 500° for 15 hours.

Major impurities
0.001-0.01% each: Al,Ca,Fe,Mg,Mo,Rb,Sb,Sn

Color
Pale pink.

Optical data
Isotropic. N=1.576.

Space group
T^4-$P2_13$ (198), Z=4 [Bellanca, 1947].

Structure
Isostructural with $K_2Mg_2(SO_4)_3$, langbeinite. [Gattow and Zemann, 1958].

Lattice constants

	a(Å)
Bellanca [1947]	10.034*
Gattow and Zemann [1958]	10.114 ±.004
NBS, sample at 25°C	10.1143 ±.0001

*from kX

Density
(calculated) 3.057 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 3.1$

Additional patterns
1. PDF 18-1036, Kohler and Franke, Mineralogisches Institut, Freie Universität Berlin, Germany.
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Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.839	10	111	15.16
4.521	8	210	19.62
4.128	14	211	21.51
3.372	4	221	26.41
3.198	100	310	27.87
3.047	17	311	29.29
2.806	8	320	31.87
2.702	50	321	33.12
2.453	4	410	36.60
2.385	<2	411	37.69
2.320	2	331	38.78
2.260	<2	420	39.85
2.208	2	421	40.84
2.156	3	332	41.86
2.064	13	422	43.82
2.024	2	430	44.74
1.984	13	510	45.69
1.947	3	511	46.62
1.878	8	520	48.42
1.846	2	521	49.31
1.761	7	522	51.89
1.734	3	530	52.74
1.7092	<2	531	53.57
1.6854	<2	600	54.39
1.6625	2	610	55.20
1.6401	15	611	56.02
1.5994	5	620	57.58
1.5793	4	621	58.38
1.5606	4	541	59.15
1.5421	<2	533	59.93
1.5249	<2	622	60.68
1.5076	4	630	61.46
1.4912	4	631	62.20
1.4596	2	444	63.70
1.4451	2	632	64.42
1.4302	2	710	65.17
1.4165	<2	711	65.88
1.4029	<2	640	66.60
1.3892	2	720	67.35
1.3765	4	721	68.05

d (Å)	I	hkl	2θ(°)
1.3517	2	642	69.48
1.3397	2	722	70.19
1.3277	<2	730	70.92
1.3168	2	731	71.60
1.2949	<2	650	73.00
1.2843	<2	732	73.70
1.2646	<2	800	75.05
1.2547	<2	810	75.74
1.2453	<2	811	76.42
1.2360	<2	733	77.10
1.2265	<2	820	77.81
1.2177	<2	821	78.48
1.2090	<2	653	79.15
1.1920	2	822	80.51
1.1835	<2	830	81.21
1.1757	3	831	81.86
1.1682	<2	751	82.50
1.1530	<2	832	83.83
1.1455	<2	752	84.51
1.1312	<2	840	85.83
1.1238	<2	841	86.53
1.1170	<2	910	87.19
1.1101	2	911	87.87
1.1034	<2	842	88.54
1.0973	<2	920	89.17
1.0905	2	921	89.87
1.0785	<2	664	91.15
1.0720	3	922	91.86
1.0660	2	930	92.53
1.0603	<2	931	93.18
1.0490	<2	852	94.49
1.0431	<2	932	95.19
1.0323	<2	844	96.52
1.0268	<2	940	97.20
1.0218	2	941	97.85
1.0164	<2	933	98.54
1.0116	<2	10·0·0	99.18
1.0064	2	10·1·0	99.87
1.0016	<2	10·1·1	100.53
0.9917	<2	10·2·0	101.92
.9870	2	10·2·1	102.60
.9825	<2	950	103.25
.9777	<2	951	103.97
.9733	<2	10·2·2	104.63
.9687	<2	10·3·0	105.33
.9643	<2	10·3·1	106.02
.9515	<2	10·3·2	108.10
.9472	<2	871	108.81
.9432	<2	953	109.50
.9390	<2	10·4·0	110.23
.9351	<2	10·4·1	110.92
.9311	<2	10·3·3	111.63
.9234	<2	10·4·2	113.06
.9197	<2	962	113.76
.9158	<2	11·1·0	114.51
.9119	<2	11·1·1	115.27
.9047	<2	11·2·0	116.72
.9011	<2	11·2·1	117.47
.8940	<2	880	118.98
.8906	<2	11·2·2	119.73
.8872	<2	11·3·0	120.50
.8839	<2	11·3·1	121.26
.8802	<2	10·4·4	122.10
.8769	<2	964	122.90
.8739	2	11·3·2	123.63
.8673	<2	10·6·0	125.27
.8642	<2	11·4·0	126.08
.8610	<2	11·4·1	126.92
.8579	<2	11·3·3	127.76
.8518	<2	11·4·2	129.46
.8488	<2	965	130.30
.8428	<2	12·0·0	132.09
.8399	<2	12·1·0	132.99
.8371	<2	12·1·1	133.90
.8343	<2	11·5·1	134.81
.8314	<2	12·2·0	135.78
.8286	<2	12·2·1	136.74
.8258	<2	11·5·2	137.72
.8203	<2	12·2·2	139.75
.8177	<2	12·3·0	140.77
.8150	<2	12·3·1	141.85
.8124	<2	11·5·3	142.91
.8072	<2	12·3·2	145.19
.8047	<2	11·6·1	146.37
.7996	<2	12·4·0	148.86
.7971	2	12·4·1	150.19
.7922	<2	991	152.96
.7898	<2	12·4·2	154.45
.7874	<2	10·8·1	156.07
.7850	2	11·6·3	157.76

Potassium Manganese(II) Trifluoride, $KMnF_3$ (cubic)

Sample source
The sample was precipitated at NBS by adding $MnCl_2$ solution to an excess of KF in solution.

Major impurities
0.001-0.01% each: Si, Al, Ca, Co, Cu, Fe, Mg.

0.01 -0.1 % each: Na.

Color
Very pale pink.

Optical data
N≃1.45. The sample was too fine-grained for accurate index measurements.

Structure
Cubic perovskite [Simanov, Batsanova, and Kovba, 1957].

Space group
O_h^1-Pm3m (221), Z=1 [Knox, 1961].

Lattice constants

	a(Å)
Simanov et al. (1957)	4.186
Hoppe et al. (1961)	4.19
Knox (1961)	4.182
Okazaki and Suemune (1961)	4.190
NBS, sample at 25 °C	4.1890 ±.0001

Density
(calculated) 3.412 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 3.1$.

Polymorphism
Below about -90 °C, $KMnF_3$ is a tetragonal distorted perovskite. [Okazaki & Suemune 1961].

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

d (Å)	I	hkl	2θ(°)
4.191	27	100	21.18
2.962	100	110	30.14
2.419	13	111	37.13
2.096	64	200	43.13
1.874	9	210	48.54
1.711	30	211	53.52
1.4813	24	220	62.66
1.3966	3	300	66.94
1.3246	11	310	71.11
1.2630	1	311	75.16
1.2091	6	222	79.14
1.1619	1	320	83.05
1.1196	8	321	86.94
1.0472	3	400	94.71
1.0159	2	410	98.61
0.9873	4	411	102.55
.9610	1	331	106.55
.9366	6	420	110.64
.9142	1	421	114.82
.8931	3	332	119.18
.8551	4	422	128.53
.8377	1	500	133.68
.8215	4	510	139.31

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Potassium Nickel Sulfate, $K_2Ni_2(SO_4)_3$ (cubic)

Sample source
Prepared at NBS by heating a mixture of $NiSO_4$ and K_2SO_4 at 750 °C. The sample was cooled slowly, ground, and annealed at 550 °C for half an hour.

Major impurities
0.001-0.01% each: Al, Ca, Fe, Mg, Na, Rb, and Si.

Color
light greenish yellow

Optical data
Isotropic. N=1.620

Structure
Isostructural with $K_2Mg_2(SO_4)_3$, langbeinite. [Gattow and Zemann, 1958].

Space group
T^1-$P2_13$ (198), Z=4 [ibid.]

Lattice constants

	a(Å)
Gattow and Zemann [1958]-------	9.838 ±.008
NBS, sample at 25°C----------	9.8436 ±.0001

Density
(calculated) 3.369 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 2.1.

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

d (Å)	I	hkl	2θ(°)
5.69	14	111	15.55
4.407	11	210	20.13
4.020	10	211	22.09
3.284	4	221	27.13
3.114	100	310	28.64
2.968	16	311	30.08
2.845	1	222	31.42
2.732	9	320	32.75
2.631	57	321	34.04
2.388	6	410	37.63
2.322	1	411	38.74
2.259	3	331	39.87
2.201	2	420	40.96
2.149	3	421	42.01
2.099	4	332	43.05
2.008	15	422	45.12
1.969	4	430	46.05
1.931	14	510	47.02
1.895	3	511	47.97
1.828	10	520	49.84
1.798	2	521	50.74
1.714	9	522	53.41
1.688	3	530	54.28
1.664	1	531	55.14
1.641	1	600	55.98
1.618	4	610	56.84
1.5968	17	611	57.68
1.5565	5	620	59.32
1.5375	5	621	60.13
1.5190	5	541	60.94
1.5010	1	533	61.75
1.4841	1	622	62.53
1.4673	7	630	63.33
1.4513	6	631	64.11
1.4211	2	444	65.64
1.4063	3	632	66.42
1.3921	3	710	67.19
1.3780	1	711	67.97
1.3651	2	640	68.70
1.3518	3	720	69.47
1.3396	4	721	70.20
1.3153	2	642	71.69
1.3037	2	722	72.43
1.2926	1	730	73.15
1.2815	4	731	73.89

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.2604	2	650	75.34
1.2501	2	732	76.07
1.2209	2	810	78.23
1.2116	1	811	78.95
1.2026	1	733	79.66
1.1937	2	820	80.37
1.1852	1	821	81.07
1.1765	1	653	81.79
1.1600	2	822	83.21
1.1521	1	830	83.91
1.1443	3	831	84.62
1.1368	2	751	85.31
1.1214	1	832	86.76
1.1146	3	752	87.43
1.0938	2	841	89.53
1.0873	1	910	90.21
1.0805	2	911	90.94
1.0740	1	842	91.64
1.0677	1	920	92.34
1.0614	2	921	93.05
1.0493	1	664	94.45
1.0433	3	922	95.17
1.0376	1	930	95.86
1.0319	1	931	96.56
1.0208	2	852	97.87
1.0154	2	932	98.68
1.0048	1	844	100.10
0.9995	1	940	100.82
.9944	1	941	101.54
.9894	1	933	102.25
.9844	<1	10.0.0	102.97
.9795	3	10.1.0	103.70
.9747	2	10.1.1	104.42
.9653	1	10.2.0	105.87
.9607	2	10.2.1	106.60
.9560	2	950	107.35
.9515	1	951	108.09
.9472	1	10.2.2	108.82
.9428	1	10.3.0	109.57
.9386	1	10.3.1	110.30
.9259	1	10.3.2	112.58
.9218	1	871	113.35
.9178	1	953	114.11
.9139	1	10.4.0	114.88
.9101	2	10.4.1	115.64

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
0.9062	1	10.3.3	116.42
.8985	2	10.4.2	118.02
.8950	1	962	118.78
.8912	2	11.1.0	119.61
.8876	1	11.1.1	120.41
.8804	2	11.2.0	122.07
.8769	1	11.2.1	122.90
.8702	1	880	124.54
.8667	2	11.2.2	125.43
.8632	1	11.3.0	126.32
.8600	2	11.3.1	127.17
.8568	1	10.4.4	128.05
.8536	1	964	128.93
.8504	2	11.3.2	129.86
.8441	1	10.6.0	131.71
.8410	1	11.4.0	132.65
.8380	2	11.4.1	133.62
.8349	1	11.3.3	134.60
.8290	1	11.4.2	136.60
.8261	1	965	137.61
.8203	1	12.0.0	139.76
.8175	2	12.1.0	140.85
.8146	2	12.1.1	142.00
.8119	2	11.5.1	143.13
.8091	1	12.2.0	144.34
.8064	2	12.2.1	145.56
.8037	1	11.5.2	146.81
.7984	1	12.2.2	149.47
.7958	3	12.3.0	150.88
.7932	1	12.3.1	152.36
.7907	2	11.5.3	153.91
.7856	2	12.3.2	157.32
.7831	2	11.6.1	159.22

References

Gattow, G. and J. Zemann (1958). Über Doppelsulfate vom Langbeinit-Typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. **293**, 233-240.

Potassium Sodium Sulfate, $K_{.67}Na_{1.33}SO_4$ (trigonal)

Sample source
The sample was prepared at NBS by melting K_2SO_4 and Na_2SO_4 in stoichiometric proportions.

Major impurities
0.001-0.01% each: Al, and Ba.

0.1 -1.0 % each: Ca.

Color
Colorless.

Optical data
Uniaxial (+), N_o=1.488, N_e=1.499.

Structure
There is a range of isomorphous phases from about $K_3Na(SO_4)_2$ to $KNa_3(SO_4)_2$ [Bredig,1942]. The structure of the series was determined by Gossner [1928].

Space group
D_{3d}^3-P$\bar{3}$m1 (164), Z=2. [Gossner,1928].

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25 °C-----	5.5515 ±.0003	7.0434 ±.0004

Density
(calculated) 2.489 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	7	100	18.46
3.967	64	101	22.39
3.521	17	002	25.27
2.841	80	102	31.46
2.778	100	110	32.20
2.584	10	111	34.69
2.404	7	200	37.37
2.349	12	003	38.29
2.276	7	201	39.57
2.181	<1	112	41.37
2.110	4	103	42.83
1.985	45	202	45.66
1.817	<1	210	50.16
1.793	3	113	50.88
1.761	6	004,211	51.88
1.680	1	203	54.58
1.654	1	104	55.52
1.615	18	212	56.96
1.603	15	300	57.44
1.563	1	301	59.06
1.486	11	114	62.42
1.458	2	302	63.78
1.437	2	213	64.84
1.420	4	204	65.68
1.408	1	005	66.31
1.388	10	220	67.41
1.351	3	105	69.50
1.334	<1	310	70.56
1.323	<1	303	71.21
1.310	1	311	72.03
1.291	<1	222	73.28
1.2643	2	214	75.07
1.2566	<1	115	75.61
1.2469	6	312	76.30
1.2150	<1	205	78.68
1.1948	1	223	80.28
1.1852	4	304,401	81.07
1.1742	<1	006	81.99
1.1593	2	313	83.27
1.1405	4	106	84.96

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.1374	4	402	85.25
1.1132	2	215	87.56
1.1030	<1	320	88.58
1.0897	4	224,321	89.96
1.0814	<1	116	90.84
1.0700	<1	403	92.08
1.0628	<1	314	92.89
1.0544	3	206	93.84
1.0524	4	322	94.09
1.0493	5	410	94.46
1.0055	<1	412	100.00
0.9985	<1	323	100.96
.9926	<1	404	101.79
.9861	3	216	102.73
.9682	1	315	105.41
.9348	<1	324	110.97
.9276	1	502	112.28
.9252	1	330	112.70
.9012	2	414,421	117.45
.8799	2	422	122.18

References

Bredig,M.A.(1942). Isomorphism and allotropy in compounds of the type A_2XO_4, J. Phys. Chem. **46**, 754-764.

Gossner,B.(1928). Ueber die Kristallstruktur von Glaserit und Kaliumsulpat, Neues Jahrb. Mineral. B-Bd 57A, 89-116.

Potassium Sodium Sulfate, $KNaSO_4$ (trigonal)

Sample source

The sample was prepared at NBS by melting equimolar proportions of Na_2SO_4 and K_2SO_4 then annealing overnight at 600°C.

Major impurities

0.001-0.01% each: Al, Be

0.1 -1.0 % each: Ca

Color

Colorless.

Optical data

Uniaxial (+), N_o=1.490, N_e=1.494.

Structure

Described by Bellanca, (1943). An isomorphous series exists from $K_3Na(SO_4)_2$ to $KNa_3(SO_4)_2$.

Space group

D_{3d}^3-$P\bar{3}m1$ (164), Z=2 [ibid.].

Lattice constants

	a(Å)	c(Å)
Hilmy (1953)	5.64	7.27
Bellanca (1943)*	5.654	7.28
NBS, sample at 25°C	5.6075 ±.0001	7.1781 ±.0002

*From kX. Natural mineral, composition uncertain.

Density

(calculated) 2.687 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.6

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

d (Å)	I	hkl	2θ(°)
4.857	9	100	18.25
4.026	49	101	22.06
3.593	19	002	24.76
2.889	71	102	30.93
2.804	100	110	31.89
2.614	6	111	34.28
2.431	7	200	36.95
2.393	13	003	37.55
2.302	10	201	39.10
2.147	3	103	42.05
2.011	42	202	45.05
1.835	2	210	49.64
1.8198	4	113	50.08
1.7944	4	004	50.84
1.7784	1	211	51.33
1.7039	2	203	53.75
1.6831	2	104	54.47
1.6340	11	212	56.25
1.6184	11	300	56.84
1.5791	2	301	58.39
1.5116	7	114	61.27
1.4758	1	302	62.92
1.4562	1	213	63.87
1.4431	4	204	64.52
1.4018	8	220	66.66
1.3767	2	105	68.04
1.3409	1	303	70.12
1.3238	1	311	71.16
1.3059	2	222	72.29
1.2833	2	214	73.77
1.2611	4	312	75.29
1.2360	1	205	77.10
1.2138	1	400	78.78
1.2095	1	223	79.11
1.2019	2	304	79.71
1.1737	1	313	82.03
1.1616	1	106	83.07
1.1501	2	402	84.09
1.1310	2	215	85.85
1.1050	2	224	88.38

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
1.0771	2	314	91.30
1.0732	3	206	91.73
1.0641	3	322	92.75
1.0598	4	410	93.23
1.0482	1	411	94.58
1.0163	<1	412	98.56
1.0102	1	323	99.37
1.0056	1	404	99.98
1.0024	2	216	100.42
0.9824	1	315	103.27
.9691	1	413	105.27
.9464	1	324	108.95
.9446	1	207	109.26
.9376	2	502	110.48
.9349	2	330	110.97
.9271	1	405,331	112.37
.9124	2	414	115.18
.8950	1	217	118.76
.8944	1	316	118.85
.8891	2	422	120.06
.8801	2	325	122.14
.8545	2	118	128.68
.8522	2	406	129.32
.8475	<1	512	130.70
.8416	1	208	132.46
.8289	1	334	136.64
.8171	1	424	141.02
.8094	1	600	144.23
.8061	1	218	145.70

Additional patterns

1.PDF card 6-0461 [Winchell et al., 1951]*
2.PDF card 6-0429 [Winchell et al., 1951]*
3.Bredig [1942]*

* Composition indefinite.

References

Bellanca,A.,(1943). Sulla struttura della aftitalite, Periodico Mineral.(Rome) **14**, 67-98.

Bredig,M.A., (1942). Isomorphism and allotropy in compounds of the type A_2XO_4, J. Phys.Chem.46, 754-764.

Hilmy,M.E., (1953). Structural crystallographic relation between sodium sulfate and potassium sulfate and some other synthetic sulfate minerals, Am. Mineralogist **38**,118-135.

Winchell,H.and R.J.Benoit, (1951). Taylorite, mascagnite, aphthitalite,lecontite, and oxammite from guano, Am.Mineralogist 36,590-602.

Potassium Sodium Sulfate (aphthitalite), $K_3Na(SO_4)_2$ (trigonal)

Sample source
The sample was prepared at NBS by melting K_2SO_4 and Na_2SO_4 together in stoichiometric proportions and annealing the product at 700 °C for 72 hours. The material is also called glaserite.

Major impurities
0.001-0.01% each: Al, and Ba

0.01 -0.1 % each: Ca

Color
Colorless.

Optical data
Uniaxial (+) N_o=1.494, N_e=1.499.

Structure
Determined by Gossner [1928]. There is a range of isomorphous phases from about $K_3Na(SO_4)_2$ to $KNa_3(SO_4)_2$ [Bredig, 1942].

Space group
D_{3d}^3-$P\bar{3}ml$ (164), Z=1 [Gossner, 1928].

Lattice constants

	a(Å)	c(Å)
Gossner (1928)----------	5.65	7.3
Hilmy (1953)----------	5.66	7.33
Yanat'eva et al. (1963)--	5.662	7.297
NBS, sample at 25 °C-----	5.6769	7.3331
	±.0003	±.0004

Density
(calculated) 2.697 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.6

Internal standard W, a = 3.16504 Å
CuK_{α_1} λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.32	2	001	12.08
4.921	9	100	18.01
4.088	28	101	21.72
3.666	21	002	24.26
2.940	76	102	30.38
2.839	100	110	31.48
2.646	3	111	33.85
2.458	10	200	36.52
2.443	16	003	36.76
2.330	14	201	38.61
2.189	3	103	41.20
2.042	44	202	44.33
1.852	5	113	49.14
1.833	4	004	49.70
1.733	2	203	52.79
1.717	2	104	53.30
1.657	11	212	55.41
1.638	9	300	56.09
1.600	2	301	57.57
1.540	6	114	60.01
1.497	1	302	61.95
1.479	2	213	62.78
1.469	5	204	63.24
1.4667	4	005	63.36
1.4194	10	220	65.73
1.4054	4	105	66.47
1.3608	1	303	68.95
1.3233	1	222	71.19
1.3048	2	214	72.36
1.2778	5	312	74.14
1.2598	2	205	75.38
1.2275	2	223	77.73
1.2221	2	006,304	78.14
1.1909	1	313	80.60
1.1861	1	106	80.99
1.1654	2	402	82.74
1.1512	3	215	83.99
1.1225	2	116,224	86.66
1.0941	2	206,314	89.50
1.0783	2	322	91.18
1.0729	3	410	91.77
1.0246	1	107	97.48
1.0211	3	216,404	97.93
0.9637	1	207	106.12

Additional patterns

1.PDF card 1-0978 [Hanawalt et al.,1938].
2.PDF card 3-0723 [Bredig,1942].
3.PDF card 6-0429 [Winchell and Benoit].
4.PDF card 6-0461 [Winchell and Benoit].
5.Yanat'eva et al. [1963].

References

Bredig,M.A. (1942). Isomorphism and allotropy in compounds of the type A_2XO_4, J. Phys. Chem. **46**,754-764.

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

Hilmy, M. E. (1953). Structural crystallographic relation between sodium sulfate and potassium sulfate and some other synthetic sulfate minerals, Am. Mineralogist **38**,118-135.

Winchell, H. and R.J. Benoit (1951). Taylorite, mascagnite, aphthitalite,lecontite, and oxammite from guano, Am. Mineralogist **36**,590-602.

Yanat'eva,O.K.,V.T.Orlova, and V.G.Kuznetsov (1963). The glaserite phase in the K_2SO_4-Na_2SO_4-H_2O system, Russ.J.Inorg. Chem. **8**, 910-915 (Trans. from Zh. Neorg. Khim. **8**, 1756-1766.)

Potassium Zinc Sulfate, $K_2Zn_2(SO_4)_3$ (cubic)

Sample source
The sample was prepared at NBS by melting K_2SO_4 and $ZnSO_4$ together, grinding the product and remelting.

Major impurities
0.001-0.01% each: Ca,Cs,Fe,Mg,Rb, and Ti.

0.01 -0.1 % each: Al.

Color
Colorless.

Optical data
Isotropic N=1.592.

Structure
Isostructural with $K_2Mg_2(SO_4)_3$ (langbeinite) [Gattow and Zemann,1958].

Space group
T^4-$P2_13$ (198), Z=4 [ibid.].

Lattice constants

	a(Å)
Gattow and Zemann [1958]--------	9.925 ±.006
NBS, sample at 25°C----------	9.9247 ±.0001

Density
(calculated) 3.376 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 1.7$

References
Gattow,G. and J.Zemann (1958).Über Doppelsulfate vom Langbeinit-Typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. **293**, 233-240.

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

d (Å)	I	hkl	2θ(°)
5.734	15	111	15.44
4.433	14	210	20.01
4.048	10	211	21.94
3.307	14	221	26.94
3.136	100	310	28.44
2.992	14	311	29.84
2.864	1	222	31.20
2.752	8	320	32.51
2.654	55	321	33.74
2.407	3	410	37.33
2.340	1	411	38.44
2.277	2	331	39.54
2.219	1	420	40.62
2.165	2	421	41.68
2.116	3	332	42.69
2.025	15	422	44.71
1.985	4	430	45.66
1.947	13	510	46.62
1.911	3	511	47.55
1.843	8	520	49.42
1.812	2	521	50.30
1.754	1	440	52.09
1.728	7	522	52.94
1.702	3	530	53.82
1.678	2	531	54.64
1.654	1	600	55.51
1.632	2	610	56.33
1.609	12	611	57.19
1.569	4	620	58.79
1.550	4	621	59.59
1.531	4	541	60.39
1.513	1	533	61.20
1.497	1	622	61.95
1.480	5	630	62.73
1.464	4	631	63.51
1.433	2	444	65.02
1.418	3	632	65.79
1.404	2	710	66.57
1.390	1	711	67.29
1.377	1	640	68.03
1.3635	1	720	68.79
1.3508	2	721	69.53
1.3266	1	642	70.99
1.3149	1	722	71.72
1.3034	1	730	72.45

Potassium Zinc Sulfate, $K_2Zn_2(SO_4)_3$ (cubic) – continued

d (Å)	I	hkl	2θ(°)
1.2925	2	731	73.16
1.2708	1	650	74.62
1.2607	2	732	75.32
1.2310	1	810	77.47
1.2217	<1	811	78.17
1.2126	1	733	78.87
1.2037	1	820	79.57
1.1951	1	821	80.26
1.1862	<1	653	80.98
1.1696	1	822	82.38
1.1617	<1	830	83.06
1.1538	2	831	83.76
1.1461	2	751	84.45
1.1309	<1	832	85.86
1.1237	1	752	86.54
1.1028	<1	841	88.61
1.0958	<1	910	89.32
1.0893	1	911	90.00
1.0830	1	842	90.67
1.0767	<1	920	91.35
1.0703	<1	921	92.05
1.0580	<1	664	93.44
1.0520	2	922	94.14
1.0461	2	930	94.83
1.0404	<1	931	95.52
1.0293	1	852	96.89
1.0236	<1	932	97.61
1.0130	<1	844	98.99
1.0079	1	940	99.67
1.0026	1	941	100.39
0.9975	<1	933	101.10
.9926	<1	10·0·0	101.79
.9876	2	10·1·0	102.51
.9829	<1	10·1·1	103.19
.9734	<1	10·2·0	104.62
.9684	1	10·2·1	105.38
.9640	1	950	106.08
.9595	1	951	106.79
.9550	1	10·2·2	107.52
.9508	1	10·3·0	108.22
.9462	<1	10·3·1	108.98
.9336	1	10·3·2	111.18
.9296	<1	871	111.91
.9253	1	953	112.69
.9215	<1	10·4·0	113.41

d (Å)	I	hkl	2θ(°)
.9175	2	10·4·1	114.18
.9137	1	10·3·3	114.91
.9061	1	10·4·2	116.43
.9024	<1	962	117.21
.8986	<1	11·1·0	117.99
.8949	2	11·1·1	118.79
.8877	1	11·2·0	120.39
.8842	1	11·2·1	121.19
.8771	<1	880	122.84
.8738	1	11·2·2	123.65
.8705	<1	11·3·0	124.46
.8671	<1	11·3·1	125.31
.8638	1	10·4·4	126.17
.8606	1	964	127.02
.8574	2	11·3·2	127.88
.8511	<1	10·6·0	129.66
.8479	1	11·4·0	130.59
.8449	<1	11·4·1	131.48
.8417	1	11·3·3	132.44
.8358	<1	11·4·2	134.31
.8328	<1	965	135.32
.8270	<1	12·0·0	137.29
.8241	<1	12·1·0	138.33
.8214	1	12·1·1	139.36
.8186	1	11·5·1	140.43
.8158	<1	12·2·0	141.51
.8131	1	12·2·1	142.63
.8104	<1	11·5·2	143.78
.8050	<1	12·2·2	146.23
.8023	1	12·3·0	147.48
.7998	1	12·3·1	148.76
.7971	1	11·5·3	150.17
.7920	<1	12·3·2	153.07
.7896	1	11·6·1	154.58
.7846	<1	12·4·0	158.05
.7821	1	12·4·1	159.99

Rhodium Vanadium 1:3, RhV_3 (cubic)

Sample source
The sample was prepared by R. M. Waterstrat at NBS by arc-melting and it was annealed at 1100 °C for two weeks.

Major impurities
0.001-0.01% each: Ag, Cu, Ir, Ni, Pb, and Si.

0.01 -0.1 % each: Cr, Fe, and Ti.

Color
Metallic dark grey and opaque.

Structure
A-15 type "β-W" [Greenfield and Beck, 1956]

Space group
O_h^3-Pm3n, Z=2 [ibid.]

Lattice constants

	a(Å)
Greenfield and Beck [1956]------	4.767
NBS, sample at 25 °C----------	4.7852 ±.0001

Density
(calculated) 7.751g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 1.8$

Internal standard W, a = 3.16504 Å
CuK_{α_1} λ = 1.5405 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
3.381	34	110	26.34
2.393	50	200	37.55
2.141	64	210	42.18
1.9540	100	211	46.43
1.6920	6	220	54.16
1.5136	6	310	61.18
1.3819	2	222	67.75
1.3267	11	320	70.98
1.2790	42	321	74.06
1.1964	10	400	80.15
1.1279	4	330	86.14
1.0700	11	420	92.09
1.0443	8	421	95.05
1.0203	9	332	98.04
0.9769	3	422	104.09
.9385	4	510	110.32
.8886	10	520	120.18
.8736	13	521	123.69
.8458	10	440	131.20
.8207	3	530	139.62
.7975	12	600	149.95
.7867	3	610	156.54

Additional patterns
1. PDF card 8-339 [Greenfield and Beck, 1956]

References
Greenfield, P. and P. A. Beck, (1956). Intermediate phases in binary systems of certain transition elements, Trans. AIME **206**, 265-76.

Rubidium Cobalt(II) Trichloride, $RbCoCl_3$ (hexagonal)

Sample source
The sample was prepared at NBS by heating co-precipitated RbCl and $CoCl_2$ in a sealed glass tube at 500 °C. The salt is moderately hygroscopic.

Major impurities
0.001-0.01% each: Ca, Cr, Cu, Fe and Sn.

0.01 -0.1 % each: Al, Na and Si.

0.1 -1.0 % each: Cs, K and Ni.

Color
Unground-strong blue; ground-pale blue.

Optical data
Uniaxial (+), N_e=1.740, N_o=1.668

Structure
Determined by Engberg and Soling(1963). Isostructural with $CsCoCl_3$ and other similar ABX_3 compounds.

Space group
D^4_{6h}-$P6_3/mmc$ (194), Z=2 [Engberg and Soling, 1963].

Lattice constants

	a(Å)	*c*(Å)
Engberg and Soling [1963]	6.999	5.996
NBS, sample at 25 °C	7.0013 ±.0004	6.002 ±.001

Density
(calculated) 3.268 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 4.3

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

d (Å)	*I*	*hkl*	2θ(°)
6.066	31	100	14.59
4.269	27	101	20.79
3.502	48	110	25.41
3.031	15	200	29.44
3.000	25	002	29.75
2.707	100	201	33.06
2.292	4	210	39.27
2.134	31	202	42.32
2.022	11	300	44.78
1.901	8	103	47.81
1.822	11	212	50.02
1.7505	22	220	52.21
1.6811	8	310	54.54
1.6698	11	203	54.94
1.6197	4	311	56.79
1.5122	7	222	61.24
1.5001	5	004	61.79
1.4696	12	401,312	63.22
1.3911	2	320	67.24
1.3792	1	114	67.90
1.3534	5	321,402	69.38
1.3229	7	410	71.22
1.2923	<1	411	73.17
1.2879	1	313	73.46
1.2620	2	322	75.23
1.2079	4	403	79.24
1.1670	2	330	82.60
1.1392	4	224	85.08
1.1254	6	421	86.38
1.0702	2	422	92.06
1.0104	3	600	99.34

References
Engberg, Å. and H. Soling, (1963). The crystal structure of $RbCoCl_3$, Acta Cryst. **16** A27.

Rubidium Nickel(II) Trichloride, $RbNiCl_3$ (hexagonal)

Sample source
The sample was prepared at NBS by heating co-precipitated RbCl and $NiCl_2$ in a sealed glass tube at 500 °C. The salt is moderately hygroscopic.

Major impurities
0.001-0.01% each:Al,Ba and Si.

0.01 -0.1 % each:Cs.

0.1 -1.0 % each:K and Na.

Color
Unground - Medium reddish brown.
Ground - Brownish orange.

Optical data
Uniaxial positive N_o=1.693, N_e=1.796.Weak pleochroism with the stronger absorption perpendicular to c.

Structure
Isostructural with $RbCoCl_3$ and similar ABX_3 compounds.

Space group
D_{6h}^4-$P6_3/mmc$ (194), Z=2 by analogy with $CsNiCl_3$

Lattice constants

	a(Å)	c(Å)
Allamagny[1960]----------	6.95	11.777
NBS, sample at 25 °C-----	6.9534 ±.0004	5.906 ±.001

No lines were found at NBS that would require the double "c" cell constant reported by Allamagny [1960].

Density
(calculated) 3.365 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 3.3$

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

d (Å)	I	hkl	2θ(°)
6.02	22	100	14.71
4.217	17	101	21.05
3.477	42	110	25.60
3.008	10	200	29.67
2.952	15	002	30.25
2.684	100	201	33.36
2.276	1	210	39.57
2.123	8	211	42.55
2.109	32	202	42.84
2.0073	9	300	45.13
1.8030	13	212	50.58
1.7384	26	220	52.60
1.6704	6	310	54.92
1.6472	13	203	55.76
1.6075	5	311	57.26
1.5051	7	400	61.56
1.4984	7	222	61.87
1.4588	12	401	63.74
1.3815	2	320	67.77
1.3452	3	321	69.86
1.3416	3	402	70.08
1.3139	7	410	71.78
1.1590	1	105,330	83.30
1.1174	6	421	87.15

Additional patterns
1. PDF card 16-110 [Allamagny,1960].

References
Allamagny, P.(1960). Synthèses de fluorures de deux métaux par réactions entre le gaz HF et des chlorures cristallisés, Bull. Soc. Chim. France **1960**, 1099.

Sodium Calcium Sulfate (glauberite), $Na_2Ca(SO_4)_2$ (monoclinic)

Sample source
The sample was prepared at NBS by reaction of $CaCl_2$ and Na_2SO_4 in solution at 80 °C. Gypsum is formed as an intermediate product. The glauberite obtained when the reaction is continued for several hours was washed with alcohol.

Major impurities
0.001-0.01% each: Al, Cu, Fe, Ni, and Si.

0.01 -0.1 % each: Sr.

Color
Colorless.

Optical data
Biaxial (-), N_α=1.511, N_β=1.530, N_γ=1.532
2V is small. Tabular-shaped crystals.

Structure
Determined by Cocco et al. [1965].

Space group
C_{2h}^6-C2/c (15), Z=4, [Pardillo,1934].

Density
(calculated) 2.782 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 0.8.

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

d (Å)	*I*	*hkl*	2θ(°)
6.214	22	110	14.24
4.689	18	200	18.91
4.381	47	111	20.25
4.148	12	020	21.40
3.945	47	002	22.52
3.792	17	$\bar{2}02,\bar{1}12$	23.44
3.175	74	$\bar{2}21$	28.08
3.126	100	$\bar{3}11$	28.53
3.110	80	220	28.68
3.008	35	112	29.67
2.926	15	310	30.53
2.861	49	022	31.24
2.808	65	$\bar{2}22$	31.84
2.677	62	$\bar{1}13,221$	33.44
2.579	1	202	34.76
2.475	27	311	36.27
2.466	12	$\bar{4}02$	36.40
2.435	8	131	36.88
2.346	19	400	38.33
2.319	3	$\bar{2}23$	38.85
2.223	2	023	40.55
2.191	7	222	41.17
2.140	14	$\bar{3}31$	42.19
2.122	8	$\bar{4}22$	42.57
2.102	6	132	42.99
2.074	16	040,330	43.61
2.036	19	$\bar{1}14$	44.46
2.006	38	041	45.15
1.997	20	$\bar{3}14$	45.37
1.975	62	$\bar{1}33,004$	45.90
1.958	13	$\bar{5}12$	46.33
1.908	14	$\bar{4}04$	47.63
1.897	8	240,$\bar{2}24$	47.91
1.858	3	$\bar{5}13$	48.99
1.836	11	042,421	49.61

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)	β(°)
Pardillo [1935]	10.01*	8.21*	8.43*	112°11′
Corazza and Sabelli [1965]	10.158	8.333	8.551	112°20′
Klebtsova and Borisob [1966]	10.30	8.32	8.60	112°
Araki and Zoltai [1967]	10.129 ±.002	8.306 ±.002	8.533 ±.002	112°11.4′ ±0.6′
NBS, sample at 25°C (synthetic)	10.134 ±.001	8.297 ±.001	8.532 ±.001	112°12.7′ ±0.5′

*from kX

d (Å)	I	hkl	2θ(°)
1.830	9	510	49.77
1.799	12	223	50.70
1.777	21	133	51.38
1.747	3	402	52.33
1.688	4	$\bar{6}02,\bar{5}14$	54.28
1.671	6	$\bar{1}34,332$	54.89
1.656	3	$\bar{3}15$	55.44
1.6316	13	$\bar{1}15$	56.34
1.6231	14	$\bar{5}31$	56.66
1.6150	11	204	56.97
1.6111	10	422	57.12
1.5793	2	151	58.38
1.5632	7	$\bar{6}22,600$	59.04
1.5530	1	440,530	59.47
1.5296	3	$\bar{6}23$	60.47
1.5140	2	$\bar{4}43,\bar{4}25$	61.16
1.5047	1	224	61.58
1.4865	1	$\bar{2}44$	62.42
1.4767	1	025,152	62.88
1.4662	2	512,350	63.38
1.4607	2	$\bar{3}52,333$	63.65
1.4421	10	$\bar{3}35$	64.57
1.4389	7	243	64.73
1.4310	5	$\bar{1}53,044$	65.13
1.4265	7	$\bar{1}35$	65.36
1.4142	4	$\bar{2}06$	66.00
1.4048	1	423	66.50
1.3975	<1	351	66.89
1.3830	<1	060	67.69
1.3583	1	$\bar{1}16,\bar{7}14$	69.09
1.3364	4	$442,\bar{5}35$	70.39
1.3318	8	$\bar{2}61$	70.67
1.3248	<1	$\bar{5}16$	71.10
1.3161	3	006	71.64
1.3123	2	532	71.88
1.3014	6	$\bar{1}54,352$	72.58
1.2975	5	135	72.83
1.2952	2	$513,\bar{6}41+$	72.98
1.2814	2	$\bar{7}32,\bar{5}52$	73.90
1.2796	3	$\bar{4}45$	74.02
1.2752	3	$\bar{7}15$	74.32
1.2741	3	$\bar{2}44$	74.39
1.2641	<1	$\bar{3}36$	75.08
1.2547	2	026	75.74
1.2388	4	$\bar{2}63$	76.89
1.2311	3	424	77.46
1.2271	2	$\bar{1}16$	77.76
1.2156	<1	$\bar{6}26$	78.64
1.2057	4	$730,\bar{3}17$	79.41
1.1850	<1	533	81.08
1.1795	7	641	81.54
1.1754	<1	$\bar{1}55$	81.89
1.1625	2	$\bar{4}27,\bar{1}17$	82.99
1.1579	1	$\bar{2}27,\bar{4}46$	83.40
1.1476	1	514	84.32
1.1421	<1	$\bar{1}72$	84.82
1.1317	3	136,245	85.78
1.1277	3	335	86.16
1.1155	1	$\bar{9}13,\bar{3}37$	87.34
1.1125	1	172	87.63
1.1002	<1	155	88.87
1.0951	1	444	89.39
1.0887	2	027,354	90.06
1.0675	2	316	92.36

Additional patterns

PDF card 2-0556 [Imperial Chemical Industries, Northwich, England]; Corazza and Sabelli [1965]; Rassonskaya and Semendyaeva [1961].

References

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Sodium Cobalt(II) Sulfate Tetrahydrate, $Na_2Co(SO_4)_2 \cdot 4H_2O$ (monoclinic)

Sample source
The sample was prepared at NBS by crystallization from an aqueous solution of its components at room temperature.

Major impurities
0.001-0.01% each: Al,Fe,Mn,Si,and Sr.

0.01 -0.1 % each: Ca,Mg,and Ni.

Color
Light purplish pink.

Optical data
Biaxial(-) N_α=1.512, $N_\beta \cong$1.517, N_γ=1.520; 2V is large.

Structure
Isostructural with $Na_2Mg(SO_4)_2 \cdot 4H_2O$ (bloedite) [Giglio, 1958].

Space group
C_{2h}^5-$P2_1/a$ (14), Z=2 [ibid].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25°C	11.104 ±.001	8.249 ±.001	5.541 ±.001	100°21.6′ ±.5′

Density
(calculated) 2.455 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.4

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

d (Å)	I	hkl	2θ(°)
6.58	13	110	13.45
5.453	16	200,001	16.24
4.553	79	210,011	19.48
4.440	14	$\bar{1}11$	19.98
4.259	39	$\bar{2}01$	20.84
4.128	2	020	21.51
3.990	16	111	22.26
3.857	3	120	23.04
3.786	16	$\bar{2}11$	23.48
3.552	2	201	25.05
3.329	28	$\bar{3}10$	26.76
3.288	100	220,021	27.10
3.257	54	211,$\bar{1}$21	27.36
3.078	8	$\bar{3}11$	28.98
2.963	12	$\bar{2}21$	30.13
2.731	12	400,320	32.76
2.726	14	002	32.83
2.692	15	221	33.25
2.667	11	130	33.57
2.639	25	$\bar{4}01$	33.94
2.622	7	$\bar{1}12$	34.17
2.586	12	012,$\bar{3}$21	34.66
2.512	1	$\bar{4}11$,$\bar{2}12$	35.71
2.456	2	230,031	36.56
2.436	4	$\bar{1}31$	36.86
2.428	4	112	36.99
2.356	4	131	38.17
2.319	4	321	38.80
2.311	6	$\bar{2}31$	38.94
2.302	8	$\bar{3}12$	39.10
2.296	10	$\bar{1}22$	39.21
2.280	15	202	39.49
2.277	16	420	39.55
2.199	1	411,212	41.00
2.174	7	231	41.51
2.162	5	122	41.74
2.130	6	$\bar{4}02$	42.40
2.113	8	510	42.76
2.097	3	$\bar{5}11$	43.10
2.063	3	$\bar{4}12$,040	43.84
2.027	22	140	44.66
1.996	3	421,222	45.41
1.963	9	331	46.20
1.958	7	312	46.33
1.950	2	$\bar{1}32$	46.52

d (Å)	*I*	*hkl*	2θ(°)
1.937	9	430,032	46.87
1.932	6	520,240	47.00
1.919	4	$\bar{5}21$	47.34
1.903	1	$\bar{4}31,\bar{2}32$	47.75
1.893	2	$\bar{4}22$	48.03
1.865	8	132	48.79
1.857	2	$\bar{2}41$	49.00
1.826	2	$\bar{2}03$	49.90
1.816	2	003	50.18
1.810	2	322	50.36
1.807	4	$\bar{3}32$	50.46
1.802	4	$\bar{1}13$	50.60
1.783	9	241,$\bar{2}$13	51.18
1.777	7	610,402	51.37
1.755	2	431,232	52.07
1.735	1	412,521	52.72
1.718	3	$\bar{3}13$	53.27
1.703	3	$\bar{5}31$	53.79
1.671	9	$\bar{6}21$	54.89
1.666	8	620	55.08
1.658	8	$\bar{6}02$	55.38
1.645	2	440,042	55.84
1.640	2	601	56.02
1.631	3	150,422	56.35
1.625	2	$\bar{6}12$,332,+	56.58
1.609	2	611	57.22
1.605	4	123	57.36
1.600	3	142	57.55
1.570	4	531	58.78
1.563	2	$\bar{3}42$	59.03
1.551	7	151,$\bar{5}$32	59.56
1.545	4	512	59.82
1.537	6	$\bar{4}23$	60.17
1.533	7	710,$\bar{1}$33	60.33
1.530	5	441,242	60.47
1.522	6	$\bar{6}31$,223	60.82
1.518	4	630	61.00
1.502	4	350	61.68
1.499	3	540	61.83
1.495	3	313	62.02
1.491	2	432	62.20
1.482	2	$\bar{4}42$	62.65

References

Giglio,M. (1958). Die Kristallstruktur von $Na_2Zn(SO_4)_2 \cdot 4H_2O$(Zn-Blödit), Acta Cryst. 11, 789-794.

Sodium Mangesium Sulfate Tetrahydrate, bloedite*, $Na_2Mg(SO_4)_2 \cdot 4H_2O$ (monoclinic)

Sample source
Natural mineral from Soda Lake, Calif. National Museum No. 93869.

*also known as astrakhanite.

Major impurities
0.001-0.01% each: Al, K, Mo, Ni, and Ti.

0.01 -0.1 % each: Ca, Co, Fe, Si, and Sr.

Color
Colorless.

Optical data
Biaxial(-), N_α=1.484, N_β=1.488, N_γ=1.492. 2V is large.

Structure
Determined by Rumanova and Malitskaya [1959]. There are a number of isostructural hydrated double sulfates, [Giglio, 1958].

Space group
C_{2h}^5-$P2_1/a$ (14), Z=2 [Lauro, 1940].

Density
(calculated) 2.218 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.0.

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

d (Å)	*I*	*hkl*	2θ(°)
5.463	2	200	16.21
4.555	94	210,011	19.47
4.442	5	$\bar{1}11$	19.97
4.281	29	$\bar{2}01$	20.73
4.126	10	020	21.52
3.981	9	111	22.31
3.860	6	120	23.02
3.800	25	$\bar{2}11$	23.39
3.333	21	310	26.72
3.289	95	220,021	27.09
3.252	100	$\bar{1}21$,211	27.40
3.091	4	$\bar{3}11$	28.86
3.055	3	121	29.21
2.971	40	$\bar{2}21$	30.05
2.732	40	400,320	32.75
2.724		002	32.85
2.687	14	221	33.32
2.667		130	33.57
2.651	38	$\bar{4}01$	33.78
2.644		311,$\bar{2}$02	33.88
2.623	2	$\bar{1}12$	34.16
2.586	22	012	34.65
2.518	3	$\bar{2}12$	35.62
2.454	4	230,031	36.58
2.420	2	112	37.11
2.314	11	$\bar{2}31$,321	38.89
2.297	12	$\bar{1}22$	39.18
2.276	19	420,401	39.56
2.271		022,202	39.65
2.194	6	330,411	41.10

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)	β(°)
Lauro [1940]	11.06*	8.17*	5.50*	100°39′
Rumanova and Malitskaya [1959]	11.05	8.16	5.50	100°40′
NBS, sample at 25°C	11.128 ±.001	8.246 ±.001	5.543 ±.001	100°51.9′ ±0.8′

*from kX

d (Å)	*I*	*hkl*	2θ(°)
2.170	15	231	41.58
2.157	5	122	41.84
2.141	8	$\bar{4}02$	42.17
2.113	9	510	42.75
2.103	1	$\bar{5}11$	42.96
2.080	3	$\bar{3}22$	43.46
2.062	4	040	43.88
2.025	30	140	44.71
1.992	7	421	45.49
1.988		222	45.58
1.959	15	331	46.30
1.951	5	$\bar{1}32,312$	46.50
1.937	16	430	46.86
1.933		032	46.97
1.921	14	$\bar{1}41$	47.27
1.907	5	$\bar{4}31$	47.64
1.901		$\bar{4}22$	47.81
1.876	3	141	48.48
1.858	10	$511,\bar{2}41$	48.99
1.834	5	$\bar{6}01$	49.67
1.812	4	$\bar{3}32$	50.31
1.803	3	$\bar{1}13$	50.59
1.790	10	$\bar{6}11$	50.97
1.785	11	$\bar{2}13$	51.13
1.779		610	51.30
1.753	5	$\bar{3}41,431$	52.14
1.732	4	521	52.82
1.723	2	$\bar{3}13$	53.12
1.711	1	530	53.52
1.706	3	$\bar{5}31$	53.69
1.700	<1	113	53.87
1.685	1	$\bar{1}23$	54.39
1.676	10	$\bar{6}21$	54.73
1.665	12	$620,\bar{6}02$	55.11
1.661	10	023	55.26
1.644	1	042	55.88
1.631	3	$150,\bar{4}13$	56.35
1.6252	1	$\bar{2}42,422$	56.58
1.6200	1	$332,\bar{3}23$	56.78
1.6053	1	611	57.35
1.6012	6	123,213	57.51
1.5988	3	142	57.60
1.5671	5	$531,\bar{3}42$	58.88
1.5501	7	151	59.59
1.5419	5	$\bar{4}23$	59.94
1.5278	3	441	60.55
1.5181	10	630,223	60.98
1.4994	7	540	61.82

Additional patterns

1. PDF card 4-0549 [Michigan Alkali Co., Wyandotte, Mich.].
2. Druzhinin et al. [1961].

References

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Rumanova, I. M. and G.I. Malitskaya (1959). Revision of the structure of astrakhanite by weighted phase projection methods, Soviet-Phys. Cryst. **4**, 481-95 (Trans. from Kristallografiya **4**, 501-515).

Sodium Manganese(II) Trifluoride, $NaMnF_3$ (orthorhombic)

Sample source
The sample was precipitated at NBS by adding $MnCl_2$ to an excess of NaF in solution.

Major impurities
0.001-0.01% each: Co, Cs, Fe, K, and Mg.

0.01 -0.1 % each: Al, Ba, Ca, and Si.

Color
Very pale pink.

Optical data
Almost isotropic, N=1.425. Perfect cubes about 10μ in size.

Structure
Orthorhombic distorted perovskite [Simanov, Batsanova, and Kovba, 1957]. Assumed to be isostructural with $CaZrO_3$.

Space group
D_{2h}^{16}-Pnma (62), Z=4 by analogy with $CaZrO_3$

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

d (Å)	*I*	*hkl*	2θ(°)
4.00	96	101	22.23
3.571	4	111	24.91
2.876	28	200	31.07
2.826	100	121	31.63
2.776	20	002	32.22
2.553	4	201	35.12
2.500	9	102	35.89
2.433	10	211	36.92
2.405	19	031	37.36
2.386	12	112	37.66
2.282	1	022	39.45
2.219	8	131	40.63
2.152	8	221	41.94
2.121	2	122	42.58
1.997	60	202	45.37
1.956	2	230	46.38
1.938	3	212	46.85
1.843	2	231	49.40
1.823	2	132	49.97
1.811	13	301	50.34
1.788	28	141	51.03
1.7666	8	311	51.70
1.7612	8	103	51.87
1.7193	<2	113	53.23
1.6499	23	321	55.66
1.6426	19	240	55.93
1.6229	17	042	56.67
1.6119	33	123	57.09
1.5565	2	203	59.32
1.5384	<2	051	60.09
1.4981	2	331	61.88
1.4696	2	133	63.22
1.4669	2	322	63.35
1.4371	4	400	64.82
1.4133	15	242	66.05
1.3911	2	401	67.24
1.3873	2	004	67.45
1.3566	3	332,251	69.19
1.3525	3	420	69.43
1.3481	3	152	69.69
1.3431	7	341	69.99
1.3303	<2	114	70.76
1.3222	2	143	71.26
1.3112	2	024	71.95
1.2763	3	402	74.24
1.2650	12	161,430	75.02
1.2630	9	323	75.16
1.2497	5	204	76.10
1.2160	5	422	78.61

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
Simanov [1957]---	11.520	8.000	11.136
NBS, sample 25°C-	5.7485	8.0045	5.5509*
	±.0004	±.0008	±.0004

*Smaller cell indexed all NBS powder lines

Density
(calculated) 3.508 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.5

Additional patterns
1.Simanov et al. [1957].

References
Simanov,Yu.P.,L.P.Batsanova,and L.M.Kovba, (1957).X-ray investigation of the binary fluorides of bivalent manganese, Russ. J. Inorg. Chem. 2, 207-215. (Trans. from Zh. Neorg. Khim. 2 No.10, 2410-2415).

Sodium Mercury(II) Trichloride Dihydrate, $NaHgCl_3 \cdot 2H_2O$ (orthorhombic)

Sample source
The sample was prepared at NBS by crystallization from an aqueous solution of equal molecular amounts of NaCl and $HgCl_2$.

Major impurities
0.001-0.01% each: Fe.

0.01 -0.1 % each: Al.

Color
Colorless.

Optical data
Biaxial(+), N_α=1.634, N_β=1.652, N_γ=1.680, 2V is large.

Structure
Determined by Malčič [1959].

Space group
D_{2h}^{16}-Pnam (62), Z=4, [Ninković,1957].

Lattice constants

	a(Å)	b(Å)	c(Å)
Ninković [1957]--	9.372 ±.003	18.71 ±.02	4.037 ±.002
NBS, sample at 25 °C----------	9.3803 ±.0005	18.732 ±.001	4.0301 ±.0004

Density
(calculated) 3.433 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 2.3$

Additional patterns
1.Ninković [1957].

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

d (Å)	I	hkl	2θ(°)
9.36	14	020	9.44
8.39	100	110	10.54
6.62	40	120	13.36
5.199	4	130	17.04
4.681	56	200,040	18.94
4.551	18	210	19.49
4.193	14	220,140	21.17
3.943	24	011	22.53
3.749	59	230	23.71
3.633	19	111	24.48
3.479	62	150	25.58
3.444	80	121	25.85
3.387	51	031	26.29
3.315	9	240	26.87
3.186	14	131	27.98
3.121	6	060	28.58
3.085	2	310	28.92
3.058	42	201	29.18
3.016	51	211	29.59
2.963	44	320,160	30.13
2.906	56	221,141	30.74
2.797	4	330	31.97
2.745	38	231,051	32.59
2.634	11	151	34.00
2.600	46	340,260	34.47
2.572	20	170	34.85
2.559	16	241	35.03
2.449	40	311	36.66
2.401	6	350	37.42
2.386	5	321,161	37.67
2.344	6	400,080	38.37
2.324	27	270	38.71
2.297	3	331	39.18
2.272	8	180	39.64
2.229	14	071	40.44
2.208	16	360	40.83
2.195	39	430	41.08
2.169	9	171	41.61
2.095	4	440,280	43.14
2.062	46	351	43.86

d (Å)	*I*	*hkl*	2θ(°)
2.031	16	370,190	44.57
2.027	16	401	44.67
2.015	26	002	44.95
1.988	13	450	45.60
1.979	46	181	45.81
1.959	13	112	46.30
1.937	3	361	46.86
1.928	9	122,431	47.10
1.902	11	290	47.77
1.874	24	460,380,+	48.53
1.860	17	441,281	48.93
1.850	24	042,091,+	49.22
1.840	10	520	49.50
1.815	2	371,191,+	50.22
1.797	3	530	50.77
1.774	9	232	51.46
1.763	6	470	51.81
1.741	11	540,2·10·0	52.51
1.722	3	242	53.14
1.700	19	461,381	53.90
1.687	4	312	54.32
1.675	26	1·11·0	54.76
1.666	8	322,162	55.08
1.616	4	471	56.94
1.608	1	560,3·10·0	57.26
1.592	18	342,262,+	57.86
1.561	5	0·12·0	59.13
1.548	11	551	59.66
1.537	1	570	60.15
1.523	8	412,272	60.78
1.508	3	422,182	61.43
1.4888	6	362	62.31
1.4830	14	640	62.58
1.4638	5	580,4·10·0	63.50
1.4531	4	611,442	64.02
1.4435	2	650	64.50
1.4385	8	1·12·1	64.75
1.4312	4	372,192	65.12
1.4194	6	631	65.73
1.4016	5	3·11·1	66.67
1.3979	7	660	66.87
1.3900	2	2·12·1	67.30
1.3832	4	292	67.68
1.3755	11	581,4·10·1	68.11
1.3723	15	462,382,+	68.29
1.3689	4	512	68.48
1.3576	6	1·10·2	69.13
1.3563	7	0·13·1	69.21
1.3402	2	013	70.16
1.3381	3	0·14·0	70.29
1.3274	5	472,720,+	70.94
1.3245	4	1·14·0	71.12
1.3169	6	591,2·10·2,+	71.59
1.3136	5	392,033	71.80
1.3039	2	3·13·0,4·11·1	72.42
1.2884	7	213,1·11·2,+	73.43
1.2797	4	671,482,+	74.01
1.2647	4	233,053	75.04
1.2603	9	721	75.35
1.2535	3	2·11·2,153	75.83
1.2448	2	243,3·13·1	76.45
1.2376	4	1·15·0,681	76.98
1.2347	5	602	77.19
1.2304	6	3·14·0	77.51
1.2278	6	4·13·0	77.71
1.2069	2	2·15·0	79.32
1.2034	3	5·11·1	79.59
1.2004	5	6·10·0,5·12·0	79.83
1.1982	4	770	80.01
1.1936	7	691,343,+	80.38
1.1844	2	582,4·10·2	81.13
1.1833	1	1·15·1	81.22
1.1725	5	800,353	82.13
1.1707	3	0·16·0,810	82.29
1.1629	1	1·13·2,780,+	82.96
1.1599	1	3·15·0	83.22
1.1559	4	183,2·15·1	83.57
1.1522	3	830	83.90
1.1488	2	662,771	84.21
1.1369	1	840,2·13·2,+	85.30

References

Malčič, S. S.(1959). Die Kristallstruktur des Natriumtrichloromercurat(II) - Dihydrats, Bull. Inst. Nucl. Sci. "Boris Kidrich" (Belgrade) [9], 115-122.

Ninković,D.V.(1957).Die Elementarzelle und die Raumgruppe von Natrium Quecksilber (II) Chlorid-Dihydrat, Bull. Inst. Nucl. Sci. "Boris Kidrich"(Belgrade).**7**, 81-82.

Sodium Nickel(II) Sulfate Tetrahydrate, $Na_2Ni(SO_4)_2 \cdot 4H_2O$ (monoclinic)

Sample source
The sample was prepared at NBS by crystallization from an aqueous solution of its components at room temperature.

Major impurities
0.001-0.01% each: Al,Ca,Co,Fe,K,Si,and Sr

0.01 -0.1 % each: Mg

Color
Very light green.

Optical data
Biaxial(-) N_α=1.518, N_β=1.520, N_γ=1.522, 2V is large.

Structure
Isostructural with $Na_2Mg(SO_4)_2 \cdot 4H_2O$ (bloedite) [Giglio,1958].

Space group
C_{2h}^5-$P2_1/a$ (14), Z=2 [ibid].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25°C	11.045 ±.001	8.193 ±.001	5.535 ±.001	100°29.9′ ±0.5′

Density
(calculated) 2.487 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.5

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

d (Å)	I	hkl	2θ(°)
6.53	9	110	13.54
5.430	9	001,200	16.31
4.523	62	011,210	19.61
4.433	13	$\bar{1}11$	20.01
4.249	25	$\bar{2}01$	20.89
4.099	2	020	21.66
3.976	14	111	22.34
3.834	3	120	23.18
3.773	13	$\bar{2}11$	23.56
3.538	3	201	25.15
3.309	27	310	26.92
3.270	100	021,220	27.25
3.243	55	211	27.48
3.236		$\bar{1}21$	27.54
3.066	7	$\bar{3}11$	29.10
3.043	2	121	29.32
2.951	13	$\bar{2}21$	30.26
2.713	17	400,320	32.99
2.677	20	221	33.45
2.647	13	130	33.84
2.628	31	$\bar{4}01$	34.08
2.582	17	012	34.71
2.506	2	$\bar{2}12$	35.80
2.441	3	031,230	36.78
2.420	7	112	37.12
2.342	3	131	38.41
2.306	7	321	39.03
2.298	1	$\bar{3}12,\bar{2}31$	39.16
2.290	13	$\bar{1}22$	39.31
2.271	21	202,401	39.65
2.266		022	39.75
2.214	1	$\bar{2}22$	40.71
2.190	2	212	41.18
2.180	4	330	41.38
2.161	13	231	41.76
2.155		122	41.88
2.124	9	$\bar{4}02$	42.53
2.099	10	510	43.05
2.087	4	$\bar{5}11$	43.31
2.068	2	$\bar{3}22$	43.73
2.049	4	040	44.16
2.012	17	140	45.01
1.987	6	222	45.61
1.950	17	331,312	46.52
1.927	16	032,430	47.13

d (Å)	*I*	*hkl*	2θ(°)
1.908	7	$\bar{1}41,\bar{5}21$	47.61
1.893	<1	$\bar{4}31$	48.02
1.887	4	$\bar{4}22$	48.18
1.867	2	141	48.74
1.857	9	132	49.02
1.852	9	511	49.15
1.846	7	$\bar{2}41$	49.33
1.824	1	$\bar{5}12,\bar{2}03$	49.96
1.819	3	$\bar{6}01$	50.10
1.813	4	003	50.27
1.803	9	322	50.58
1.777	13	$\bar{6}11$	51.38
1.772		241,013	51.52
1.768	4	402,610	51.64
1.747	3	232,431	52.33
1.741	1	$\bar{3}41$	52.51
1.725	3	521	53.05
1.716	4	$\bar{3}13$	53.35
1.700	5	113,530	53.88
1.693	5	$\bar{5}31$	54.11
1.663	13	$\bar{6}21$	55.20
1.658	11	023	55.35
1.655	12	620,$\bar{4}03$	55.48
1.651		$\bar{6}02$,341	55.60
1.636	5	042,440	56.19
1.632	3	601	56.34
1.620	5	$\bar{4}13$,150,+	56.76
1.616	3	332,$\bar{2}42$,+	56.93
1.600	6	123,611	57.55
1.593	2	142	57.85
1.569	4	051,250	58.81
1.564	7	$\bar{1}51$	59.01
1.560		531	59.17
1.556	7	$\bar{3}42$	59.33
1.542	13	151,$\bar{7}11$	59.95
1.537	10	512	60.16
1.533	8	$\bar{4}23,\bar{6}22$	60.32
1.5285	7	$\bar{2}51,\bar{1}33$	60.52
1.5208	13	242,441	60.86
1.5167	6	223,$\bar{2}33$	61.04
1.5082	5	630	61.42
1.4927	8	350	62.13
1.4903	5	540,313	62.24
1.4841	9	432	62.53
1.4750	3	$\bar{4}42$	62.96
1.4662	2	133	63.38
1.4507	2	720	64.14
1.4451	3	$\bar{7}12$	64.42
1.4385	4	$\bar{5}23$	64.75
1.4336	3	342	65.00
1.4152	2	$\bar{4}33$	65.95
1.4095	3	$\bar{1}52$	66.25
1.4037	3	711,052	66.56
1.4000	3	631	66.76
1.3955	3	$\bar{6}13$,403	67.00
1.3614	1	$\bar{2}43,\bar{2}14$	68.91
1.3602	6	004,$\bar{6}41$,+	68.98
1.3568		532,640	69.18
1.3486	6	730	69.66
1.3386	3	$\bar{6}23$,442	70.26
1.3288	1	252,451	70.85
1.3246	6	333,061,+	71.11
1.3212		$\bar{1}61$,423	71.32
1.3076	2	550,161,+	72.18
1.3053		$\bar{8}21,\bar{5}51$	72.33
1.2868	2	$\bar{4}43$	73.53
1.2756	3	641	74.29

Additional patterns

1. PDF card 14-659 [Kuznetsov and Imanakunov].
2. Druzhinin et al.[1961].

References

Druzhinin, I. G., B. Imanakunov, and V. G. Kuznetsov (1961). Physicochemical properties of nickel astrakhanite, Russ. J. Inorg. Chem. **6**, 1302-1304. (Trans. from Zh. Neorg. Khim. **6**, 2576-2582).

Giglio,M. (1958). Die Kristallstruktur von $Na_2Zn(SO_4)_2 \cdot 4H_2O$(Zn-Blödit), Acta Cryst. **11**, 789-794.

Sodium Oxalate, $Na_2C_2O_4$ (monoclinic)

Sample source
NBS standard sample No. 40d. was used. Assay indicated 99.9 % sodium oxalate.

Color
Colorless.

Structure
Determined by Jeffrey and Parry, [1954].

Space group
C_{2h}^{5}-$P2_1/a$ (14), Z=2 [ibid.].

Density
(calculated) 2.339 g/cm^3 at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.1

Additional patterns
1.PDF card 14-0758 [Hanawalt et al., 1938]

References

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

Jeffrey, G.A., and G.S. Parry (1954). The crystal structure of sodium oxalate, J. Am. Chem. Soc. **76**, 5283-5286.

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

d (Å)	*I*	*hkl*	2θ(°)
5.202	24	200	17.03
4.686	6	110	18.92
3.700	5	210	24.03
3.474	7	001	25.62
2.965	9	$\bar{2}01$	30.11
2.895	34	011,310	30.86
2.825	100	$\bar{1}11$	31.64
2.759	9	111	32.42
2.625	10	020	34.13
2.600	56	400	34.47
2.485	8	211	36.12
2.330	44	$\bar{4}10$	38.60
2.276	2	$\bar{3}11$	39.57
2.176	17	311	41.46
2.139	7	$\bar{4}01$	42.22
2.097	<1	021,320	43.09
2.067	2	$\bar{1}21$	43.75
2.041	17	121	44.34
2.030	7	401	44.60
1.979	2	$\bar{4}11$	45.80
1.966	7	$\bar{2}21$	46.13
1.922	14	221	47.25
1.894	<1	411	47.99
1.849	5	$\bar{4}20$	49.25
1.820	11	$\bar{3}21$	50.07
1.768	8	321	51.65
1.737	6	002	52.66
1.728	9	$\bar{5}11$,130	52.94
1.675	4	$\bar{2}02$	54.74
1.659	23	230,$\bar{4}21$	55.31

-continued

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)	β(°)
Jeffrey and Parry [1954]--------	10.35 ±.02	5.26 ±.02	3.46 ±.02	92°54′ ±6′
NBS, sample at 25 °C----------	10.420 ±.001	5.2552 ±.0004	3.4799 ±.0003	93°6.0′ ±.5′

Sodium Oxalate, $Na_2C_2O_4$ (monoclinic) – continued

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.646	6	610	55.79
1.622	3	202	56.68
1.617	2	112	56.88
1.586	1	$\bar{6}01$	58.10
1.563	6	031,330	59.04
1.552	1	$\bar{1}31$	59.52
1.519	4	601,$\bar{6}11$	60.94
1.508	1	$\bar{2}31$	61.42
1.502	1	$\bar{5}21$	61.71
1.482	1	$\bar{4}02$	62.65
1.460	2	312	63.66
1.453	3	521,430	64.02
1.448	3	620	64.28
1.439	2	$\bar{3}31$	64.70
1.4304	4	710	65.16
1.4267	3	122,$\bar{4}12$	65.35
1.4131	3	331,$\bar{2}22$	66.06
1.4101	2	402	66.22
1.3478	1	$\bar{7}11$	69.71
1.3152	1	621	71.70
1.3034	2	140	72.45
1.2908	<1	$\bar{4}22$	73.27
1.2740	1	240	74.40
1.2624	2	810,$\bar{6}02$,+	75.20
1.2428	1	422	76.60
1.2403	1	$\bar{8}01$	76.78
1.2323	3	630	77.37
1.2291	2	041,340	77.61
1.2192	<1	132	78.36
1.2111	1	$\bar{2}32$	78.99
1.2074	1	$\bar{8}11$	79.28
1.1941	2	721	80.34
1.1905	2	241,232	80.63
1.1763	1	$\bar{3}32$,$\bar{6}31$	81.81
1.1728	<1	440	82.11
1.1657	2	612,820,+	82.72
1.1516	1	341	83.96
1.1485	2	332	84.24
1.1377	1	$\bar{6}22$	85.22
1.1334	2	$\bar{7}12$,730	85.62
1.1314	2	$\bar{4}32$,013,+	85.81
1.1195	1	$\bar{4}41$	86.95

Sodium Zinc Sulfate Tetrahydrate, $Na_2Zn(SO_4)_2 \cdot 4H_2O$ (monoclinic)

Sample source
The sample was prepared at NBS by crystallization from a solution of its components at room temperature.

Major impurities
0.001-0.01% each: Fe,Mg,Ni,and Si.

0.01 -0.1 % each: Al and Ca.

Color
Colorless

Optical data
Biaxial (-)N_α=1.507, N_β=1.512, N_γ=1.516, 2V is large. Tabularly shaped crystals.

Structure
Isostructural with $Na_2Mg(SO_4)_2 \cdot 4H_2O$ (bloedite) [Giglio, 1958].

Space group
C_{2h}^5-$P2_1/a$ (14), Z=2 [ibid.]

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Giglio [1958]	11.05 ±0.02	8.23 ±0.02	5.54 ±0.01	100°35′ ±05′
NBS, sample at 25°C	11.080 ±0.001	8.256 ±0.001	5.534 ±0.001	100°11.7′ ±0.6′

Density
(calculated) 2.503 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.4

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

d (Å)	I	hkl	2θ(°)
6.57	16	110	13.46
5.450	20	200,001	16.25
4.546	66	210,011	19.51
4.436	18	$\bar{1}11$	20.00
4.247	36	$\bar{2}01$	20.90
4.128	1	020	21.51
3.994	18	111	22.24
3.857	2	120	23.04
3.779	13	$\bar{2}11$	23.52
3.553	3	201	25.04
3.327	38	310	26.77
3.289	100	220,021	27.09
3.263 }	48	{ 211	27.31
3.248 }		{ $\bar{1}21$	27.44
3.069	8	$\bar{3}11$	29.07
2.961	7	$\bar{2}21$	30.16
2.728	10	320,400	32.80
2.691	15	221	33.26
2.669	10	130	33.55
2.631	24	$\bar{4}01,\bar{2}02$	34.04
2.584	10	410,012	34.68
2.509	1	$\bar{3}21,\bar{4}11$	35.76
2.456	2	230,031	36.55
2.426	4	112	37.02
2.357	3	131	38.15
2.319	3	321	38.80
2.311	4	$\bar{2}31$	38.94
2.294	10	$\bar{1}22$	39.23
2.279	12	401,202	39.50
2.273	12	420,022	39.62
2.216	1	$\bar{4}21,\bar{2}22$	40.67
2.176	5	231	41.47
2.163	4	122	41.72
2.123	7	$\bar{4}02$	42.54
2.114	8	$\bar{3}31$	42.74
2.109	7	510	42.85
2.092	3	$\bar{5}11$	43.21
2.065	3	040	43.81
2.029	6	140	44.62
1.996	3	421,222	45.39
1.963	9	331	46.21
1.958	3	312	46.33
1.935	6	032	46.91
1.930	5	240,041	47.04
1.914	4	$\bar{5}21$	47.46

Internal standard W, a = 3.16504 Å CuKα_1 λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.902	1	$\bar{4}31,\bar{2}32$	47.78
1.889	3	$\bar{4}22$	48.13
1.866	7	132	48.77
1.862	5	511	48.87
1.856	5	$\bar{2}41$	49.03
1.824	3	$\bar{6}01$	49.97
1.818	2	600	50.13
1.811	3	322	50.33
1.805	4	$\bar{3}32$	50.52
1.800	4	$\bar{1}13$	50.67
1.784	5	241	51.17
1.779	7	$\bar{2}13$	51.32
1.756	<1	431,232	52.05
1.734	1	521	52.75
1.714	3	$\bar{3}13$	53.40
1.710	3	530	53.56
1.704	2	$\bar{5}22,113$	53.74
1.700	2	$\bar{5}31$	53.90
1.668	7	$\bar{6}21$	55.01
1.663	6	620,341+	55.18
1.652	4	$\bar{6}02,\bar{1}42+$	55.58
1.639	2	601	56.06
1.632	3	150,422	56.32
1.623	3	$\bar{4}41,\bar{2}42$	56.67
1.608	3	611	57.26
1.576	2	$\bar{1}51$	58.53
1.570	3	531	58.78
1.552	4	151	59.50

References

Giglio,M. (1958). Die Kristallstruktur von $Na_2Zn(SO_4)_2 \cdot 4H_2O$(Zn-Blödit), Acta Cryst. **11**, 789-794.

Sodium Zinc Trifluoride, $NaZnF_3$ (orthorhombic)

Sample source
The sample was prepared at NBS by adding a solution of $ZnCl_2$ to a concentrated solution of NaF. The precipitate was washed and annealed at 500 °C.

Major impurities
0.001-0.01% each: Al, Mg, Mn, Mo, Si, Sr

0.01 -0.1 % each: Ba, Ca, and Fe.

Color
Colorless.

Optical data
Almost isotropic, N≅1.440.

Structure
Orthorhombic, distorted perovskite [Rüdorff et al., 1959] Isostructural with $CaZnO_3$ and $NaMnF_3$.

Space group
D_{2h}^{16}-Pnma (62)Z=4. [Rüdorff et al.,1959].

Lattice constants

	a(Å)	b(Å)	c(Å)
Rüdorff et al. (1959)---------	5.569	7.756	5.40
Tutov et al. (1966)---------	5.56	7.74	5.40
NBS, sample at 25°C--------	5.5873 ±.0003	7.775 ±.001	5.4150 ±.0002

Density
(calculated) 4.104 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 3.0.

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

d (Å)	I	hkl	2θ(°)
3.885	100	101,020	22.87
3.477	2	111	25.60
2.793	23	200	32.02
2.748	80	121	32.55
2.707	16	002	33.06
2.483	1	201	36.14
2.437	6	102	36.85
2.366	4	211	38.00
2.338	10	031	38.47
2.326	6	112	38.67
2.223	1	022	40.54
2.157	3	131	41.84
2.094	2	221	43.16
2.066	1	122	43.78
1.944	50	202,040	46.69
1.900	1	230	47.83
1.887	1	212	48.19
1.793	1	231	50.88
1.762	10	301	51.85
1.739	24	222,141	52.57
1.718	6	311,103	53.27
1.677	<1	113	54.67
1.604	14	321	57.38
1.596	12	240	57.70
1.571	22	123	58.72
1.517	1	203	61.04
1.494	<1	051	62.05
1.457	1	331	63.83
1.431	1	133	65.13
1.428	1	322	65.29
1.3966	2	400	66.94
1.3744	8	410,242	68.17
1.3534	2	004	69.38
1.3144	2	420	71.75
1.3049	4	341	72.35
1.2784	2	313,024	74.10
1.2414	1	402	76.70
1.2294	5	323,430,+	77.59
1.2182	2	204	78.44
1.1825	1	422	81.29
1.1755	<1	260	81.88
1.1691	<1	062	82.42
1.1661	<1	351	82.68
1.1627	1	224	82.98
1.1530	<1	153	83.83

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
1.1342	1	440	85.55
1.1198	<1	432	86.92
1.1107	1	044	87.81
1.0945	1	501	89.46
1.0839	1	511	90.57
1.0784	1	343,262	91.16
1.0627	1	423	92.91
1.0532	1	521,115	94.00
1.0461	2	442	94.84
1.0437	2	361	95.13
1.0347	2	163	96.22
1.0322	2	244,270	96.53
1.0256	2	125	97.36
.9720	<1	404,080	104.82
.9535	<1	541	107.76
.9500	1	503	108.33
.9429	2	424,181	109.55
.9361	1	305,064	110.74
.9228	1	523	113.16
.9176	1	601	114.15
.9162	1	363	114.42
.9144	1	082	114.77
.9102	2	325,434	115.61
.9026	1	182,006	117.15

Polymorphism

$NaZnF_3$ is reported to occur in two polymorphic forms [Schmitz-DuMont and Bornefeld, 1956] with an inversion at 683 °C. The lower form is tetragonal,but was not observed at NBS.

References

Rüdorff,W., J.Kandler,B.Lincke and D.Babel (1959). Über Doppelfluoride von Nickel und Kobalt, Angew. Chem. **71**, 672.

Schmitz-DuMont,O. and H.Bornefeld (1956). Die Systemreihe Alkalifluorid/Zinkfluorid, Z.Anorg. Allgem. Chem. **287**,120-137.

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Strontium Indium Hydroxide, $Sr_3In_2(OH)_{12}$ (cubic)

Sample source
The sample was prepared by Jun Ito.

Major impurities
NaOH was used in the preparation. Since it was not practical to wash the sample, 1-5% remained in the sample and appeared as a separate carbonate phase in the powder pattern.

Color
Yellowish white

Structure
Isostructural with other hydrogarnets [Ito and Frondel, 1967].

Space group
O_h^{10}-Ia3d (230), Z=8.
[Flint et al., 1941].

Lattice constants

	a(Å)
Ito and Frondel,[1967]----------	13.53
NBS, sample at 25 °C----------	13.5222 ±.0001

Density
(calculated) 3.742 g/cm^3 at 25° C.

Additional patterns
1.Ito and Frondel [1967].

References

Flint, E.P., H.F. McMurdie, and L.S. Wells (1941). Hydrothermal and x-ray studies of the garnet-hydrogarnet series, J.Res. Nat. 26, 13-33.

Ito,J. and C. Frondel (1967). New synthetic hydrogarnets, Am. Mineralogist 52, 1105-1109.

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

d (Å)	I	hkl	2θ(°)
5.521	65	211	16.04
4.784	85	220	18.53
3.613	39	321	24.62
3.379	65	400	26.35
3.025	51	420	29.50
2.759	100	422	32.42
2.652	8	431	33.77
2.468	40	521	36.37
2.390	7	440	37.60
2.194	36	611	41.10
2.139	18	620	42.22
1.993	8	631	45.47
1.875	18	640	48.51
1.840	15	721	49.49
1.807	74	642	50.47
1.717	10	732	53.30
1.689	13	800	54.25
1.617	4	653	56.91
1.593	9	822	57.83
1.531	2	752	60.41
1.5116	28	840	61.27
1.4754	11	842	62.94
1.4578	8	921	63.79
1.4413	23	664	64.61
1.4254	1	851	65.42
1.3946	6	932	67.05
1.3801	5	844	67.85
1.3660	1	941	68.65
1.3389	3	10·1·1	70.24
1.3262	10	10·2·0	71.01
1.3132	1	943	71.81
1.2896	8	10·3·1	73.35
1.2557	13	10·4·0	75.67
1.2453	4	10·3·3	76.42
1.2345	27	10·4·2	77.21
1.2044	8	11·2·1	79.51
1.1951	12	880	80.26
1.1683	4	11·3·2	82.49
1.1596	3	10·6·0	83.25
1.1350	1	965	85.47

Strontium Indium Hydroxide, $Sr_3In_2(OH)_{12}$ (cubic) – continued

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.1268	10	12•0•0	86.25
1.1115	3	12•2•0	87.73
1.1041	4	11•5•2	88.47
1.0966	24	12•2•2	89.24
1.0757	2	11•6•1	91.46
1.0690	2	12•4•0	92.20
1.0496	4	11•6•3	94.42
1.0431	4	10•8•2	95.19
1.0252	3	13•2•1	97.41
1.0078	6	12•6•0	99.69
0.9969	11	12•6•2	101.18
.9760	5	888	104.22
.9709	1	13•4•3	105.00
.9611	2	14•1•1	106.54
.9561	5	14•2•0	107.34
.9421	4	14•3•1	109.68
.9375	6	12•8•0	110.49
.9287	4	14•4•0	112.08
.9200	19	14•4•2	113.70
.9076	2	14•5•1	116.13
.9035	1	12•8•4	116.98
.8916	4	15•2•1	119.52
.8766	2	15•3•2	122.96
.8657	4	12•10•0	125.69
.8621	2	14•7•1	126.61
.8587	15	14•6•4	127.54
.8485	4	15•5•2	130.39
.8452	4	16•0•0	131.38
.8323	3	16•2•2	135.47
.8230	3	15•6•3	138.76
.8200	8	16•4•0	139.89
.8139	5	16•4•2	142.30
.8110	4	15•7•2	143.51
.8081	7	12•10•6	144.80
.7996	2	15•6•5	148.84
.7886	2	17•2•1	155.24
.7859	4	16•6•2	157.08

Strontium Scandium Oxide Hexahydrate, $Sr_3Sc_2O_6 \cdot 6H_2O$ (cubic)

Sample source
The sample was prepared by Jun Ito.

Major impurities
0.01 -0.1 % each: Al, Ca, Fe

0.1 -1.0 % each: Si

greater than 1%: Na*
*NaOH was used in the preparation. Since it was not practical to wash the sample, 1-5% remained in the sample and appeared as a separate carbonate phase in the powder pattern.

Color
Yellowish white

Structure
Isostructural with other hydrogarnets [Ito and Frondel, 1967].

Space group
O_h^{10}-Ia3d (230), Z=8 [Flint et al., 1941].

Lattice constants

	a(Å)
Ito and Frondel,[1967]----------	13.39
NBS, sample at 25 °C----------	13.4007 ±.0002

Density
(calculated) 3.074 g/cm³ at 25° C.

Additional patterns
1.Ito and Frondel [1967].

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

d (Å)	I	hkl	2θ(°)
5.470	100	211	16.19
4.741	4	220	18.70
3.583	80	321	24.83
3.349	51	400	26.59
2.994	100	420	29.81
2.860	3	332	31.25
2.735	41	422	32.71
2.628	11	431	34.09
2.447	72	521	36.70
2.369	2	440	37.95
2.174	65	611	41.50
2.119	1	620	42.63
2.069	3	541	43.71
1.975	5	631	45.90
1.934	10	444	46.94
1.895	3	543	47.97
1.857	31	640	49.00
1.823	23	721	49.99
1.790	39	642	50.98
1.701	11	732	53.84
1.675	11	800	54.77
1.650	3	741	55.64
1.602	2	653	57.49
1.558	2	831	59.27
1.517	3	752	61.01
1.498	7	840	61.87
1.462	7	842	63.60
1.4450	5	921	64.42
1.4285	6	664	65.26
1.4129	2	851	66.07
1.3821	5	932	67.74
1.3535	1	941	69.37
1.3267	3	10·1·1	70.98
1.3137	1	10·2·0	71.79
1.3015	3	943	72.57
1.2778	6	10·3·1	74.14
1.2442	8	10·4·0	76.50
1.2339	3	10·3·3	77.25
1.2234	5	10·4·2	78.04
1.2131	2	954	78.83
1.1941	6	11·2·1	80.34
1.1846	3	880	81.12
1.1576	4	11·3·2	83.42
1.1244	2	965	86.48
1.1167	8	12·0·0	87.22

Internal standard W, a = 3.16504 Å $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.1094	1	11·4·3	87.94
1.1015	1	12·2·0	88.74
1.0940	1	11·5·2	89.51
1.0869	5	12·2·2	90.25
1.0659	2	11·6·1	92.54
1.0401	5	11·6·3	95.56
1.0278	3	12·5·1	97.08
1.0159	2	13·2·1	98.61
1.0102	1	12·4·4	99.36
0.9988	14	12·6·0	100.92
.9934	3	13·3·2	101.67
.9879	2	12·6·2	102.47
.9824	1	13·4·1	103.27
.9672	1	888	105.57
.9524	1	14·1·1	107.95
.9337	3	14·3·1	111.17
.9292	1	12·8·0	111.98
.9204	1	14·4·0	113.63
.9118	7	14·4·2	115.29
.8994	3	14·5·1	117.84
.8837	3	15·2·1	121.30
.8686	1	15·3·2	124.93
.8579	2	12·10·0	127.75
.8510	2	14·6·4	129.68

References

Flint, E.P., H.F. McMurdie, and L.S. Wells (1941). Hydrothermal and x-ray studies of the garnet-hydrogarnet series, J.Res. Nat. 26, 13-33.

Ito,J. and C. Frondel (1967). New synthetic hydrogarnets, Am. Mineralogist 52, 1105-1109.

Ytterbium Oxide, Yb_2O_3 (cubic)

Sample source
The sample was obtained from Prof. F. H. Spedding, Iowa State College, Ames, Iowa. It was heated to 1400°C and then held at 1300°C for 48 hours.

Major impurities
0.001-0.01% each: Cu, Fe, Mg, Pb, Ti, V, and Zr

0.01 -0.1 % each: Al, Ca, Sb

Color
Colorless

Structure
Mn_2O_3 type [Pauling and Shappell 1930].

Space group
T_h^7-Ia3 (206), Z=16 [ibid.]

Lattice constants

	a(Å)
Goldschmidt et al. [1925]-------	10.41**
Bommer [1939]-------------------	10.429*
Brauer and Gradinger [1954]-----	5.219*
Templeton and Dauben [1954]-----	10.439
Staritzky [1956]----------------	10.435
NBS, sample at 25°C-------------	10.4342 ±0.0001

*from kx

**from Fe=1.934

Density
(calculated) 9.216 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 6.9

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

d (Å)	I	hkl	2θ(°)
5.20	2	200	17.02
4.25	10	211	20.87
3.010	100	222	29.65
2.788	2	321	32.08
2.608	33	400	34.35
2.460	5	411	36.50
2.333	1	420	38.56
2.225	4	332	40.51
2.130	1	422	42.40
2.047	8	431	44.21
1.9049	2	521	47.70
1.8446	34	440	49.36
1.7895	2	433	50.99
1.7390	1	600	52.58
1.6929	4	611	54.13
1.6499	1	620	55.66
1.6101	4	541	57.16
1.5734	24	622	58.62
1.5391	5	631	60.06
1.5063	5	444	61.51
1.4758	2	543	62.92
1.4471	1	640	64.32
1.4192	2	721	65.74
1.3946	1	642	67.05
1.3254	2	732	71.06
1.3045	4	800	72.38
1.2843	3	811	73.70
1.2656	2	820	74.98
1.2472	2	653	76.28
1.2296	1	822	77.57
1.2130	4	831	78.84
1.1972	5	662	80.09
1.1814	1	752	81.38
1.1665	4	840	82.65
1.1525	1	833	83.88
1.1384	1	842	85.16
1.1251	2	921	86.41
1.1123	1	664	87.65
1.0999	2	851	88.90
1.0763	2	932	91.39

d (Å)	*I*	*hkl*	2θ(°)
1.0650	4	844	92.64
1.0541	1	941	93.89
1.0436	1	10.0.0	95.13
1.0332	1	10.1.1	96.41
1.0232	2	10.2.0	97.66
1.0136	1	943	98.91
1.0042	2	10.2.2	100.18
0.9949	1	10.3.1	101.47
.9774	1	871	104.01
.9688	2	10.4.0	105.32
.9606	1	10.3.3	106.62
.9526	1	10.4.2	107.91
.9447	1	954	109.24
.9297	1	11.2.1	111.89
.9223	1	880	113.27
.9082	1	10.4.4	116.02
.9014	1	11.3.2	117.41
.8948	1	10.6.0	118.82
.8882	1	11.4.1	120.27
.8819	2	10.6.2	121.71
.8757	<1	965	123.18
.8695	1	12.0.0	124.71
.8635	1	12.1.1	126.23
.8577	1	12.2.0	127.80
.8520	1	11.5.2	129.40
.8463	2	12.2.2	131.06
.8408	1	12.3.1	132.72
.8301	1	11.6.1	136.23
.8249	1	12.4.0	138.07
.8198	1	12.3.3	139.95
.8148	2	12.4.2	141.93
.8098	1	11.6.3	144.02
.8050	1	10.8.2	146.21
.8002	1	12.5.1	148.54
.7995	<1	10.6.6	151.03
.7910	1	13.2.1	153.70
.7865	1	12.4.4	156.66
.7820	1	12.5.3	160.08

Additional patterns

1. PDF card 6-0371. [Div. Applied Physics Polytechnic Inst. of Brooklyn,N.Y.1955], Fert [1962].
2. Staritzky [1956].

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

Aluminum Nickel, AlNi (cubic)

Structure

Becker and Ebert [1923]. Isostructural with CsI and CsCl. Atoms are in special positions:

Al: 0 0 0
Ni: ½ ½ ½

Space group

O_h^1-Pm3m (221). Z=1 [ibid.].

Lattice constants

	a(Å)
Becker and Ebert (1923)--------	2.83
Bradley and Taylor (1937)------	2.887*
Guseva (1951)-----------------	2.886*

*from kX

The constant used was a=2.887

Density

(calculated) 5.913 g/cm³ at 25° C.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
2.89	27	100	30.95
2.04	100	110	44.33
1.667	5	111	55.04
1.444	13	200	64.50
1.291	5	210	73.25
1.179	22	211	81.61
1.021	7	220	97.98
0.962	2	300	106.3
.913	10	310	115.1
.870	1	311	124.5
.833	3	222	135.1
.801	2	320	148.3

Additional patterns

1.PDF 2-1261 (Bradley and Taylor, 1937).

References

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Guseva, L. N. (1951). On the nature of the β-phase in the nickel-aluminum system, Akad. Nauk SSSR, Doklady 77 , 415-418.

Gold Magnesium, AuMg (cubic)

Structure

Brauer and Haucke (1936). Isostructural with CsCl; atoms in special positions:

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

Space group

O_h^1-Pm3m (221). Z=1. (ibid.).

Lattice constants

	a(Å)
Brauer and Haucke (1936)--------	3.266*

*from kX, for the composition at 48.7 atomic percent Mg.

Density

10.55 g/cm^3, calculated using the lattice constant a_0 = 3.266 Å, and 50-50 atomic percents.

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.27	82	100	27.28
2.31	100	110	38.97
1.886	20	111	48.22
1.633	15	200	56.29
1.461	24	210	63.65
1.333	28	211	70.58
1.155	9	220	83.68
1.089	11	300	90.07
1.033	12	310	96.45
0.985	7	311	102.9
.943	4	222	109.6
.906	7	320	116.5
.873	20	321	123.9
.816	3	400	141.2
.792	15	410	153.0

Additional patterns

1. PDF card 4-0796[Brauer and Haucke, 1936].

References

Brauer, G. and W. Haucke (1936). Kristallstruktur der intermetallischen Phasen MgAu und MgHg, Z.Physik. Chem. B33, 304-310.

Structure

Brauer and Haucke (1936). Isostructural with CsCl; atoms in special positions:

Hg: 0 0 0
Mg: ½ ½ ½

Space group

O_h^1-Pm3m (221). Z=1. (ibid.).

Lattice constants

	a(Å)
Brauer and Haucke (1936)-------	3.449*

*from kX, for the composition at 50.8 atomic percent Mg.

Density

9.102 g/cm³, calculated using the lattice constant a_0 = 3.449 Å, and 50-50 atomic percents.

Additional patterns

1. PDF card 4-0775[Brauer and Haucke, 1936].

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.45	80	100	25.81
2.44	100	110	36.82
1.991	20	111	45.51
1.724	15	200	53.06
1.542	25	210	59.92
1.408	28	211	66.33
1.219	8	220	78.35
1.150	11	300	84.13
1.091	11	310	89.86
1.040	6	311	95.58
0.996	3	222	101.4
.957	6	320	107.3
.922	16	321	113.4
.862	2	400	126.6
.837	10	410	134.1
.813	11	411	142.7
.791	6	331	153.5

References

Brauer, G. and W. Haucke (1936). Kristallstruktur der intermetallischen Phasen MgAu und MgHg, Z.Physik. Chem. B33, 304-310.

Osmium Titanium, OsTi (cubic)

Structure

Laves and Wallbaum [1939]. Isostructural with CsCl; atoms in special positions:

Os: 0 0 0
Ti: ½ ½ ½

Space group

O_h^1-Pm3m (221). Z=1. (ibid.).

Lattice constants

	a(Å)
Jordan (1955)----------	3.07
Dwight (1959)----------	3.07

Density

(calculated) 13.66 g/cm^3

Additional patterns

1. PDF 18-944 [Dwight, private comm.]

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.07	50	100	29.1
2.17	100	110	41.6
1.77	12	111	51.5
1.54	14	200	60.2
1.37	14	210	68.2
1.25	26	211	75.8
1.09	8	220	90.4
1.02	7	300	97.6
0.971	12	310	105.0
.926	5	311	112.6
.886	4	222	120.7
.851	4	320	129.5
.820	21	321	139.7

References

Dwight, A. E. (1959). CsCl-type equiatomic phases in binary alloys of transition elements, Trans. AIME **215**, 283-286.

Jordan, C. B. (1955). Crystal structure of TiRu and TiOs, J. Metals **7**, 832-833.

Laves, F. and H. J. Wallbaum (1939). Zur Kristallchemie von Titan- Legierungen, Naturwissenschaften **27**, 674-675.

Ruthenium Titanium, RuTi (cubic)

Structure

Laves and Wallbaum (1939). Isostructural with CsCl; atoms in special positions:

Ru: 0 0 0
Ti: ½ ½ ½

Space group

O_h^1-Pm3m (221). Z=1. (ibid.).

Lattice constants

	a(Å)
Jordan (1955)----------	3.06
Dwight (1959)----------	3.070

The constant used was a_0=3.06 Å.

Density

8.63 g/cm³ (calculated from a_0=3.06 Å).

Additional patterns

1. PDF 18-1144 [Dwight, private comm.]

Calculated Pattern
$CuK\alpha_1$ λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.06	19	100	29.2
2.16	100	110	41.7
1.77	4	111	51.7
1.53	14	200	60.4
1.37	5	210	68.5
1.25	24	211	76.1
1.08	7	220	90.8
1.02	2	300	98.1
0.968	11	310	105.5
.923	2	311	113.2
.883	3	222	121.4
.849	2	320	130.3
.818	20	321	140.7

References

Dwight, A. E. (1959). CsCl-type equiatomic phases in binary alloys of transition elements, Trans. AIME **215**, 283-286.

Jordan, C. B. (1955). Crystal structure of TiRu and TiOs, J. Metals **7**, 832-833.

Laves, F. and H. J. Wallbaum (1939). Zur Kristallchemie von Titan- Legierungen, Naturwissenschaften **27**, 674-675.

Structure

Dwight [1959]. Isostructural with CsCl; atoms in special positions:

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

Space group

O_h^1-Pm3m (221) Z=1. (ibid.).

Lattice constants

	a(Å)
Dwight (1959)----------	3.66
Iandelli (1960)----------	3.653
Baenziger and Moriarty (1961)---	3.6476
Gschneidner (1965)----------	3.6491

The constant used was a_0 = 3.6483 Å, the average of the last two values.

Density

9.065 g/cm³ (calculated from a_0 =3.6483Å.)

Calculated Pattern
CuKα_1 λ = 1.5405 Å

d(Å)	I(Peak height)	hkl	2θ(°)
3.648	3	100	24.38
2.580	100	110	34.74
2.106	<1	111	42.90
1.824	15	200	49.95
1.632	1	210	56.34
1.489	28	211	62.28
1.290	8	220	73.33
1.216	<1	300	78.60
1.154	11	310	83.77
1.100	<1	311	88.89
1.053	3	222	94.00
1.012	<1	320	99.14
0.9750	13	321	104.36
.9121	2	400	115.24
.8848	<1	410	121.03
.8599	9	411	127.20
.8370	<1	331	133.93
.8158	6	420	141.53
.7961	<1	421	150.70

References

Baenziger,N.J. and J.L.Moriarty,Jr.(1961). Gadolinium and dysprosium intermetallic phases. II.Laves phases and other structure types, Acta Cryst. **14** 948-950.

Dwight, A. E. (1959). CsCl-type equiatomic phases in binary alloys of transition elements, Trans. AIME **215**, 283-286.

Gschneidner,K.A. Jr.(1965). Crystal Structures of some equiatomic gadolinium compounds, Acta Cryst. **18**, 1082-1083.

Iandelli, A.(1960). Su alcuni composti intermetallici e semimetallici del Gadolinio, Atti Accad. Nazl. Lincei Rend. Classe Sci. Fis. Mat. Nat. **29**, 62-69.

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

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

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CUMULATIVE INDEX—Continued

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CUMULATIVE INDEX—Continued

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CUMULATIVE INDEX—Continued

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CUMULATIVE INDEX—Continued

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A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

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A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE MINERAL INDEX

* Natural mineral.

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