



NATIONAL INSTITUTE OF STANDARDS & TECHNOLOGY Research Information Center Gaithersburg, MD 20899



25, Se . 8

UNITED STATES DEPARTMENT OF COMMERCE • Maurice H. Stans, Secretary NATIONAL BUREAU OF STANDARDS • Lewis M. Branscomb, Director

Standard X-ray Diffraction Powder Patterns

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

> Institute for Materials Research National Bureau of Standards Washington, D.C. 20234



رج ، National Bureau of Standards, Monograph 25—Section 8 Nat. Bur. Stand. (U.S.), Monogr. 25—Section 8, 171 pages (Sept. 1970) CODEN: NBSMA

Issued September 1970

NATIONAL BUREAU OF STANDARDS FEB 1 2 1971

and see

201 2

Library of Congress Catalog Card Number: 53-61386

Contents

	Page
Introduction	1
Experimental patterns:	
Ammonium Cadmium Suitate Hydrate, (NH) $Cd(SO)$.6H O	5
A mmonium Calcium Sulfate	J
(NH.), Ca. (SO.)	7
Ammonium Cobalt Fluoride, $NH_1 CoF_3$	9
Ammonium Magnesium Chromium Oxide	
Hydrate, $(NH_4)_2 Mg(CrO_4)_2.6H_2O$	10
Ammonium Manganese Sulfate Hydrate,	
$(NH_{4})_{2} Mn (SO_{4})_{2} \cdot 6H_{2}O$	12
Ammonium Mercury Chloride, NH ₁ HgCl ₃	
(revised)	14
Ammonium Nickel Chromium Oxide	
Hydrate, $(NH_4)_2 Ni(CrO_4)_2 \cdot 6H_2 O$	16
Ammonium Zinc Fluoride, NH, ZnF ₃	18
Barium Bromate Hydrate,	10
$Ba(BrO_3)_2 \cdot H_2 O \dots$	19
Barium Chlorate Hydrate,	91
Gadmium Imidagolo Nitrato	41
Cd(C H N) (NO)	23
Cesium Calcium Eluoride CsCaF.	25
Cesium Lead Fluroide, CsPbF	26
Cesium Magnesium Chromium Oxide.	
$\operatorname{Cs} \operatorname{Mg} (\operatorname{CrO}_{4})_{3}$	27
Cesium Magnesium Chromium Oxide	
Hydrate, $Cs_2Mg(CrO_4)_2$ ·6H ₂ O	29
Copper Pyrazole Chloride,	
$Cu(C_3H_4N_2)_4Cl_2$	31
Gadolinium Titanium Oxide, Gd ₂ TiO ₅	32
Gallium Phosphate Hydrate,	
$GaPO_4 \cdot 2H_2O$	34
Gold Potassium Cyanide, AuK $(CN)_2$	36
For Sulfate Hydrate (melanterite),	20
Lanthanum Nitrata Hydrata	30
$L_{a}(NO_{a})$, •6H _a O	40
Lithium Carbonate LicCO	42
Manganese Chloride (scacchite). MnCl	43
Nickel Pyrazole Chloride,	
$Ni(C_3H_4N_2)_4Cl_2$	44
Potassium Bromide Chloride,	
$KBr_{0.5}$ $Cl_{0.5}$	46
Potassium Cadmium Fluoride, KCdF	47
Potassium Calcium Carbonate (fair-	
childite), $K_2 Ca(CO_3)_2$	48
Potassium Calcium Fluoride, KCaF,	49
Potassium Magnesium Chloride Hydrate	50
Deta gium Magnagium Chromium Ovida	50
K Mg (CrO)	52
Potassium Magnesium Sulfate Hydrate	04
(picromerite). $K_2 Mg(SO_4)_2 \cdot 6H_2 O_2$	54
Potassium Vanadium Oxide, KV O	56
Rubidium Calcium Fluoride, RbCaF,	57
Rubidium Cobalt Fluoride, RbCoF	58
Rubidium Cobalt Sulfate, $Rb_2 Co_2 (SO_4)_3 \dots$	59
Rubidium Copper Sulfate Hydrate,	
$\operatorname{Rb}_{2}\operatorname{Cu}(\operatorname{SO}_{4})_{2}$ · 6H $_{2}\operatorname{O}_{4}$	61
Rubidium Fluoride, RbF	63
Rubidium Iron Sulfate Hydrate,	
$\operatorname{Rb}_{2}\operatorname{Fe}(\operatorname{SO}_{4})_{2}$ $^{\circ}\operatorname{6H}_{2}\operatorname{O}_{4}$	64
Rb My (CrO)	66
	00

	Page
Rubidium Magnesium Chromium Oxide	
Hydrate, $Rb_2Mg(CrO_4)_2\cdot 6H_2O$	68
Rubidium Magnesium Sulfate Hydrate,	50
$\operatorname{Rb}_2\operatorname{Mg}(\operatorname{SO}_4)_2 \cdot \operatorname{6H}_2\operatorname{O}_2\operatorname{O}_2$	70
Rubidium Nickel Sullate, $RD_2 NI_2 (SO_1)_3$	(2
Rubidium Nickel Sullate Hydrate,	74
$RD_2NI(SO_4)_2 \circ OR_2O$	14
Rubiaium Potassium Chioride,	76
Samarium Tin Oxide Sm Sn O	77
Silver Potassium Cyanide $A\sigma K(CN)$	78
Silver Sodium Chloride, Ago, Na Cl	79
Strontium Tin Oxide. SrSnO	80
Thallium Azide, TlN	82
Thallium Cadmium Sulfate, $Tl_2 Cd_2 (SO_4)_3$.	83
Thallium Cobalt Sulfate, $Tl_2 Co_2 (SO_4)_3 \dots$	85
Thallium Iron Sulfate Hydrate,	
$Tl_2 Fe(SO_4)_2 \cdot 6H_2O$	87
Thallium Magnesium Chromium Oxide,	
$\mathrm{Tl}_{2}\mathrm{Mg}_{2}(\mathrm{CrO}_{4})_{3}$	89
Calculated patterns:	
4-Acetyl-2' -fluorobiphenyl, C ₁₁ H ₁₁ OF	91
ℓ -Alanine, $C_3 H_7 O_2 N_{1}$	93
Ammonium Acetate, NH ₁ ·CH ₃ CO ₂	95
Ammonium Yttrium Oxalate Hydrate,	07
$\operatorname{NH}_4 \mathfrak{l} (\mathbb{C}_2 \mathbb{O}_4)_2 \operatorname{H}_2 \mathbb{O}_{\operatorname{conv}}$	91
$C_{\rm NOH}$	102
Hydrogen Jodate HI O	104
Hydroquinone gamma, C. H. O.	107
Lead Uranium Oxide. Pb. UO	109
Lithium Aluminum Fluoride, alpha,	
Li, AlF	111
Lithium Azide, LiN,	113
Lithium Borate, Li, B, O.	114
Magnesium Selenite Hydrate,	
$MgSeO_3 \cdot 6H_2O$	116
Mercury Sulfide Chloride, alpha,	
$Hg_3 S_2 Cl_2$	118
Potassium Niobium Fluoride, K ₂ NbF	120
Reservine, $C_{33} H_{10} N_2 O_9$	123
Silver Arsenic Suilide, xanthoconite,	126
Ag ₃ ASS ₃	120
Sodium Azide, alpha, Na N_3 , at = 50 to	129
Sodium Azide beta NaN	130
Sodium Calcium Aluminum Fluoride	
Hydrate, thomsenolite, NaCaAlF ₆ ·H ₂ O.	132
Sodium Calcium Bervllium Aluminum	
Fluorosilicate, meliphanite,	
$(Na_{0.63} Ca_{1.37}) Be(A1_{0.13} Si_{0.67})$	
$(O_{6,25} \mathbf{F}_{0,75})$	135
Sodium Calcium Beryllium Fluorosilicate.	
leucophanite, NaCaBeFSi ₂ O ₆	138
Sodium Silicate, alpha (III), Na Si O ₅	141
Sodium Zirconium Fluoride, Na-Zr ₆ F ₃₁	144
Strontium Azide, $Sr(N_3)_2$	140
2.4.6 Tripitronhonotolo	149
2,4,0-1 rinitrophenetole,	159
Unic Acid $C_{2}H_{2}(NO_{2})_{3}$	154
Cumulative index to Circular 539	101
Volumes 1 through 10 and Monograph 25	
Sections 1 through 8	157
Cumulative mineral index	166

Circular 539

Vol. 2 pg. 37 In the next to last column, the first value of I (at d = 4.67) should be 44.

Monograph 25

Section 3, pg. 23: the space group symbol should be C_{ch}^2 -P6 $_{\pi}/m$ (No. 176)

Section 6, pg. 32; the formula in the page heading should be $K_2 Co_2 (SO_4)_3$

Section 7, { pg. iii In both places, the formula for Azobenzene should be $C_{12} H_{10} N_2$

Section 7, pg. 78 The volume # for the Tutton (1925) reference should be 108.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Information on 13 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 Monograph 25, Section 1, Standard X-ray Diffraction Powder Patterns (Data for 46 substances) 40 cents.
- NBS Monograph 25, Section 2, Standard X-ray Diffraction Powder Patterns (Data for 37 substances) 35 cents.
- NBS Monograph 25, Section 3, Standard X-ray Diffraction Powder Patterns (Data for 51 substances) 40 cents.

NBS Circular 539, Volume 1, Standard X-ray Diffraction Powder Patterns (Data for 54 substances). NBS Circular 539, Volume 2, Standard X-ray Diffraction Powder Patterns (Data for 30 substances). NBS Circular 539, Volume 3, Standard X-ray Diffraction Powder Patterns (Data for 34 substances). NBS Circular 539, Volume 4, Standard X-ray Diffraction Powder Patterns (Data for 42 substances). 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 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). NBS Circular 539, Volume 9, Standard X-ray Diffraction Powder Patterns (Data for 43 substances).

The following four volumes in this series are available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C., 20402, as follows:

- 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.
- NBS Monograph 25, Section 6, Standard X-ray Diffraction Powder Patterns (Data for 60 substances) 60 cents.
- NBS Monograph 25, Section 7, Standard X-ray Diffraction Powder Patterns (Data for 81 substances) \$1.50.

(Order by SD Catalog No. C 13.44:25/Sec .--)

Send orders with remittance for the above four Monographs to Superintendent of Documents, U.S. Government Printing Office, Washington, D.C., 20402. Remittance from foreign countries should include an additional one-fourth of the purchase price for postage.

Those wishing to be notified of future issues should send mailing address to the Government Printing Office.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 8.-Data for 81 substances

Howard E. Swanson, Howard F. McMurdie, ¹ Marlene C. Morris,² and Eloise H. Evans²

Standard x-ray diffraction patterns are presented for 81 substances. Fifty-three of these patterns represent experimental data and 28 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer, using samples of high purity. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray power diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities were reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File is a compilation of diffraction patterns, gathered from many sources, produced, and published by the Joint Committee on Powder Diffraction Standards.³ The File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, our 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 information for 81 compounds (53 experimental and 28 calculated patterns), and is the eighteenth of the series of "Standard X-ray Diffraction Powder Patterns."

EXPERIMENTAL POWDER PATTERNS

Sample. 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. Appropriate annealing, recrystallizing, or heating in hydrothermal bombs improved the definition of most of the patterns. A check of phase purity was usually provided by indexing the x-ray pattern itself.

¹See previous page for listing of other published volumes.

<u>Optical data, color</u>. A microscopic inspection for phase purity was also made on the non-opaque 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].⁵

Structure, lattice constants. The space groups are listed with short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography Vol. I [1952].

Orthorhombic cell dimensions are presented according to the Dana convention $b \ge a \ge c$ [Palache et al., 1944].

A computer program [Evans et al., 1963] assigned *hkl*'s and refined the lattice constants. Cell refinement was based only upon 2θ values which could be indexed without ambiguity. The number of significant figures reported for d-values varies with the symmetry and crystallinity of each sample. Unit cell constants and their standard errors are based on least squares refinement of the variancecovariance matrix derived from the unweighted $\Delta\theta$ residuals.

Previously published unit cell data in kX units were converted to angstrom units using the factor 1.00206 reported by Bearden [1964]. Some literature references do not specify the wavelength with the unit cell; such lattice constants were reported here as originally published.

Densities. These were calculated from the NBS lattice constants, the Avogadro number

^{1, 2} Consultant and Research Associates, respectively, at the National Bureau of Standards, sponsored by the Joint Committee on Powder Diffraction Standards.

³Joint Committee on Powder Diffraction Standards, 1845 Walnut St., Philadelphia, Pa., 19103. This Pennsylvania nonprofit corporation functions in cooperation with the American Society for Testing and Materials, the American Crystallographic Association, The Institute of Physics, and the National Association of Corrosion Engineers.

⁵ Dates in brackets indicate the literature references at the end of each section of this paper.

(6.02252 x 10 23), and atomic weights based on carbon 12 [International Union, 1961].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with approximately 5 wt. percent tungsten powder that served as an internal standard. When tungsten lines were found to interfere, 25 wt. percent silver was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid aberrations at the very top of the peak, the reading of 2θ was taken at a position about 20 percent of the way down from the top, and in the center of the peak width. The internal standard correction appropriate to each region was then applied to the measured value of 2θ . We have reported all data as a_1 peaks because the internal standard corrections for all regions were established in terms of the Ka_1 wavelength. The lattice constants used for the internal standards were 3.16516Å for tungsten, 4.08641Å for silver, and 4.69576Å for cadmium oxide, all at 25 ^oC. The following angles for high-purity tungsten, silver, and cadmium oxide were computed using cell dimensions without index of refraction corrections.

Calculated 2θ Angles

CuKa ₁ = 1.54056 Å						
hkl	W a = 3.16516 Å	Ag a = 4.08641 Å	CdO a = 4.69576 Å			
110 111 200 211 220 310 311 222 321 400 331 420 422 511 440 531 600	40.262 58.251 73.184 86.996 100.632 114.923 131.171 153.535	38.112 44.295 64.437 77.390 81.533 97.875 110.499 114.914 134.871 156.737	33.013 38.304 55.287 65.920 69.255 82.014 91.290 94.378 106.954 116.939 136.230 152.077 159.618			

All of our patterns were made at 25 $^{\rm O}$ C on a diffractometer. This was equipped with a monochromator having a curved lithium fluoride crystal located between the sample and the Geiger counter. Copper radiation was used and the wavelength K_{a₁} was assumed to be 1.54056 A [Bearden, 1964).

<u>Intensity</u> measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than

10 μ^{m} , as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see fig. 1), and the powdered sample was 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 could be exposed to the x-ray beam (as shown in fig. 2). If the sample powder did not flow readily, or was 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. At least three patterns for intensity measurements were prepared for each sample to check reproducibility.

Reference intensity. For reference intensity measurements, αAl_2O_3 (corundum) was chosen as an internal standard to be mixed 1:1 by weight with the sample. This mixture was mounted in our regular intensity sample holder (see figs. 1 and 2). Only the portion of the x-ray pattern that included the strongest line of each component was run; for the standard, the hexagonal (113) reflection with d=2.085 Å was used. The direct ratio of the heights of the two lines was then reported as $I/I_{corundum}$. In a few instances, the strongest line of one of the materials coincided with a line of the other. In that case, the second strongest line was measured, and on the basis of previous knowledge of the relative peak heights, the value for the strongest line was calculated.

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, and were computed with a FORTRAN program developed by Smith [1967], and modified here.

Lattice parameters. Before the computations of the patterns, corrections were made as necessary in the published parameters to make them consistent with the Bearden [1964] value of the copper wavelength; specifically, the published parameter in Å was multiplied by 1.00004. Both the altered parameter and the original published value are given.

<u>Scattering factors</u>. Whenever possible, the same scattering factors were used which the author of

the reference article specified. Otherwise, the factors were used directly from the International Tables for X-ray Crystallography Vol. III [1962] on pages 202 (Table #3.3.1A), 210 (#3.3.1B), 213 (#3.3.2A), and 214 (#3.3.2B). Corrections were made for dispersion if the authors had done so.

Thermal parameters. The Smith computer program uses thermal parameter data of two forms, the isotropic B's and anisotropic β 's. The isotropic parameters are easier to use and were used directly, if given by the structure reference. Initially, in a few of our patterns, anisotropic parameters were also used directly as given by the structure reference. In later work, in place of using given anisotropic parameters, we used approximately equivalent isotropic parameters, calculated from the equation:

$$\mathbf{B} = [\boldsymbol{\beta}_{11} \boldsymbol{\beta}_{22} \boldsymbol{\beta}_{23}]^{1_3}$$

Integrated intensities. Intensity calculations were based on the copper K_{r_1} wavelength, 1.54056 A, determined by Bearden [1964]. The integrated intensities were computed from the formula:

$$I = F = (Lp) (FAC)$$

where F is the standard structure factor

FAC is the powder multiplicity

and
$$Lp = \frac{1 \cdot 2\cos^2 2\theta}{\sin^2 \theta \cos \theta}$$

The intensities were scaled to the strongest line as 100. Reflections which had intensities of 0.7 or less were not reported.



<u>Scale factors</u>. For each compound, this factor when multiplied by the integrated intensities will reproduce the unscaled intensities which had been derived from the structure factors for a unit cell. The scale factors are not usable for comparisons between compounds since they have not been standardized for the effects of volume and absorption.

Peak intensities. In the Smith program, the integrated intensities can be transformed to a Cauchy profile with an appropriate half-width designated to simulate a diffractometer tracing. The value of the half-width used here was 0.075° at 40° (2 θ). The program then summed the intensities from the overlapping peak profiles, and scaled the resulting peak intensities to the strongest peak height. Reflections were not reported which had peak heights of 0.7 or less. When adjacent peaks had nearly equal 2θ values, resolution of individual peaks in the powder pattern would be unlikely; therefore, one composite peak was given. The angle of this peak was assigned the hkl of the reflection having the greatest integrated intensity; a plus sign (+) was used to indicate additional hkl's.

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



- Alexander, L., H. P. Klug, and E. Kummer (1948). Statistical factors affecting the intensity of x-rays diffracted by crystalline powders, J. Appl. Phys. 19, No. 8, 742-753.
- Bearden, J. S. (1964). X-ray Wavelengths, U.S. At. Energy Comm. NYO-10586.
- Evans, H. T., Jr., D. E. Appleman, and D. S. Handwerker (1963). The least-squares refinement of crystal unit cells with powder diffraction data by an automatic computer indexing method, (abs.) Am. Crystal. Assoc. Annual Meeting, Cambridge, Mass. Program, 42-43.
- International Tables for X-ray Crystallography, 1 (1952). (The Kynoch Press, Birmingham, England.) Ibid. III (1962). Pgs. 202, 210, 213, 214.

- International Union of Pure and Applied Chemistry, (1961). Chem. Eng. News 39 (4), Nov. 20, 42.
- ISCC-NBS Controid Color Charts, SRM 2106, obtained from the Office of Standard Reference Materials, Room B328, Chemistry Building, National Bureau of Standards, Washington, D.C. 20234. \$5.00 per set.
- Palache, C., H. Berman, and C. Frondel (1944). Dana's System of Mineralogy (John Wiley & Sons, New York, 7th Ed.), I, 6.
- Smith, D. K. (1967). A Revised Program for Calculating Powder Diffraction Patterns, UCRL 50264, University of California, Lawrence Radiation Laboratory, Livermore, Calif. 94551.

The sample was made by slow evaporation at room temperature of a l : l aqueous solution of $(NH_4) \ge SO_4$ and $CdSO_4$. The material loses water slowly in dry air.

Color

Colorless

Optical data

Biaxial(+), N_{α} =1.486, N_{β} =1.488, N_{γ} =1.494 2V is large.

Structure

Monoclinic, P2,/a (14), Z=2, structure determined by Montgomery and Lingafelter [1966].Isostructural with other "Tutton" salts [Tutton, 1916].

	$a(\mathring{A})$ $b(\mathring{A})$		c(Å)	β(°)
Hofmann [1931] Montgom-	9.35*	12.705*	6.27*	106°41 ′ *
ery et al.[1966] NBS, sample	9.43	12.82	6.29	106°52′
at 25 °C	9.395 ±.001	12.776 ±.002	6.299 ±.001	106°43′ ±1′

*as published

Density

(calculated) 2.058 g/cm³ at 25° C.

Reference intensity

 $1/1_{corundum} = 1.8$

Internal standard Ag, $a = 4.08641 \text{ Å}$ CuK $a_1 \lambda = 1.54056 \text{ Å}$; temp. 25 °C					
$d(\mathring{A})$ I hkl $20(\circ)$					
7.37	40	110	12.00		
6.39	40	020	13.85		
6.03	40	001	14.68		
5.45	35	011	16.26		
5.32	35	111	16.66		
5.21	17	120	17.00		
4.500	40	200	19.71		
4.388	40	021	20.22		
4.316	30	Ī21	20.56		
4.239	100	210,201	20.94		
4.205	75	111	21.11		
4.022	8	211	22.08		
3.849	100	130	23.09		
3.678	30	220	24.18		
3.655	10	121	24.33		
3.531	18	221	25.20		
3.478	12	031	25.59		
3.442	35	I31	25.86		
3.193	6	040,201	27.92		
3.099	19	211	28.78		
3.077	8	131	28.99		
3.057	60	112	28.19		
3.014	4	002	29.61		
3.006	4	231	29.70		
2.934	10	012	30.44		
2.921	20	202,310	30.58		
2.855	35	221	31.30		
2.823	20	041,122	31.67		
2.759	7	321	32.42		
2.729	5	022	32.79		
2.659	11	222	33.68		
2.603	15	240	34.43		
2.584	9	112	34.68		
2.552	8	231,241	35.13		
2.529	4	132	35.46		
2.485	40	331	36.11		
2.471	7	312	36.32		
2.458	14	150	36.52		
2.431	14	330	36.60		
2.380	5	311	37.77		

Internal standard Ag, $a = 4.08641 \text{ Å}$					
$\frac{d(\hat{A})}{d(\hat{A})} = \frac{I}{I} + \frac{1}{2\theta(2)}$					
2.339	8	151,401	38.46		
2.264	20	321	39.78		
2.258	12	241	39.89		
2.243	6	132,142	40.17		
2.227	3	202	40.48		
2.215	9	151,410	40.70		
2.193	18	212,042	41.13		
2.187	15	251,340	41.24		
2.169	6	332	41.61		
2.156	15	242	41.87		
2.122 2.103 2.072 2.068 2.044	20 3 5 2	420 222 160,203 I13 213	42.56 42.98 43.64 43.74 44.28		
2.009	15	061	45.10		
1.992	3	I23	45.50		
1.960	9	351	46.29		
1.945	7	350	46.66		
1.926	14	260,252	47.16		
1.919	7	023	47.33		
1.902	7	261	47.77		
1.888	3	441	48.17		
1.879	6	133	48.40		
1.859	8	511	48.95		
1.850	7	421	49.21		
1.833	8	113	49.70		
1.827	7	242	49.86		
1.795	6	352	50.83		
1.782	9	510	51.22		
1.773	6	403,333	51.49		
1.770	4	261,512	51.59		
1.757	7	351,413	52.00		
1.746	1	361,071	52.35		
1.737	9	243,360	52.66		
1.719	6	531	53.25		

Hofmann,	₩.	(1931).	I	Die	Struk	tur	der	Tut-
tonsche	en i	Salze,	\mathbf{Z} .	Kri	.st.,	78,	279-	-333.

- Montgomery, H.,and E.C. Lingafelter(1966). The crystal structure of Tutton's salts. IV.Cadmium ammonium sulfate hexahydrate, Acta Cryst. 20, 728 - 730.
- Tutton, A.E. (1916). The monoclinic double sulphates containing ammonium. Completion of the double sulphate series, Trans. Roy. Soc. London Ser.A 216, 1-62.

ſ

The sample was made by refluxing at 100 °C for five hours, a mixture of 2.66% $CaSO_4$, 41.11% $(NH_4)_2SO_4$ and 56.22% H_2O (by weight). The slurry was then filtered off rapidly. This is the method given by Hill and Yanick [1935].

Color

Colorless

Optical data

Isotropic, N=1.532

Structure

Cubic, $P2_1 3$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The structure of langbeinite, $K_2 Mg_2 (SO_4)_3$, was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
Gattow and Zemann [1958]	10.536 ±.008
NBS, sample at 25 °C	10.5360 ±.0002

Density

(calculated) 2.297 g/cm³ at 25° C.

Reference intensity

 $I/I_{contradum} = 2.3$

Additional patterns

1. PDF card ll-241, [M. Hoshino, Dept. Applied Chem., Tohoku Univ., Sendai, Japan].

Internal standard Ag, a = 4.08641 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C				
d (Å)	I	hkl	26(°)	
6.08	20	111	14.56	
4.72	16	210	18.80	
4.300	45	211	20.64	
3.725	7	220	23.87	
3.515	11	221	25.32	
3.334	100	310	26.72	
3.176	9	311	28.07	
2.924	6	320	30.55	
2.815	45	321	31.76	
2.555	4	410	35.09	
2.485	1	411	36.12	
2.417	2	331	37.17	
2.356	1	420	38.17	
2.300	3	421	39.14	
2.247	2	332	40.10	
2.149	11	422	42.00	
2.107	5	430	42.89	
2.066	9	510	43.78	
2.028	5	511	44.65	
1.956	11	520	46.38	
1.924	3	521	47.20	
1.835	8	522	49.65	
1.806	4	530	50.48	
1.7808	1	531	51.27	
1.7321	2	610	52.81	
1.7093	12	611	53.57	
1.6657	3	620	55.09	
1.6456	2	621	55.82	
1.6256	2	541	56.57	
1.6066	1.	533	57.30	
1.5878 1.5706 1.5535 1.5206 1.5052	1 4 1 2	622 630 631 444 632	58.04 58.74 59.45 60.87 61.56	
1.4900	2	710	62.26	
1.4757	1	711	62.93	
1.4610	2	640	63.64	
1.4475	3	720	64.30	
1.4338	4	721	64.99	

Ammonium Calcium Sulfate,	(NH_4)) ₂ Ca ₂ (SO ₄).	3 (cubic)	 continued
---------------------------	----------	--	-----------	-------------------------------

Internal standard Ag, a = 4.08641 Å					
CuKa	$\lambda = 1.5$	54056 A; temp. 25	5 °C		
$d(\mathring{A})$ I hkl $2\theta(\circ)$					
1.4081	2	642	66.33		
1.3956	1	722	67.00		
1.3713	2	731	68.35		
1.3490	2	650	69.64		
1.3379	2	732	70.30		
1.3067 1.2967 1.2871 1.2776 1.2682	2 1 1 1	810 811 733 820 821	72.24 72.89 73.52 74.16 74.80		
1.2593	1	653	75.42		
1.2415	2	822	76.70		
1.2329	1	830	77.33		
1.2249	3	831	77.93		
1.2168	1	751	78.55		
1.2007	2	832	79.81		
1.1930	1	752	80.43		
1.1778	1	840	81.69		
1.1706	1	841	82.30		
1.1564	1	911	83.53		
1.1497	2	842	84.13		
1.1430	1	920	84.74		
1.1363	2	921	85.36		
1.1233	1	664	86.59		
1.1169	2	922	87.21		
1.1106	2	930	87.83		
1.1046	1	931	88.43		
1.0926	1	852	89.66		

- Gattow, G.and J.Zemann(1958). Über Doppelsulfate vom Langbeinit-Typ, A⁺₂ B²⁺₂ (SO₄)₃, Z. Anorg. Allgem. Chem. 293, 233 - 240.
- Hill, A.E., and N.S. Yanick (1935). Ternary systems, XX. Calcium sulfate, ammonium sulfate and water, J. Am. Chem. Soc. 57, 645 - 651.
- Zemann,A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit,K₂Mg₂ (SO₄)₃, Acta Cryst. 10, 409 - 413.

The material was formed by the reaction of methanol solutions of $CoBr_2$ and $NH_4 F$, according to the method of Haendler et al. [1958]. In moist air $CoF_2 \cdot 4H_2O$ slowly develops as a decomposition product.

Color

Light purplish pink

Optical data

Isotropic, N=1.506

Structure

Cubic, perovskite type, Pm3m (221), Z=1 [Rüdorff et al., 1959].

Lattice constants

	a(Å)
Rüdorff et al.[1959] Crocket and Haendler[1960] NBS, sample at 25 °C	4.129 4.129 4.1320 ±.0001

Density

(calculated) 3.153 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 2.2$

Internal standard W, a = 3.16516 Å			
CuK	$\alpha_1 \lambda = 1$.54056 Å; temp. 2	5 °C
d (Å)	Ι	hkl	20(°)
4.133	100	100	21.48
2.921	65	110	30.58
2.386	7	111	37.67
2.066	65	200	43.78
1.848	40	210	49.27
1.686	20	211	54.36
1.4611	30	220	63.63
1.3774	16	300	68.01
1.3064	6	310	72.26
1.1925	8	222	80.47
1.1461	5	320	84.46
1.1045	6	321	88.44
1.0330	4	400	96.44
1.0020	6	410	100.48
.9740	5	411	104.53
.9238	5	420	112.99
.9017	6	421	117.36

- Crocket, D. S., and H. M. Haendler (1960). Synthesis of fluorometallates in methanol. Some structure relationships, J.Am. Chem. Soc. 82, 4158-62.
- Haendler, H. M., F. A. Johnson, and D. S. Crocket (1958). The synthesis of ammonium fluorometallates in methanol, J. Am. Chem. Soc. 80, 2662-64.
- Rüdorff, W., J. Kändler, G. Lincke, and D. Babel (1959). Über Doppelfluoride von Nickel und Kobalt, Angew. Chem. 71, 672.

The sample was prepared at room temperature by slow evaporation of an aqueous equimolar solution of $(NH_4)_2 CrO_4$ and $MqCrO_4$.

Color

Unground: vivid yellow Ground: vivid greenish yellow

Optical data

Biaxial(+) $\rm N_{\alpha}{=}1.637$, $\rm N_{\beta}{=}1.638$, $\rm N_{\gamma}{=}1.653$, 2V is small.

Structure

Monoclinic, P_{2_1}/a (14), Z=2. Isostructural with other "Tutton Salts" [Tutton and Porter, 1912]. The structure of a "Tutton Salt", $(NH_4)_2 Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton (1962).

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.508 ±.001	12.674 ±.002	6.246 ±.001	106°14′ ±1′

Density

(calculated) 1.840 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 0.9$

Internal standard Ag, a = 4.08641 Å				
CuK a_1 $\lambda = 1.54056$ Å; temp. 25 °C				
d (Å)	Ι	hkl	20(°)	
7.41	8	110	11.94	
6.33	6	020	13.98	
6.00	4	001 `	14.76	
5.41	50	011	16.36	
5.208	35	120	17.01	
4.562	14	200	19.44	
4.352	9	021	20.39	
4.285	100	121	20.71	
4.249	70	201	20.89	
4.213	30	111	21.07	
4.026	8	211	22.06	
3.832	80	130	23.19	
3.649	19	121	24.37	
3.453	20	031	25.78	
3.414	12	131	26.08	
3.222	18	201	27.66	
3.167	30	040	28.15	
3.123	16	211	28.56	
3.071	5	131	29.05	
3.029	30	112	29.46	
2.996	20	311,231,+	29.80	
2.957	3	310	30.20	
2.907	13	202	30.73	
2.873	13	221	31.10	
2.832	2	212	31.57	
2.798	25	041,Ī22	31.96	
2.774	15	321	32.24	
2.742	5	320	32.63	
2.710	1	022	33.02	
2.586	7	141,112	34.66	
2.563	11	231	34.98	
2.541	6	241	35.29	
2.491	25	331	36.02	
2.445	3	032	36.72	
2.394	3	232	37.53	

Intern	hal stand	ard Ag, a = 4.0864	41 Å	
CuKa	$\lambda = 1.3$	54056 Å; temp. 25	5 ℃	
$d(A)$ I hkl $2\theta(\circ)$				
2.282	6	400	39.46	
2.260	15	241	39.86	
2.246	5	410	40.12	
2.216	7	250,421	40.68	
2.195	9	340	41.09	
2.178	14	042,251	41.43	
2.147	12	420	42.05	
2.121	4	331	42.60	
2.028	4	213,142	44.64	
2.000	2	003	45.31	
1.994	6	251,061	45.46	
1.959	6	401,351	46.32	
1.939	4	341	46.81	
1.917	10	260,313	47.39	
1.911	8	252,161	47.53	
1.852	8	323,440	49.15	
1.847	7	233	49.30	
1.828	3	113,152	49.83	
1.822	2	521	50.03	
1.807	12	510,033	50.46	
1.775	2	123	51.45	
1.750	3	162	52.23	
1.730	4	522,451,+	52.88	
1.725	5	243	53.05	
1.696	3	450	54.03	
1.678	6	171	54.65	
1.667	3	441,271	55.06	
1.652	2	213,343	55.56	

- Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.
- Tutton, A. E. H., and M. W. Porter (1912). Crystallographic constants and isomorphous relations of the double chromates of the alkalis and magnesium, Min. Mag. 16, 169-196.

The sample was prepared at room temperature by slowly evaporating a 1:1 aqueous solution of $(NH_4)_2 SO_4$ and $MnSO_4$.

Color

Pale pink

Optical data

Biaxial (+) ${\rm N}_{\alpha}{=}1.482$, ${\rm N}_{\beta}{=}1.456$, ${\rm N}_{\gamma}{=}1.492$ 2V is large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2, isomorphous with other "Tutton Salts" [Tutton,1916]. The structure was determined by Montgomery et al. [1966].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Cipriani [1958] Montgom-	9.29	12.66	6.211	107.05°
ery et al.[1966] NBS,	9.40	12.74	6.26	107°
sample at 25 °C	9.374 ±.002	12.676 ±.002	6.253 ±.001	106°49 ′ ±1′

Density

(calculated) 1.827 g/cm³ at 25° C.

Additional patterns

1. PDF card 11-134. [Cipriani, 1958]

Internal standard Ag, $a = 4.08641 \text{ Å}$					
	$d(\dot{A})$ I bbl 20(°)				
7.31	6	110	12.09		
6.34	20	020	13.95		
5.98	16	001	14.80		
5.41	45	011	16.38		
5.28	12	111	16.77		
5.18	25	120	17.10		
4.491	20	200	19.75		
4.356	25	021	20.37		
4.287	50	121	20.70		
4.227	100	210,201	21.00		
4.172	45	111	21.28		
4.010	11	211	22.15		
3.824	80	130	23.24		
3.664	10	220	24.27		
3.627	10	121	24.52		
3.517	6	221	25.30		
3.453	16	031	25.78		
3.422	19	131	26.02		
3.177	25	201	28.06		
3.079	25	211,230	28.98		
3.031	45	Ī12	29.44		
2.986	8	140,231	29.90		
2.965	7	311	30.12		
2.911	15	012,310	30.69		
2.834	20	212	31.54		
2.801	25	Ī22,041	31.93		
2.749	12	321	32.54		
2.703	3	022,320	33.11		
2.643	5	222	33.89		
2.587	10	240	34.64		
2.576	7	141	34.80		
2.539	11	231	35.32		
2.475	30	331	36.27		
2.439	6	330,150	36.82		
2.397	4	232	37.49		
2.336	5	051,401	38.51		
2.295	3	411	39.23		
2.242	15	241,400	40.19		
2.228	6	132	40.45		
2.208	7	410,250	40.84		

Internal standard Ag, a = $4.08641 \stackrel{\circ}{A}$					
CuKa	$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. } 25 \text{ °C}$				
d (Å)	Ι	hkl	26(°)		
d (Å) 2.199 2.176 2.157 2.143 2.114 2.052 2.029 2.004 1.991 1.959 1.950 1.950 1.934 1.902 1.890 1.879 1.854 1.849 1.814 1.783	I 6 20 6 7 14 5 4 6 12 6 7 8 6 3 8 8 7 8 8 7 8 8 6	hkl $151, \overline{3}41$ $042, 340$ $\overline{3}32$ $\overline{2}42$ $420, 060$ $\overline{1}13$ $\overline{2}13$ $\overline{4}22$ 061 232 $\overline{3}51$ $052, 350$ $411, 023$ $\overline{2}61, \overline{4}32$ $\overline{4}41$ $\overline{5}11, \overline{3}23$ $\overline{2}33$ 440 242 $\overline{3}52$	$26(\circ)$ 41.01 41.47 41.84 42.14 42.74 44.10 44.62 45.21 45.52 46.30 46.54 46.94 47.78 48.10 48.39 49.09 49.23 49.76 50.26 51.18		
1.776 1.764 1.749 1.725	8 4 7 8	510,170 403,123 162,413 360,243,+	51.41 51.77 52.26 53.03		

- Cipriani, C. (1958). Manganese boussinggaultite of Larderello (Tuscany), Rend. Soc. Mineral. Ital. 14, 124 - 137.
- Montgomery, H., R. V. Chastain and E. E. Lingafelter (1966). The crystal structure of Tutton's salts. V. Manganese ammonium sulfate hexahydrate, Acta Cryst. 20, 731 - 733.
- Tutton, A.E.H. (1916). The monoclinic double sulphates containing ammonium, Trans. Roy. Soc. London Ser.A 216, 1-62.

The sample was precipitated from solutions of ammonium chloride and mercury chloride. Spectrographic analysis showed the only impurity greater than 0.001 percent to be 0.01 to 0.1 percent silicon.

Color

Colorless

Optical data

Uniaxial (+) N =1.793, N =1.84. (The higher index could not be measured accurately because the index liquid and sample reacted.)

Structure

Tetragonal, P***, Z=1, space group not resolved by Harmsen [1938].

Lattice constants

	a(Å)	c(Å)
Harmsen [1938] NBS, sample at 25 °C	4.20 4.1977 ±.0001	7.96 7.9353 ±.0002

Density

(calculated) 3.859 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 3.1$

Additional patterns

1. PDF 18-116 [Swanson et al., 1967]

*Intensity values reported earlier by NBS have been modified.

Internal standard Ag, $a = 4.08641 \text{ Å}$ CuK $a_1 \lambda = 1.54056 \text{ Å}$; temp. 25 °C			
d (Å)	Ι	hkl	2ê(°)
7.93	100	001	11.15
4.199	65	100	21.14
3.967	25	002	22.39
3.711	40	101	23.96
2.969	60	110	30.07
2.883	6	102	30.99
2.782	30	111	32.15
2.645	20	003	33.86
2.377	17	112	37.81
2.239	20	103	40.25
2.099	13	200	43.06
2.029	9	201	44.62
1.983	9	004	45.71
1.974	20	113	45.93
1.877	8	210	48.45
1.855	6	202	49.06
1.827	7	211	49.88
1.793	8	104	50.88
1.6966	2	212	54.00
1.6491	10	114	55.69
1.6445	10	203	55.86
1.5868	1	005	58.08
1.5308	7	213	60.42
1.4843	4	105,220	62.52
1.4588	3	221	63.74
1.4417	3	204	64.59
1.3994	3	115,300	66.79
1.3899	2	222	67.31
1.3781	2	301	67.96
1.3635	3	214	68.79
1.3274	4	310	70.94
1.3227	2	006	71.23
1.3092	3	311	72.08
1.2943	2	223	73.04
1.2658	2	205	74.96
1.2616 1.2587 1.2366 1.2116	4 4 2 1 2	106 312 303 215	75.25 75.46 77.05 78.95 79.22

Interr	Internal standard Ag, a = 4.08641 Å			
CuKa	$\lambda = 1.5$	54056 A; temp. 25	5 °C	
d (Å)	Ι	hkl	20(°)	
1.1881	2	224	80.83	
1.1865	2	313	80.96	
1.1646	1	320	82.81	
1.1518	1	321	83.94	
1.1434	1	304	84.70	
1.1333	1	007	85.63	
1.1190	1	206	87.00	
1.1032	2	314	88.56	
1.0944	2	107	89.47	
1.0837	<1	225	90.59	
1.0810	2	216	90.88	
1.0656	1	323	92.58	
1.0590	2	117	93.33	
1.0496	1	305,400	94.42	
1.0184	2	315,410	98.29	
1.0095	1	411	99.46	
1.0043	2	324	100.16	
0.9975	2	207	101.10	
.9920	1	008	101.88	
.9893	1	330	102.26	
.9874	1	226	102.54	
.9756	1	403	104.28	
.9706	2	217	105.05	
.9655	2	108	105.84	
.9612	2	306	106.51	
.9502	<1	413	108.32	
.9408	1	118	109.91	

- Harmsen, E. J. (1938). The crystal structure of NH_4HgCl_3 , Z. Krist. 100A, 208 211.
- Swanson, H.E., H.F. McMurdie, M.C. Morris, and E.H. Evans (1967). Standard x-ray diffraction powder patterns, Nat'l. Bur. Std. U.S. Mono. 25, Sec.5, 9-10.

The sample was prepared by slow evaporation at room temperature of an aqueous solution of $(NH_4)_2 CrO_4$ and $NiCrO_4$.

Color

Unground: deep yellowish green Ground: brilliant greenish yellow

Optical data

Biaxial, N $_{\alpha}=1.656,$ N $_{\gamma}=1.676,~2V$ is very large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2. Isostructural with other "Tutton Salts", by comparison of the powder patterns. The structure of a "Tutton Salt", $(NH_4)_2$ -Mg(SO₄)₂.6H₂O, was determined by Margulis and Templeton [1962].

Lattice constants

	$a(\stackrel{\circ}{A})$	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.420 ±.001	12.603 ±.002	6.275 ±.001	105°54′ ±1′

Density

(calculated) 2.016 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 1.3$

Internal standard Ag, $a = 4.08641 \text{ \AA}$				
CuKa	$\lambda = 1.5$	54056 Å; temp. 2	5 °C	
d (Å)	Ι	hkl	20(°)	
6.31	16	020	14.03	
6.04	12	001	14.66	
5.45	40	011	16.26	
5.28	7	111	16.78	
5.18	25	120	17.11	
4.530	25	200	19.58	
4.358	18	021	20.36	
4.269	95	121,210	20.79	
4.227	100	111,201	21.00	
4.003	8	211	22.19	
3.811	75	130	23.32	
3.657	19	121	24.32	
3.508	4	221	25.37	
3.449	18	031	25.81	
3.406	16	131	26.14	
3.226	10	201	27.63	
3.152	14	040	28.29	
3.124	14	211	28.55	
3.041	40	112	29.35	
2.977	8	231,140	29.99	
2.936	10	310,012	30.42	
2.908	8	202	30.72	
2.872	18	221	31.12	
2.805	15	122	31.88	
2.772	7	141	32.27	
2.753 2.722 2.638 2.597 2.579	8 6 3 6	321 320,022 222 112 141	32.50 32.88 33.96 34.51 34.75	
2.556	8	231	35.08	
2.525	4	241	35.53	
2.470	20	331	36.34	
2.451	7	330,032	36.64	
2.427	2	150	37.01	
2.399 2.388 2.326 2.280 2.252	3 3 3 15	311 232 322,051 321 241	37.45 37.64 38.67 39.49 40.01	

Interr	Internal standard Ag, a = 4.08641 Å					
d (Å)	$\begin{array}{c c c c c c c c c c c c c c c c c c c $					
2.230	4	410	40.41			
2.202	6	250	40.95			
2.193	7	421,341	41.12			
2.178	16	340,042	41.43			
2.163	6	251	41.72			
2.131 2.112 2.079 2.061 2.033	12 2 2 3	420 222,331 412 113,203 213	42.39 42.77 43.49 43.90 44.54			
2.011	4	003	45.05			
2.001	3	422	45.29			
1.984	5	061,123	45.70			
1.976	5	161	45.88			
1.944	6	351	46.68			
1.934	7	350,052	46.93			
1.914	9	313	47.47			
1.903	6	252,161	47.75			
1.880	3	261,441	48.37			
1.863	4	511	48.85			
1.849	7	233	49.23			
1.839	8	113,440	49.53			
1.827	4	242,152	49.86			
1.816	5	033	50.21			
1.811	4	322	50.34			
1.793	7	510	50.87			
1.783	2	123	51.20			
1.777	2	352	51.37			

Margulis,	T.N.	and D.	н.	Templeton	(1962).
Crystal	struc	ture	and	hydrogen	bonding
of mag	nesium	ammor	nium	sulfate	hexahy-
drate, 2	Z. Kri	st. 11	17, 3	334-357.	

,

The sample was precipitated by mixing methanol solutions of ZnBr_2 and NH_4HF_2 , as described by Haendler et al. [1958].

Color

Colorless

Structure

Cubic, Pm3m (221), Z=1, perovskite type. Isostructural with KZnF₃ [Crocket and Haendler, 1960]

Lattice constants

	$a(\mathring{A})$
Crocket and Haendler[1960] NBS, sample at 25°C	4.115 4.1162 ±.0001

Density

(calculated) 3.343 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 3.8$

- Crocket, D.S., H.M. Haendler (1960). Synthesis of fluorometallates in methanol. Some structure relationships, J. Am. Chem. Soc. 82, 4158-4162.
- Haendler, H. M., F. A. Johnson and D. S. Crocket (1958). The synthesis of ammonium fluorometallates in methanol, J. Am. Chem. Soc. 80, 2662-2664.

Internal standard W, a = 3.16516 Å				
Cuk	$a_1 \land = 1$.54050 A; temp. 2		
d (Å)	I	hkl	20(°)	
4.118 2.910 2.376 2.0580 1.8409 1.6800 1.4552 1.3718 1.3014	100 70 <1 50 35 18 20 13 6	100 110 111 200 210 211 220 300 310	21.56 30.70 37.84 43.96 49.47 54.58 63.92 68.32 72.58	
1.2409 1.1884 1.1417 1.1001 1.0290 0.9984	<1 5 4 5 2 5	311 222 320 321 400 410	76.74 80.81 84.86 88.88 96.93 100.98	
.9702 .9204 .8982 .8775 .8402 .8232 .8072	2 4 3 2 4 2 4	411 420 421 332 422 430 510	105.11 113.62 118.10 122.75 132.91 138.67 145.19	

The sample was a reagent grade material from Mallinckrodt Chemical Works, St. Louis, Missouri.

Color

Colorless

Optical data

Biaxial (+) $\rm N_{\alpha}{=}1.650\,,\ \rm N_{\gamma}{=}1.738,\ 2V$ is small.

Structure

Monoclinic, I2/c (15), Z=4. The structure of Ba(BrO₃)₂·H₂O was determined by Kartha [1953].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Kartha [1953] NBS,	9.06	7.92	9.66	93°5'
sample at 25℃	9.069 ±.001	7.901 ±.001	9.639 ±.001	93°16.9′ ±.4′

Density

(calculated) 3.960 g/cm^3 at 25° C.

Reference intensity

 $I/I_{corundum} = 2.8$

Additional patterns

 PDF card 16-247 [Weigel et al., 1962]. (In this reference and on the card, the formula was inadvertently given as BaBrO₃ •H₂O).

Inte	rnal stan	dard W, a = 3.165	16 Å			
CuK a_1 λ = 1.54056 Å; temp. 25 °C						
d (Å)	Ι	hkl	20(°)			
5.94	55	110	14.90			
4.53	9	200	19.57			
3.950	25	020	22.49			
3.815	12	<u>1</u> 12	23.30			
3.705	50	<u>2</u> 11	24.00			
3.679	15	$ \begin{array}{r} 112 \\ 211 \\ \overline{1}21 \\ \overline{2}02 \\ 121 \end{array} $	24.17			
3.576	25		24.88			
3.415	50		26.07			
3.396	55		26.22			
3.363	13		26.48			
3.208	60	202	27.79			
3.055	40	022	29.21			
2.977	100	220	29.99			
2.819	7	310	31.72			
2.575	4	222	34.81			
2.542	15	031	35.28			
2.531	13	130	35.44			
2.493	12	312,222	36.00			
2.430	6	123	36.96			
2.407	6	004	37.33			
2.374	25	$ \begin{array}{r} 123 \\ \overline{3}21 \\ 321 \\ 400, \overline{1}14 \\ \overline{2}31 \end{array} $	37.87			
2.353	10		38.21			
2.302	9		39.09			
2.262	40		39.81			
2.231	13		40.40			
2.225	12	132	40.51			
2.203	9	114,231	40.94			
2.178	11	204	41.43			
2.148	6	411	42.02			
2.076	, 6	204	43.57			
2.036	4	033	44.45			
1.985	3	330	45.67			
1.964	14	323,420	46.18			
1.907	4	224	47.66			
1.896	6	141	47.93			
1.888	18	$ \begin{array}{r} 141 \\ \overline{2}33,314 \\ \overline{3}32 \\ \overline{4}22 \\ \overline{4}13 \\ \end{array} $	48.15			
1.882	11		48.33			
1.859	8		48.96			
1.850	15		49.20			
1.848	15		49.27			

Barium Bromate H	Hydrate, E	$Ba(BrO_3)$	2·H20	(monoclinic) -	continued
------------------	------------	-------------	-------	----------------	-----------

Internal standard W, a = 3.16516 Å CuKa, $\lambda = 1.54056 \text{ Å}$; temp. 25 °C				
d (Å)	I	hkl	2θ(°)	
1.831	16	233	49.75	
1.827	16	042	49.88	
1.810	13	332,240	50.36	
1.788	8	422	51.04	
1.784	8	314	51.15	
1.765	15	510	51.76	
1.758	18	134,413	51.97	
1.715	4	125	53.37	
1.703	6	431	53.80	
1.695	12	215	54.07	
1.678	7	431	54.66	
1.637	8	341,521	56.14	
1.628	4	512	56.48	
1.609	5	521	57.19	
1.6040	6	006,404	57.40	
1.5566	7	150	59.32	
1.5535	13	035	59.45	
1.5359	5	325	60.20	
1.5267	4	044	60.60	
1.5092	4	600	61.38	
1.5032	5	334 235 152,206 611,152 602	61.65	
1.4908	4		62.22	
1.4848	8		62.50	
1.4776	6		62.84	
1.4644	8		63.47	
1.4624	9	244,514	63.57	
1.4526	6	611	64.05	
1.4376	8	442	64.80	
1.4340	7	226,523	64.98	
1.4309	5	244	65.14	
1.4170	5	053,602	65.86	
1.4094	8	620	66.26	
1.4069	9	442,532	66.39	
1.3995	5	350	66.79	
1.3729	4	622	68.26	
1.3629	4	316,253	68.83	
1.3534	5	352	69.38	
1.3434	5	253	69.97	
1.3348	5	352	70.49	
1.3297	4	541	70.80	

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C				
d (Å)	Ι	hkl	20(°)	
1.3170 1.3143 1.3094 1.3062 1.3010 1.2894 1.2784	4 7 6 6 4	$ \begin{array}{r} 060 \\ 541 \\ \overline{4}35 \\ \overline{6}31 \\ 154 \\ 161, \overline{4}51 \\ 451, 217 \\ 406 \\ \end{array} $	71.58 71.76 72.07 72.27 72.61 73.37 74.10 74.35	
1.2545 1.2510	4 4 3	435 712,543	74.35 75.76 76.01	
1.2339 1.2281 1.2244 1.2173 1.2139	4 3 5 5 4	633 721,262 354 712,327 246,543	77.26 77.69 77.97 78.51 78.77	
1.2112 1.1992 1.1919 1.1887 1.1693 1.1658	4 4 7 6 4 5	721,Ī63 640 237,633,+ 624 723 552	78.98 79.93 80.52 80.78 82.41 82.71	

Kartha, G.(1953). Structure of halogenates of the type A(BO₃)₂·H₂O, Proc. Indian Acad. Sci. Sect. A38, 1 - 12.

Weigel,D., B. Imelik and M. Prettre (1962) Hydrates des sels oxygénés de nickel, Bull. Soc. Chim. France 1962, 1427-1434.

The sample was obtained from Matheson. Coleman and Bell, Co., East Rutherford, N.J.

Color

Colorless

Optical data

Biaxial (+) $N_{\alpha} {=} 1.564$, $N_{\beta} {=} 1.58$, $N_{\gamma} {=} 1.634$, 2V is medium.

Structure

Monoclinic, I2/c (15), Z=4. The structure of Ba(ClO₃)₂ \cdot H₂O was determined by Kartha [1952].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Kartha [1952]	8.86 ±.02	7.80 ±.02	9.35 ±.02	93°30′
NBS, sample at 25 °C	8.938 ±.001	7.837 ±.001	9.418 ±.001	93°42.6′ ±.4′

Density

(calculated) 3.251 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 1.8$

Additional patterns

1. PDF card 1-0155 [Hanawalt et al., 1938]

Internal standard Ag, a = 4.08641 \mathring{A}				
$CuKa_1 \lambda = 1.54056 \text{ \AA}; \text{ temp. } 25 \text{ °C}$				
d (Å)	Ι	hkl	28(°)	
6.01	40	011	14.73	
5.88	100	110	15.05	
4.69	12	002	18.90	
4.462	3	200	19.88	
3.923	10	020	22.65	
3.753	25		23.69	
3.658	50		24.31	
3.601	15		24.70	
3.517	20		25.30	
3.382	40		26.33	
3.343	55	202	26.64	
3.321	30	121	26.82	
3.136	60	202	28.44	
3.011	30	022	29.64	
2.944	40	220	30.34	
2.910	40	$ \begin{array}{c} 013\\ 310\\ 031\\ 130, \overline{2}13\\ \overline{3}12 \end{array} $	30.70	
2.779	10		32.18	
2.517	18		35.64	
2.510	19		35.75	
2.458	6		36.52	
2.391	10	ī23	37.58	
2.373	6	213	37.89	
2.350	10	004	38.27	
2.327	55	321	38.66	
2.269	8	321	39.69	
2.229	25	400,Ī32	40.43	
2.216	25	Ī14	40.69	
2.209	25	231	40.81	
2.195	6	132	41.09	
2.175	.14	231	41.48	
2.151	6	114	41.96	
2.137	18	204	42.26	
2.120	7	411	42.61	
2.067	4	402	43.76	
2.026	8	204	44.69	
2.006	7	$ \begin{array}{r} 033 \\ 402 \\ 040 \\ 420, \overline{3}23 \\ 141 \end{array} $	45.16	
1.966	5		46.14	
1.959	4		46.31	
1.938	10		46.85	
1.870	5		48.65	

Barium Chlorate Hydrate	, Ba(CIO ₃) 2.H ₂ C) (monoclinic) -	continued
-------------------------	--	------------------	-----------

Internal standard Ag, a = 4.08641 Å				
CuKa	$CuKa_1 \ \lambda = 1.54056 \ \text{\AA}; \text{ temp. 25 °C}$			
d (Å)	Ι	hkl	20(°)	
1.860	10	233	48.94	
1.850	7	314	49.22	
1.845	6	3 2 3	49.35	
1.827	8	422,015	49.86	
1.823	6	413	49.98	
1.809	11	042	50.40	
1.802	12	233	50.60	
1.794	10	240	50.86	
1.785	5	332	51.14	
1.758	8	422	51.98	
1.743	4	314	52.45	
1.739	5	510	52.60	
1.731	9	134,215	52.86	
1.721	5	413	53.19	
1.691	2	242	54.21	
1.683	8	431,125	54.47	
1.673	4	404	54.84	
1.665	6	512	55.10	
1.661	5	242	55.25	
1.656	8	215,431	55.45	
1.643	4	Ī43	55.90	
1.622	2	341	56.72	
1.616	4	521	56.93	
1.598	3	512	57.62	
1.584	3	521	58.21	
1.567	6	404	58.87	
1.544	4	150	59.86	
1.539	3	334.424	60.06	
1.530	4	I 16	60.47	
1.526	8	035	60.62	
1,523	8	433	60.75	
1.511	3	325	61.30	
1 505	2	044	61 58	
1 /00	2	116	61 90	
1 176	6	334	62 92	
1.4/0	0	334	02.92	

Internal standard Ag, a = 4.08641 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C				
d (Å)	I	hkl	20(°)	
1.472	7	440,343,+	63.12	
1.462	4	152,433	63.60	
1.457	4	611	63.83	
1.449	4	206	64.22	
1.444	6	602,244	64.46	
1.436	5	325	64.86	
1.428	4	532	65.27	
1.422	5	442,235	65.62	
1.408	6	523,226,+	66.33	
1.402	4	053,316	66.68	
1.392	6	602	67.21	
1.387	8	442	67.45	
1.371	1	415	68.34	
1.358	2	514,613	69.14	
1.350	2	145	69.59	
1.3408 1.3312 1.3234 1.3189 1.3062	2 2 6 2	352 145,316 017 352 060	70.13 70.71 71.19 71.47 72.27	
1.2974	4	541,Ī54	72.84	
1.2910	6	435,217	73.26	
1.2835	3	154	73.76	
1.2784	4	161	74.10	
1.2717	3	444	74.56	
1.2681	4	127	74.81	
1.2578	1	710	75.53	

- 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.
- Kartha, G. (1952). Structure of barium chlorate monohydrate,Ba(ClO₃)₂·H₂O, Acta Cryst. 5, 845 - 846.

The sample was prepared by C.W. Reimann by precipitation from a water solution of $C_3H_4N_2$ and $Cd(NO_3)_2$.

Color

Colorless

Optical data

Uniaxial (-) $N_e = 1.558$, $N_o = 1.564$

Structure

Hexagonal, $R\overline{3}$ (148), Z=3, isostructural with imidazole nickel nitrate, the structure for which was reported by Santoro et al. [1969].

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25 $^\circ$ C	12.636 ±.001	15.044 ±.001
Density (calculated) 1.544 g/cm ³	at 25° C.	

Reference intensity

 $I/I_{corundum} = 2.3$

Polymorphism

A polymorph precipitated concurrently with this hexagonal form.

References
Santoro, A., A.D. Mighell, M. Zocchi and C.
W. Reimann (1969). The crystal and mo-
lecular structure of hexakis(imidazole)
nickel(II) nitrate, $(C_3H_4N_2)_cNi(NO_3)_2$,
Acta Cryst. B25, 842-847.

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C				
d (Å)	Ι	hkl	26(°)	
8.83	40	101	10.01	
6.31	95	110	14.02	
6.201	100	012	14.27	
5.139	13	021	17.24	
5.015	1	003	17.67	
4.425	1	202	20.05	
3.992	35	211	22.25	
3.924	40	113	22.64	
3.626	45	122	24.53	
3.559	3	104	25.00	
3.161	7	220	28.21	
3.100	2	024	28.78	
2.975	12	131	30.01	
2.949	10	303	30.28	
2.901	9	015	30.79	
2.815	7	312	31.76	
2.786	2	214	32.10	
2.675	8	223	33.47	
2.639	4	205	33.94	
2.571	<1	042	34.87	
2.477 2.433 2.387 2.383 2.362 2.332	5 6 7 5 1	321 125 410 232 134 116	36.23 36.91 37.65 37.72 38.06 38.58	
2.214	1	404	40.72	
2.166	4	051	41.67	
2.157	6	413	41.84	
2.136	. 3	315	42.27	
2.108	2	107,330	42.86	
2.102	2	502	42.99	
2.089 2.066 2.049 2.024 2.000	2 2 1 2	324 306 241 045 027	43.28 43.78 44.17 44.73 45.31	
1.995	2	422	45.42	
1.963	1	226	46.20	
1.949	2	511	46.57	
1.941	2	333	46.75	
1.927	1	235	47.13	

Internal standard W, a = 3.16516 Å CuKa, λ = 1.54056 Å: temp. 25 °C			
d (Å)	I	hkl	20(°)
1.907 1.901 1.853 1.824 1.811	1 1 1 1 1	217 152 018 600 244	47.65 47.80 49.13 49.95 50.33
1.787 1.779 1.771 1.753 1.741	1 2 3 2	431 208 505 137,520 514	51.07 51.30 51.57 52.12 52.51
1.730 1.712 1.690 1.659 1.654	2 2 1 1 1	416 128 407 161 523	52.89 53.47 54.23 55.33 55.50
1.633 1.616 1.599 1.554 1.544	1 <1 1 1	327 119 318 351 345	56.30 56.92 57.60 59.41 59.86
1.531 1.525 1.519 1.506 1.490	1 <1 <1 <1 <1 <1	072 164 309 443 1.0.10,247	60.43 60.68 60.92 61.50 62.26
1.459 1.450 1.437 1.413 1.407	<1 1 <1 1 <1	615 0·2·10,517,+ 526 2·1·10 624	63.71 64.16 64.84 66.04 66.40
1.392 1.369 1.357	1 <1 <1	713 419 0·1·11	67.18 68.48 69.18

The sample was prepared by treating Cs_2CO_3 and $CaCO_3$ with HF solution, drying, and heating the product to 1000 °C for two hours in a stream of nitrogen gas. The sample was somewhat hygroscopic.

Color

Colorless

Optical data

Isotropic, N=1.466

Structure

Cubic, perovskite type, Pm3m (221), Z=1 [Ludekens and Welch, 1952]

Lattice constants

	$a(\mathring{A})$
Ludekens and Welch [1952] Klasens et al. [1953] NBS, sample at 25 °C	4.523* 4.52 4.5244 ±.0001

*from kX units

Density

(calculated) 4.123 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 3.4$

References

Klasens, H. A., P. Zalm and F. O. Huysman (1953). The manganese emission in ABF₃ compounds, Philips Res. Rep. 8, 441-451.

Ludekens, W.L.W., and A.J.E. Welch (1952).
Reactions between metal oxides and fluorides: some new double-fluoride structures of the type ABF₃, Acta Cryst. 5,
841.

Interr	Internal standard Ag, a = 4.08641 Å			
CuKa	$\lambda = 1.5$	54056 A; temp. 25	5 °C	
d (Å)	I	hkl	2°(°)	
4.53	17	100	19.57	
3.202	100	110	27.84	
2.612	30	111	34.30	
2.262	45	200	39.82	
2.023	9	210	44.76	
1.847	35	211	49.31	
1.599	20	220	57.58	
1.508	5	300	61.45	
1.430	13	310	65.17	
1.364	9	311	68.78	
1.306	5	222	72.30	
1.255	4	320	75.71	
1.2092	13	321	79.14	
1.1312	3	400	85.83	
1.0975	2	410	89.15	
1.0664	6	411	92.49	
1.0382	3	331	95.79	
1.0117	6	420	99.17	
.9873	2	421	102.56	
.9646	3	332	105.99	
.9235	3	422	113.04	
.9046	1	500	116.72	
.8872	7	510	120.51	
.8706	2	511	124.44	
.8403	1	520	132.90	
.8259	4	521	137.69	

The sample was prepared by treating $C_{S_2}CO_3$ with HF and adding PbF_2 . The mixture was heated at 450 °C for 17 hours. Since the material was somewhat hygroscopic, the patterns were prepared with the sample in a dry mount.

Color

Colorless

Optical data

Isotropic, N=1.599

Structure

Cubic, Pm3m (221), Z=1, perovskite type, [Schmitz-Dumont and Bergerhoff, 1956].

Lattice constants

	a(Å)
Schmitz-Dumont and	4.81*
Bergehoff [1956]	4.7990
NBS, sample at 25 °C	±.0002

k	fr	om	kΧ

Density

(calculated) 5.966 g/cm³ at 25° C.

Reference intensity

I/I_{corundum =} 7.1

Additional patterns

1. Schmitz-Dumont and Bergerhoff [1956]

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C				
d (Å)	Ι	hkl	20(°)	
4.79	7	100	18.51	
3.39	100	110	26.26	
2.400	25	200	37.44	
2.147	4	210	42.05	
1.959	30	211	46.32	
1.696	12	220	54.01	
1.598	1	300	57.60	
1.517	10	310	61.01	
1.447	1	311	64.33	
1.386	3	222	67.54	
1.2826 1.1996 1.1641 1.1314 1.0732	8 1 3 3	321 400 410 330 420	73.82 79.90 82.84 85.82 91.74	
1.0231	2	332	97.68	
.9796	1	422	103.69	
.9413	3	510	109.83	
.8760	2	521	123.11	

Polymorphism

According to Schmitz-Dumont and Bergerhoff [1956] this cubic phase is metastable at room temperature; being stable only between 615 °C and its congruent melting point at 725 °C.

References

Schmitz-Dumont,O.,and G.Bergerhoff (1956). Die Systeme Alkalifluorid/Bleifluorid, Z. Anorg. Allgem. Chem., 283, 314-328.

The sample was prepared by heating a mixture of Cs_2CrO_4 and $MgCrO_4$ for one half hour at 440 °C in nitrogen.

Color

Vivid greenish yellow.

Optical data

Isotropic, N=1.890

Structure

Cubic, P2₁3 (198), Z=4, langbeinite type by analogy with langbeinite, $K_{\&}$ Mg₂ (SO₄)₃, and similar sulfates. The structure of langbeinite was determined by Zemann and Zemann [1957].

Lattice constants

	$a(\mathring{A})$				
NBS, sample at 25 $^\circ$ C	10.5543 ±.0002				
Density (calculated) 3.742 g/cm ³ at 25° C.					
Reference intensity I/I _{corundum} = 3.2					
References Zemann,A. and J. Zemann (1957). Die Kris- tallstruktur vom Langbeinit,K ₂ Mg ₂ (SO ₄) ₃ , Acta Cryst. 10, 409 - 413.					

Internal standard Ag, a = 4.08641 Å				
CuK a_1 λ = 1.54056 A; temp. 25 °C				
d (Å)	Ι	hkl	2θ(°)	
6.091	16	111	14.53	
5.279	6	200	16.78	
4.719	16	210	18.79	
4.308	6	211	20.60	
3.731	11	220	23.83	
3.517	11	221	25.30	
3.336	100	310	26.70	
3.182	25	311	28.02	
3.050	6	222	29.26	
2.928	40	320	30.51	
2.820	50	321	31.70	
2.638	3	400	33.95	
2.560	25	410	35.02	
2.487	3	411	36.08	
2.422	16	331	37.09	
2.360	5	420	38.10	
2.304	9	421	39.07	
2.250	7	332	40.04	
2.154	11	422	41.90	
2.111	5	430	42.80	
2.070	25	510	43.69	
2.031	4	511	44.58	
1.960	10	520	46.28	
1.927	4	521	47.12	
1.837	7	522	49.57	
1.809	2	530	50.39	
1.784	3	531	51.16	
1.759	2	600	51.95	
1.735	, 8	610	52.72	
1.712	19	611	53.48	
1.668	3	620	54.99	
1.648	16	621	55.73	
1.628	8	541	56.47	
1.609	3	533	57.19	
1.591	2	622	57.91	
1.573	7	630	58.64	
1.556	5	631	59.34	
1.523	4	444	60.76	
1.507	3	632	61.48	
1.492	4	710	62.16	
1.477	2	711	62.85	
1.463	2	640	63.54	
1.4493	3	720	64.21	
1.4360	7	721	64.88	
1.4101	3	642	66.22	

Internal standard Ag, a = 4.08641 Å CuKa, λ = 1.54056 Å; temp. 25 °C				
d (Å)	Ι	hkl	2θ(°)	
1.3976	2	722	66.89	
1.3856	2	730	67.55	
1.3741	5	731	68.19	
1.3514	4	650	69.50	
1.3403	4	732	70.16	
1.3091	3	810	72.09	
1.2988	2	811	72.75	
1.2894	1	733	73.37	
1.2796	1	820	74.02	
1.2705	4	821	74.64	
1.2615	3	653	75.27	
1.2437	2	822	76.54	
1.2268	5	831	77.79	
1.2187	2	751	78.40	
1.2110	1	662	79.00	
1.2027 1.1952 1.1727 1.1657 1.1586	2 2 1 2 2 2	832 752 841 910 911	79.65 80.25 82.12 82.72 83.34	
1.1516	2	842	83.96	
1.1447	1	920	84.58	
1.1381	2	921	85.19	
1.1253	1	664	86.39	
1.1189	2	922	87.01	
1.1127	3	930	87.62	
1.0945	1	852	89.46	
1.0888	3	932	90.06	
1.0719	1	940	91.88	
1.0660	2	941	92.53	
1.0609 1.0555 1.0503 1.0452 1.0349	1 1 1 1	933 10.0.0 10.1.0 10.1.1 10.2.0	93.11 93.73 94.34 94.94 96.20	
1.0299	2	10·2·1	96.82	
1.0252	2	950	97.42	
1.0205	2	951	98.02	
1.0154	1	10·2·2	98.68	
1.0111	1	10·3·0	99.25	
1.0063	2	10.3.1	99.89	
The sample was prepared at room temperature by slow evaporation of a 1:3 aqueous solution of Cs_2CrO_4 and $MgCrO_4$.

Color

Unground: brilliant yellow Ground: light greenish yellow

Optical data

Biaxial(+) N_{\alpha}=1.635, N_{\beta}=1.640, N_{\gamma}=1.665. 2V is large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2. Isostructural with other "Tutton Salts" [Tutton and Porter, 1912]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.604 ±.001	12.953 ±.001	6.369 ±.001	106°6′ ±1 ′

Density

(calculated) 2.749 g/cm³ at 25° C.

Reference intensity

 $I/I_{a = 2.2}$

- Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.
- Tutton, A. E. H. and M. W. Porter (1912). Crystallographic constants and isomorphous relations of the double chromates of the alkalis and magnesium, Min. Mag. 16, 169-196.

Internal standard W, a = 3.16516 Å					
CuK a_1 λ = 1.54056 A; temp. 25 °C					
d (Å)	Ι	hkl	20(°)		
7.51	35	110	11.77		
6.47	5	020	13.67		
6.11	8	001	14.48		
5.54	6	011	15.99		
5.38	4	111	16.46		
5.30	9	$120 \\ 200 \\ 021 \\ 210 \\ \overline{2}01, 111$	16.70		
4.62	3		19.20		
4.445	7		19.96		
4.350	19		20.40		
4.302	100		20.63		
4.085	7	211	21.74		
3.911	70	130	22.72		
3.722	4	121	23.89		
3.584	3	221	24.82		
3.488	7	131	25.52		
3.272	30	201	27.23		
3.240	30	040	27.51		
3.174	13	211	28.09		
3.151	15	230	28.30		
3.131	25	131	28.48		
3.087	25	Ī12	28.90		
3.058	6	002,140	29.18		
3.031	19	311	29.44		
2.991	7	310	29.85		
2.980	9	012	29.96		
2.956	20	202	30.21		
2.923	11	221	30.56		
2.880	4	212	31.03		
2.854	,20	122	31.32		
2.842	12	141	31.45		
2.810	5	321	31.82		
2.776	5	320	32.22		
2.688	2	222	33.30		
2.638	3	141	33.95		
2.606	5	231	34.38		
2.587	13	241	34.64		
2.560	12	132	35.02		
2.527	25	331	35.49		
2.505	8	330,312	35.82		
2.483	7	122	36.14		

,				
Internal standard W, a = 3.16516 Å CuK α , λ = 1.54056 Å; temp. 25 °C				
d (Å)	Ι	hkl	20(°)	
2.388	8	\$\overline{4}01,051\$ \$\overline{3}22,\$\overline{1}51\$ \$\overline{4}11\$ \$\overline{2}1\$ \$\overline{2}1\$	37.64	
2.376	7		37.84	
2.348	5		38.31	
2.318	6		38.81	
2.302	18		39.10	
2.276	4	202	39.56	
2.258	4	250	39.89	
2.220	9	251	40.61	
2.182	7	242	41.34	
2.173	7	420	41.53	
2.158	5	$ \begin{array}{r} 060\\ 331, \overline{4}02\\ \overline{4}12\\ 160\\ \overline{1}13, \overline{4}31 \end{array} $	41.82	
2.153	5		41.93	
2.121	2		42.59	
2.102	2		42.99	
2.091	3		43.24	
2.066 2.039 2.032 2.015 2.009	2 5 3 2	213 003 251 013,Ī23,+ Ī52	43.78 44.40 44.55 44.95 45.08	
1.991	3	351,223	45.51	
1.977	6	052	45.85	
1.947	4	252,313,+	46.61	
1.929		261	47.06	
1.925	3	432	47.18	
1.904	4	Ī33	47.73	
1.899	3	511,312,+	47.87	
1.885	5	323	48.25	
1.880	8	440	48.38	
1.844	1	033	49.38	
1.840	4	521,322	49.50	
1.827	3	510	49.87	
1.815	5	170	50.22	
1.810	6	123	50.37	
1.804	6	431,261	50.56	
1.793	6	351,333	50.87	
1.775	2	520,361,+	51.45	
1.754	5	531,332	52.11	
1.727	4	133,043	52.99	
1.713	5	171	53.44	
1.697	3	$530 \\ 162, \overline{3}43, + \\ \overline{5}32 \\ \overline{5}41, 342 \\ 402 $	53.99	
1.684	2		54.44	
1.677	4		54.70	
1.651	2		55.62	
1.637	2		56.14	

The sample was prepared by C. W. Reimann at NBS by evaporating an aqueous solution of CuCl₂ and pyrazole at room temperature.

Color

Unground: vivid purplish blue Ground: brilliant purplish blue

Optical data

Biaxial(-) $\mathrm{N}_{\alpha}{=}1.648$, $\mathrm{N}_{\beta}{=}1.660$, $\mathrm{N}_{\gamma}{=}1.670.$ 2V is large.

Structure

Monoclinic, C2/c (15), Z=4. Isostructural with Ni($C_3 H_4 N_2$)₄ Cl₂, the structure for which was determined by Reimann et al., [1967].

	a(Å)	b (Å)	c(Å)	β(°)
NBS sample at 25°C	13.657 ±.002	9.200 ±.002	14.737 ±.002	116°50′ ±1′

Lattice constants

Density

(calculated) 1.544 g/cm³ at 25° C.

Reference intensity

 $I/I_{conundum} = 2.0$

References

Reimann, C.W., A.D. Mighell, and F.A.Mauer (1967). The crystal and molecular structure of tetrakispyrazole-nickel chloride Ni(C₃H₄ N₂)₄ Cl₂, Acta Cryst. 23, 135-141.

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	I	hkl	20(°)
7.30	70	Ī11	12.12
6.58	20	002	13.45
6.10	12	200	14.52
6.03	9	202	14.69
5.78	40	111	15.32
4.60	5	020	19.30
4.348	4	112,021	20.41
4.314	6	113	20.57
4.035	5	311	22.01
3.813	14	221	23.31
3.770 3.663 3.413 3.245 3.201	8 100 6 1	022 204,222 402 311 314	23.58 24.28 26.09 27.46 27.85
3.171	1	023	28.12
3.046	3	400	29.30
3.015	2	404	29.60
2.888	4	222	30.94
2.830	4	132	31.59
2.781	5	312	32.16
2.741	6	422	32.64
2.722	2	115	32.88
2.690	2	421	33.28
2.674	6	024	33.49
2.609	5	512 513,132 331 424,511 206	34.34
2.603	8		34.42
2.534	19		35.40
2.520	14		35.59
2.444	10		36.75
2.439	5	333	36.82
2.389	4	313	37.62
2.384	5	402	37.70
2.352	9	406	38.23
2.346	10	133	38.34
2.337	9	421,134	38.49
2.311	3	425	38.94
2.296	4	331	39.20
2.239	2	604	40.25
2.173	3	224	41.52
2.159	3	226	41.81
2.150	3	240,242	41.98
2.094	2	134,426	43.16
2.054	3	317	44.06
2.033	6	533	44.52

The sample was made at NBS by J. S. Waring, by heating a mixture of Gd_2O_3 and TiO_2 at 1550 °C for 16 hours.

Color

Colorless

Structure

Orthorhombic, Pnam(62) or $Pna2_1$ (33) Z=4, isostructural with $Y_2 TiO_5$ [Mumme and Wadsley, 1968]. The structure of $Y_2 TiO_5$ was determined by Mumme and Wadsley [1968].

Lattice constants

	a(Å)	b(Å)	c(Å)
Mumme and Wadsley [1968] NBS, sample at	10.48	11.33	3.76
25 °C	10.4788 ±.0004	11.328 ±.001	3.7547 ±.0002

Density

(calculated) 6.593 g/cm³ at 25° C.

Polymorphism

 Gd_2TiO_5 undergoes a reversible phase transition at 1712°C [Waring and Schneider,1965]. The structure above that temperature has not been determined.

Additional patterns

- 1. PDF card 16-393 [Queyroux, Laboratoire de Vitry du C.N.R.S.]
- PDF card 18-528 [Waring and Schneider, 1965]
- *Intensity values were obtained from the spacing pattern and may be subject to preferred orientation.

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C				
d(A)	I *	hkl	20(°)	
7.69	15	110	11.50	
5.65	2	020	15.66	
5.24	6	200	16.92	
4.98	8	120	17.81	
4.754	10	210	18.65	
3.849	3	220	23.09	
3.553	20	130	25.04	
3.376	5	111	26.38	
3.337	2	310	26.69	
3.063	90	230	29.13	
3.053	100	201	29.23	
2.999	4	121	29.77	
2.971	10	320	30.05	
2.945	10	211	30.32	
2.832	2	040	31.57	
2.736	2	140	32.70	
2.661	15	031	33.65	
2.619	10	400	34.21	
2.579	6	131	34.75	
2.562	6	330	34.99	
2.552	4	410	35.13	
2.495	4	311	35.97	
2.331	10	321	38.59	
2.214	5	150	40.72	
2.151	1	430	41.97	
2.118	12	331	42.66	
2.110	8	411	42.82	
2.076	4	241	43.55	
2.062	2	510	43.88	
2.009	8	421	45.08	
1.965	3	520	46.16	
1.924	4	440	47.21	
1.908	3	151	47.62	
1.898	4	341	47.88	
1.889	4	060	48.14	
1.878	15	002	48.43	
1.867	20	431	48.73	
1.859	3	160	48.97	
1.833	<1	530	49.70	
1.8068	3	511	50.47	
1.7453	2	600,212	52.38	
1.7416	4	521	52.50	
1.7257	1	610	53.02	
1.7117	1	441	53.49	
1.6958	2	351	54.03	

	-			
Internal standard W, a = 3.16516 Å				
$CuKa_1 \lambda = 1.54056 A; temp. 25 C$				
d (Å)	I *	hkl	20(°)	
1.6843	1	540	54.43	
1.6687	4	620	54.98	
1.6654	8	161	55.10	
1.6607	7	360,132	55.27	
1.6472	2	531	55.76	
1.6364	<1	312	56.16	
1.6053	5	261	57.35	
1.6009	15	232,170	57.52	
1.5838	12	601	58.20	
1.5684	3	611	58.83	
1.5382 1.5261 1.5188 1.5152 1.4863	3 5 5 2	550 402,621 361 332 640,071	60.10 60.63 60.95 61.11 62.43	
1.4837	2	710	62.55	
1.4473	1	720	64.31	
1.4320	1	152	65.08	
1.4030	1	180,560	66.60	
1.3917	1	730	67.21	
1.3879	1 .	512	67.42	
1.3827	1	650,641	67.71	
1.3577	<1	522	69.13	
1.3434	2	442	69.97	
1.3312	2	062	70.71	
1.3203	4	162	71.38	
1.3140	2	181,561	71.78	
1.3100	1	800	72.03	
1.3013	<1	810	72.59	
1.2705	<1	612	74.64	
1.2539	1	542	75.80	
1.2497	2	190	76.10	
1.2472	2	622	76.28	
1.2438	1	013,362	76.53	
1.2349	<1	113	77.18	
1.2293 1.2176 1.2111 1.1931 1.1880	1 4 1 3	811 172,203 632 272,091 033	77.60 78.49 78.99 80.42 80.84	
1.1852	5	751	81.07	
1.1753	1	831	81.90	
1.1645	2	712	82.82	
1.1462	<1	722	84.45	
1.1405	<1	920	84.97	

*Intensity values were obtained from the spacing pattern and may be subject to preferred orientation.

- Mumme, W. G., and A. D. Wadsley (1968). The structure of orthorhombic Y₂TiO₅, an example of mixed seven and fivefold coordination, Acta Cryst. B24, 1327-1333.
- Waring, J. L., and S. J. Schneider (1965). Phase equilibrium relationships in the system Gd₂O₃-TiO₂, J.Res.NBS 69A,255-61.

The sample was prepared by Alvin Perloff at NBS, from Ga_2O_3 dissolved in dilute $H_3 \ PO_4$. This solution was then layered with water slightly alkaline with NH₄OH.

Color

Colorless

Optical data

Biaxial, $N_{\alpha}=1.605$, $N_{\gamma}=1.610$

Structure

Monoclinic, $P2_1/n$ (14), Z=8. The structure of $GaPO_4 \cdot 2H_2O$ was determined by Mooney-Slater [1966].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Mooney- Slater [1966] NBS,	9.77	9.64	9.68	102°42′
at 25 °C	9.754 ±.001	9.639 ±.001	9.690 ±.002	102°52′ ±1′

Density

(calculated) 3.002 g/cm³ at 25° C.

References

Mooney-Slater, R.C.L. (1966). The crystal structure of hydrated gallium phosphate of composition GaPO₄ · 2H₂O, Acta Cryst. 20, 526-534.

Internal standard Ag, a = 4.08641 Å				
d (Å)	I - 1.0	hkl	20(°)	
7.60	50	101	11.64	
6.76	95	110,011	13.09	
6.06	65	101	14.61	
5.97	100	111	14.83	
5.13	<1	111	17.28	
4.75	25	200	18.67	
4.298	18	120,021	20.65	
4.265	20	210	20.81	
4.241	14	012	20.93	
4.198	18	112	21.15	
4.072	20	$ \begin{array}{r} 121 \\ 202 \\ 121 \\ 112 \\ $	21.81	
3.800	5		23.39	
3.775	4		23.55	
3.614	13		24.61	
3.382	8		26.33	
3.359	12	221	26.51	
3.229	2	301	27.60	
3.209	6	103	27.78	
3.061	35	311	29.15	
3.035	45	221,122	29.40	
3.009	15	310	29.66	
2.984	35	222	29.92	
2.959	30	I31	30.18	
2.891	30	212	30.91	
2.838	14	I31	31.50	
2.820 2.707 2.684 2.673 2.663	45 8 16 14	312,301 311 321 123 230	31.70 33.06 33.36 33.50 33.62	
2.647	14	320, 132	33.83	
2.564	15	222	34.96	
2.534	10	303	35.39	
2.514	4	223	35.69	
2.479	7	132	36.20	
2.453	5	232,313	36.61	
2.434	8	321	36.89	
2.426	12	123	37.02	
2.409	6	040	37.30	
2.378	6	400	37.80	
2.336	11	140,041	38.51	
2.321	4	213	38.76	
2.296	3	141	39.20	
2.278	3	331,412	39.52	
2.249	6	030	40.05	

Internal standard Ag, a = 4.08641 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C				
d (Å)	I	hkl	20(°)	
2.205	1	232	40.89	
2.175	4	421,332	41.48	
2.148	4	240,042	42.03	
2.138	8	411	42.23	
2.121	1	024,331	42.60	
2.108	3	422	42.87	
2.089	4	413	43.28	
2.084	5	314	43.39	
2.050	3	241,142	44.13	
2.036	1	242	44.46	
2.020	1	303	44.82	
1.996	2	421	45.40	
1.990	8	333	45.54	
1.978	9	313	45.84	
1.955	8	423,402	46.40	
1.942	1	431	46.75	
1.931	2	341	47.01	
1.927	5	143	47.11	
1.918	9	233,340	47.35	
1.911	9	511,430+	47.53	
1.901	6	404,115	47.81	
1.887	7	234,242	48.18	
1.881	6	512	48.34	
1.866	4	510,243+	48.77	
1.833	4	341	49.71	
1.807	11	521,224	50.45	
1.787	8	250	51.07	
1.784	8	513,052+	51.16	
1.779	7	105,315+	51.31	
1.769	4	520,424	5,1.64	
1.7587	3	$\begin{array}{r} 025,511\\ \overline{3}43\\ 251,152\\ \overline{4}41\\ 413,\overline{3}25 \end{array}$	51.95	
1.7462	3		52.35	
1.7278	2		52.95	
1.7140	1		53.41	
1.6944	10		54.08	
1.6761	4	521,244	54.72	
1.6549	6	351	55.48	
1.6475	7	532,350+	55.75	
1.6356	4	530,434	56.19	
1.6211	6	441,423	56.74	
1.6148	4	602,352	56.98	
1.5997	1	611,443	57.57	
1.5841	10	600,160+	58.19	
1.5633	5	610,531	59.04	
1.5547	10	522,016	59.40	

This compound was obtained from Pfaltz and Bauer Inc., Flushing, N.Y. The sample was recrystallized from an aqueous solution.

Color

Colorless

Optical data

Uniaxial (+) $N_0 = 1.602$, $N_e = 1.695$

Structure

Hexagonal, $R\overline{3}$ (148) Z=9, structure determined by Rosenzweig and Cromer [1959].

Lattice constants

	a(Å)	c(Å)
Staritzky and Ellinger [1956] NBS, sample at 25 °C	7.28 7.3026 ±.0004	26.36 26.357 ±.002
Density		

(calculated) 3.537 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 4.2$

Additional patterns

1.PDF card 9-370. [Staritzky and Ellinger
1956]

Internal standard W, a = 3.16504 Å CuK a_1 λ = 1.5405 Å; temp. 25 °C				
d (Å)	Ι	hkl	20(°)	
8.790	100	003	10.08	
6.146	40	101	14.40	
5.705	25	012	15.52	
4.565	18	104	19.43	
4.390	55	006	20.21	
4.053	14	015	21.91	
3.655	5	110	24.33	
3.373	45	113	26.40	
3.236	5	107	27.54	
3.141	65	021	28.39	
3.076	55	202	29.00	
2.928	19	009	30.50	
2.920	10	018	30.59	
2.850	30	024	31.36	
2.710	20	205	33.03	
2.433	9	1.0.10	36.92	
2.422	20	027	37.09	
2.380	5	211	37.77	
2.351	5	122	38.25	
2.282	30	119,208	39.45	
2.248	4	214	40.08	
2.242	7	0·1·11	40.19	
2.196	10	0·0·12	41.07	
2.177	5	125	41.45	
2.050	8	303	44.13	
2.025	10	$ \begin{array}{c} 0 \cdot 2 \cdot 10 \\ 217 \\ 128 \\ 2 \cdot 0 \cdot 11 \\ 1 \cdot 1 \cdot 12 \\ \end{array} $	44.71	
2.018	7		44.88	
1.934	3		46.94	
1.910	8		47.57	
1.881	2		48.34	
1.825	7	220	49.92	
1.804	2	0·1·14	50.56	
1.788	8	223	51.05	
1.771	3	2·1·10	51.57	
1.757	3	0·0·15	51.99	
1.750	3	131	52.22	
1.738	2	312	52.62	
1.711	4	309	53.52	
1.706	4	0·2·13	53.68	
1.694	3	134	54.09	

Internal standard W, a = 3.16504 Å CuK α_1 λ = 1.5405 Å; temp. 25 °C				
d (Å)	Ι	hkl	20(°)	
1.691 1.6857 1.6643 1.6177 1.5903	5 14 2 7 2	1.2.11 226 315 2.0.14 137	54.18 54.38 55.14 56.87 57.94	
1.5786 1.5698 1.5495 1.5375 1.5143	4 3 3 2	401 042 229 404 045	58.41 58.77 59.62 60.13 61.15	
1.5059 1.4646 1.4611 1.4577 1.4258	2 3 5 4 2	0·1·17 0·0·18 0·2·16,1·3·10 407 048	61.53 63.46 63.63 63.80 65.40	
1.4160 1.4039 1.3798 1.3634 1.3553	2 6 1 2 3	$3 \cdot 1 \cdot 11 \\ 2 \cdot 2 \cdot 12 \\ 410 \\ 413 \\ 4 \cdot 0 \cdot 10, 1 \cdot 0 \cdot 9$	65.91 66.55 67.87 68.80 69.27	
1.3197	2	0•4•11	71.42	

References

Staritzky, E., and F. H. Ellinger (1956). Potassium gold dicyanide,KAu(CN)₂, Anal. Chem. (Crystallographic Data) 28, 420-1.

Rosenzweig, A., and D.T. Cromer (1959). The crystal structure of KAu(CN)₂, Acta Cryst. 12, 709-12.

The sample was obtained from Fisher Scientific Co., New York, N.Y. The sample was recrystallized and maintained in a moist atmosphere.

Color

Pale bluish green

Optical data

Biaxial, N_{α} =1.471, N_{β} =1.478, N_{γ} =1.484 2V is very large.

Structure

Monoclinic, $P2_1/c$ (14), Z=4 [Ness, 1940], structure determined by Baur [1964].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Leonard & Ness [1947]* Keating	15.33	6.50	20.08	104.26°
[1953] Baur	14.11	6.51	11.02	105°15'
[1964] NBS,	14.072	6.503	11.041	105°34'
at 25 °C	14.077 ±.002	6.509 ±.001	11.054 ±.001	105°36' ±1'

*as published

Density

(calculated) 1.893 g/cm³ at 25° C.

Polymorphism

The mineral,tauriscite,has been reported as an orthorhombic polymorph, but its composition has been questioned [Palache et al. 1944].

Internal standard W, a = 3.16516 Å			
Cuk 	$a_1 \land = 1$	hkl	2ê(o)
6.79	8	200	13.03
5.88	<2	110	15.06
5.56	8	011	15.94
5.49	11	102	16.14
5.41	3	111	16.36
5.33	7	002	16.62
4.90	100	111	18.10
4.87	50	202	18.19
4.56	9	102	19.44
4.20	<2	112	21.15
4.028	14	$211 \\ 311 \\ 112,202 \\ 400 \\ 402,311$	22.05
3.776	60		23.54
3.732	20		23.82
3.393	8		26.24
3.291	15		27.07
3.256	5	020	27.37
3.209	11	I13	27.78
3.125	7	213	28.54
3.117	6	013,021	28.61
3.084	3	I21	28.93
3.062	5	302	29.14
3.009	6	410	29.66
2.980	<2	121	29.96
2.937	4	412,220	30.41
2.905	<2	313	30.75
2.799	9	I22	31.95
2.772	7	312	32.27
2.757	8	I04	32.45
2.731	10	502,411	32.77
2.704	<2	222	33.10
2.665	3	321,004	33.60
2.649	7	122	33.81
2.643	9	320	33.89
2.625	8	413,304	34.13
2.564	<2	402	34.97
2.531	3	322	35.43
2.527	3	214	35.50
2.488	4	104	36.07
2.475	3	321	36.26
2.453	2	222	36.60

Internal standard W, a = 3.16516 Å						
	$\frac{d(\mathring{A})}{I} \qquad I \qquad hkl \qquad 2\theta(\circ)$					
2.434	5	$ \overline{404}, \overline{314} $ 023 420 513 422,511	36.90			
2.399	4		37.46			
2.346	2		38.33			
2.336	2		38.50			
2.314	11		38.89			
2.277	2	204	39.54			
2.190	<2	502	41.19			
2.181	5	612	41.36			
2.149	<2	423,214	42.00			
2.117	<2	131	42.67			
2.096	<2	$ \frac{\overline{2}24}{\overline{1}15} 413,304 \overline{3}15 015 $	43.12			
2.081	7		43.44			
2.063	2		43.84			
2.054	2		44.06			
2.023	5		44.76			
2.014	7	422	44.97			
1.999	<2	231,611	45.33			
1.977	<2	124,323	45.86			
1.964	9	331	46.18			
1.951	8	424	46.51			
1.931	6	115	47.03			
1.913	5	711,712	47.50			
1.885	10	331	48.23			
1.865	10	224,404	48.79			
1.856	8	710,620	49.05			
1.841	5	206,513	49.48			
1.826	2	306,430+	49.89			
1.820	<2	125	50.08			
1.804	2	333	50.55			
1.800	3	133,325	50.66			
1.780	<2	406	51.28			
1.775	<2	006	51.44			
1.758	<2	431,802	51.96			
1.753	5	711	52.12			
1.710	2	506,624	53.55			
1.692	3	315	54.15			

Additional patterns

- 1. Keating and Berry [1953]
- PDF card 1 255 [Hanawalt, Rinn, and Frevel, 1938]

References

- Baur, W.H. (1964). On the crystal chemistry of salt hydrates. III. The determination of the crystal structure of FeSO₄. 7H₂O (melanterite). Acta Cryst. 17,1167-1174.
- 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.

Keating, L.F. and L.G. Berry (1953). Pisanite from Flin Flon, Manitoba, Am. Mineralogist 38, Nos. 5&6, 501 - 505.

Leonard, J. and I. Ness (1947)or(1950). Strukturvorschlag fur FeSO₄ • 7H₂O, Fortschr. Mineral. 26, 83 - 85.

Ness, I. (1940). Zum Gitterbau des monoklinen FeSO₄ ·7H₂O (Eisenvitriol, Melanterit), Naturwissenschaften 28, 78.

Palache,C.,H. Berman and C. Frondel(1944). Dana's System of Mineralogy (John Wiley & Sons, New York, 7th Ed.), II, 519.

Sample The sample was obtained from Pfaltz and Bauer, Inc. Flushing, N.Y. The material	Inte CuK	Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
tion at room temperature.	d (\mathring{A})	Ι	hkl	2∂(°)	
Color Colorless	8.71 6.70 6.389 5.985	25 100 45 60	100 110 001 011	10.15 13.20 13.85 14.79	
Optical data	5.749	40	ĪOl	15.40	
Biaxial (-) N_{α} =1.458, N_{β} =1.552, N_{γ} =1.593 2V is small Structure	5.443 5.254 5.046 4.714	40 40 40 95	Ī11 020 0Ī1 ĪĪ1,101	16.27 16.86 17.56 18.81	
Triclinic, Pl (2),Z=2 [Iveronova et al., 1955].	4.500	35	021,120	19.71	
	4.362 4.035 4.006 3.894 3.787	55 18 20 14 14	200 210 201 211 121	20.34 22.01 22.17 22.82 23.47	
	3.728 3.591 3.508 3.383 3.355	5 4 4 20 20	021 121 030 221 031,220	23.85 24.77 25.37 26.32 26.55	
	3.256 3.232 3.191 3.062 3.021	35 25 10 14 13	Ī12,130 012 002 2Ī1 131,221	27.37 27.58 27.94 29.14 29.54	
Density (calculated) 2.358 g/cm ³ at 25° C.	3.013 2.993 2.928	16 20 25	122 022 112	29.62 29.83 30.51	
Reference intensity I/I _{corundum} = 1.3	2.906	30 8	300,0Ī2 202	30.74 31.11	

Lattice constants

	$a(\stackrel{\circ}{A})$	b(Å)	$c(\stackrel{\circ}{A})$	a(°)	β(°)) (°)
Iveronova et al. [1955] NBS, sample at 25 °C	8.914* 8.924 ±.001	10.699* 10.711 ±.002	6.646* 6.650 ±.001	78°54′ 78°53′ ±1′	102°6′ 102°5′ ±1′	92°30′ 92°2′ ±1′

* from kX

Lanthanum Nitrate Hydrate	La(NO ₃) 3.6H 20	(triclinic) — co	ntinued
---------------------------	------------------------------	------------------	---------

Internal standard W, a = 3.16516 Å			
$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. } 25 \text{ °C}$			
d (Å)	Ι	hkl	28(°)
2.849	20	031	31.37
2.843	20	112	31.44
2.805	13	310,231	31.88
2.797	8	310	31.97
2.722	13	311,222	32.88
2.677	8	122,221	33.45
2.660	25	212	33.66
2.626	19	040	34.12
2.617	25	321	34.24
2.612	20	112,041	34.30
2.557	14	$ \begin{bmatrix} \overline{1}41 \\ \overline{122}, \overline{320} \\ 231 \\ \overline{231} \\ 301 $	35.07
2.539	12		35.32
2.533	17		35.41
2.501	13		35.88
2.462	14		36.47
2.447 2.431 2.411 2.362 2.355	11 10 10 9	141,321 232 302 222 311,202	36.70 36.94 37.26 38.07 38.18
2.323	16	122,241	38.73
2.318	20	331,322	38.82
2.299	25	321	39.16
2.288	30	231	39.35
2.274	12	222	39.60
2.254	20	142,240	39.96
2.231	7	330,212	40.39
2.214	8	113	40.71
2.208	11	401	40.83
2.188	11	411	41.22

Internal standard W, a = $3.16516 \stackrel{\circ}{A}$			
СиК	$a_1 \lambda = 1$.54056 Å; temp. 2	25 °C
d (Å)	Ι	hkl	2. (*)
2.173	9	132,103	41.53
2.167	18	141,321,+	41.65
2.139	14	410	42.22
2.133	20	410	42.33
2.129	19	332,003	42.43
2.118	17	051,023	42.66
2.105	7	142	42.92
2.091	14	203,241,+	43.24
2.078	10	223	43.51
2.060	7	232	43.92
2.043	15	222	44.30
2.011	6	412,420	45.04
2.008	9	113	45.12
2.004	10	402	45.20
1.994	5	033,421	45.46
1.982	6	213	45.73
1.967	4	123,312	46.12
1.960	9	233,241	46.28
1.947	7	401,340,+	46.62
1.933	8	052	46.98
1.929 1.915 1.890 1.884 1.868	5 5 9 9	412 342 250 312,123 133,341,+	47.07 47.44 48.11 48.26 48.71

References

Iveronova, V.I., V.P. Tarosova, Z.K. Zolina, G. V. Markhasin and I. M. Sukhodreva (1955). Structures of nitrates of rareearth elements, Zh. Fiz. Khim. 29, 314 -315.

The sample was reagent grade, obtained from Baker and Adamson, General Chemical Division, Allied Chemical and Dye Corp., New York, N.Y.

Color

Colorless

Optical data

Biaxial (-) $N_{\rm C}{=}1.430$, $N_{\rm \beta}{=}1.567$, $N_{\rm \gamma}{=}1.570$, 2V is medium.

Structure

Monoclinic, C2/c (15), Z=4, structure determined by Zemann [1957].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)	
Zemann [1957] NBS,	8.39	5.00	6.21	114.5°	
sample at 25 °C	8.359 ±.001	4.9767 ±.0004	6.194 ±.001	114°43′ ±1'	
Density (calculated) 2.096 g/cm ³ at 25° C.					
Reference I/I _{corundu}	intensity _{m =} 0.9				
Additional 1. PDF ca	patterns ard 9-359),[Zemanr	n, 1957].		
References Zemann, J.(1957). Die Kristallstruktur von Li ₂ CO ₃ , Acta Cryst. 10, 664-666.					

Intern	Internal standard Ag, a = 4.08641 Å			
CuK a	CuKa ₁ λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)	
4.164	85	110	21.32	
3.797	19	200	23.41	
3.029	25	111	29.46	
2.918	80	202	30.61	
2.812	100	002	31.80	
2.627	30	ī12	34.10	
2.488	18	020	36.07	
2.431	40	311	36.95	
2.276	20	021	39.57	
2.256	12	310	39.92	
2.116	4	112,221	42.69	
2.081	7	220	43.44	
2.012	2	402	45.02	
1.910	2	202	47.56	
1.893	2	222	48.02	
1.867	17	311	48.74	
1.8205	1	221	50.06	
1.8121	4	313	50.31	
1.6208	4	130	56.75	
1.5959	7	421,131	57.72	
1.5858	2		58.12	
1.5804	4		58.34	
1.5723	4		58.67	
1.5652	8		58.96	
1.5469	10		59.73	
1.5154	6	222	61.10	
1.5092	5	420	61.38	
1.4980	1	023	61.89	
1.4669	4	513	63.35	
1.4622	3	132	63.58	
1.4359	1	114	64.88	
1.4250	5	331	65.44	
1.4066	<1	004	66.41	
1.3923	2	602	67.18	
1.3879	1	330	67.42	
1.3754 1.3529 1.3497 1.3361 1.3132	1 	332 132 421 402 224	68.12 69.41 69.60 70.41 71.83	
1.3042	<1	514	72.40	
1.2872	1	511	73.51	
1.2842	3	133	73.71	
1.2807	3	331	73.95	
1.2655	3	600	74.99	

The sample was prepared by dehydrating MnCl₂ \cdot 4H₂O in vacuum above 650 °C.

Color

Unground: deep pink Ground: light pink

Optical data

Uniaxial(-) $N_0 = 1.708$, $N_e = 1.622$

Structure

Hexagonal, $R\overline{3}m$ (166), Z=3, isostructural with CdCl₂ and NiCl₂ [Ferrari et al., 1963]. The structure of CdCl₂ was determined by Pauling and Hoard [1930].

Lattice constants

	a(Å)	c(Å)
Ferrari et al. [1963] NBS, sample at 25 °C	3.711 3.7061 ±.0004	17.59 17.569 ±.001

Density

(calculated) 3.000 g/cm^3 at 25° C.

Additional patterns

- 1. Ferrari et al. [1929]
- 2. PDF card 1-0172 [Hanawalt et al., 1938]

$V_{\rm rescaled} = 16516$			
Internal standard w, $a = 3.10510 \text{ A}$			
CuK	$a_1 \lambda = 1.$	54056 A; temp. 25	5 °C
d (Å)	Ι	hkl	20(°)
5.85	100	003	15.14
3.161	25	101	28.21
3.013	4	012	29.62
2.929	6	006	30.49
2.592	80	104	34.58
2.371	8	015	37.91
1.977	11	107	45.85
1.9521	2	009	46.48
1.8529	25	110	49.13
1.8118	25	018	50.32
1 7660	1.0	110	c]]]
L.7663	13	113	51.71
1.5074		024	61.46
1.4638	TO	0.0.12	63.50
1.4299	5	0.1.11	65.19
1.2959	6	208	12.94
1,1713	6	0.0.15	82.24
1,1488	8	$1 \cdot 1 \cdot 12$	84.21
1.0617	3	128	93.02
1.0390	3	1.0.16	95.70

- Ferrari,A.,A. Celeri and F. Giorgi (1929). Sulla importanza della forma cristallina nella formazione di soluzioni solide. V. Analisi termica e röntgenografica dei sistemi CoCl₂-FeCl₂ e MnCl₂-FeCl₂ anidri. Atti reale accad. naz. Lincei [6] 9, 782 - 789.
- Ferrari, A., A. Braibanti and G. Bigliardi (1963). Refinement of the crystal structure of NiCl₂ and of unit-cell parameters of some anhydrous chlorides of divalent metals, Acta Cryst. 16, 846 -847.
- 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.
- Pauling, L., and J. L. Hoard (1930). The crystal structure of cadmium chloride, Z. Krist 74, 546 - 551.

The sample was prepared by C. W. Reimann at NBS by evaporating an aqueous solution of NiCl₂ and pyrazole at room temperature.

Color

Unground: deep blue Ground: light greenish blue

Optical data

Biaxial, $N_{\rm C}{=}1.636$, $N_{\rm \beta}{=}1.654$, $N_{\rm \gamma}{=}1.670$ 2V is large.

Structure

Monoclinic, C2/c (15), Z=4, structure determined by Reimann et al.[1967].

	a(Å)	b (Å)	c(Å)	β(°)
Reimann et al. [1967] NBS,	13.876	9.263	14.451	116°50'
sample at 25°C	13.878 ±.002	9.261 ±.002	14.435 ±.003	116°52′ ±1′

Lattice constants

Density

(calculated) 1.613 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 1.9$

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
7.40	100	110	11.95
6.43	16	002	13.75
6.18	14	200	14.31
6.02	18	202	14.70
5.78	8	111	15.33
5.679	30	112	15.59
4.624	8	020	19.18
4.362	5	021	20.34
4.320	8	112	20.54
4.249	5	113	20.89
4.103	3	$ \begin{array}{r} 3 \\ 3 \\ 1 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2$	21.64
4.066	7		21.84
3.849	18		23.09
3.762	10		23.63
3.703	70		24.01
3.670	45	222	24.23
3.597	10	204	24.73
3.466	9	402	25.68
3.346	4	113	26.62
3.270	5	311	27.25
3.181	3	314	28.03
3.149	5	023	28.32
3.010	4	404	29.65
2.992	3	130,Ī31	29.84
2.891	2	222	30.90
2.839 2.788 2.708 2.637 2.593	4 5 6 4	224,I32 312 315 513 I33	31.49 32.08 33.05 33.97 34.56
2.572	7	$ \begin{array}{r} 420 \\ \overline{3}32 \\ \overline{4}24 \\ 223 \\ \overline{2}25, \overline{3}33 \end{array} $	34.85
2.550	16		35.17
2.524	7		35.54
2.491	3		36.02
2.448	6		36.68

Internal standard W, a = 3.16516 Å				
CuK	$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. 25 °C}$			
d (Å)	I	hkl	20(°)	
2.440	6	204	36.81	
2.398	8	402	37.48	
2.359	10	421	38.11	
2.324	8	134,316,+	38.72	
2.281	6	334,041	39.48	
2.261	3	604	39.83	
2.161	5	242	41.76	
2.124	4	332,226,+	42.52	
2.077	5	426	43.54	
2.064	6	600,314	43.82	
2.034 1.996 1.979 1.948 1.928	7 4 4 6	624 534 512 026,244 333,714,+	44.51 45.40 45.81 46.58 47.09	
1.886	3	620	48.22	
1.880	2	044	48.37	
1.857	4	135	49.01	
1.853	4	440,404	49.13	
1.833	4	711,150	49.70	
1.796	3	716	50.80	
1.763	4	208,621	51.80	
1.736	3	710	52.67	
1.732	2	152	52.82	
1.714	2	337,352	53.42	
1.689	3	802	54.28	
1.677	3	428	54.69	
1.672	4	226	54.87	
1.662	4	246	55.21	

References

Reimann, C.W., A.D. Mighell, and F.A.Mauer (1967). The crystal and molecular structure of tetrakispyrazole-nickel chloride Ni $(C_3 H_4 N_2)_4 Cl_2$, Acta Cryst. 23, 135-141.

The sample was prepared from a 1:1 molar mixture of KBr and KCl by melting, quenching, and annealing at 600 $^\circ C$ for 3 days.

Color

Colorless

Optical data

Isotropic, N=1.528

Structure

Cubic, Fm3m (225), NaCl type, Z=4. This l:l composition is the midpoint in the complete solid solution series between KBr and KCl.

Lattice constants

	a(Å)
NBS, sample at 25 °C	6.4484 ±.0002

Internal standard W, a = 3.16504 Å CuKa, $\lambda = 1.5405$ Å; temp. 25 °C			
	α1 · · · · ·	10100 m, compt =0	C
d (Å)	Ι	hkl	20(°)
3.723	7	111	23.88
3.226	100	200	27.63
2.281	55	220	39.47
1.945	2	311	46.67
1.861	16	222	48.90
1.612	7	400	57.10
1.480	1	331	62.73
1.4417	14	420	64.59
1.3160	8	422	71.65
1.2412	1	511	76.72
1.1402	2	440	85.00
1.0748	4	600	91.56
1.0198	2	620	98.10
0.9722	1	622	104.81
.8942	1	640	118.96
.8617	3	642	126.74

Density

(calculated) 2.397 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 5.9$

The sample was prepared by the reaction of a 1:2 molar mixture of K_2CO_3 and $CdCO_3$ with HF. This product was dried and heated at 700 °C in an atmosphere of nitrogen for 5 hours.

Color

Colorless

Optical data

Almost isotropic, $N \approx 1.464$

Structure

Orthorhombic, Pnma (62) Z=4, distorted perovskite, by analogy with RbCaCl₃ and other ABX₃ compounds. KCdF₃ has been reported as cubic by Brisi [1952], and as pseudocubic by Klasens et al.[1952] and by Martin et al. [1956].

Lattice constants

	a(Å)	b(Å)	c(Å)
Brisi [1952] Klasens et al.	4.293*		
[1953] Martin et al.	4.33**		
[1956] NBS, sample at	4.33**		
25 °C	6.124 ±.001	8.665 ±.001	6.104 ±.001

* as published, reported as cubic **reported as pseudocubic

Density

(calculated) 4.275 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 5.1$

References

- Brisi, C (1952). Sulla struttura cristallina dei composti KCdF₃ e KCaF₃, Ann. Chim. Rome 42, 356-60.
- Klasens, H. A., P. Zalm, and F. O. Huysman (1953). The manganese emission in ABF₃ compounds, Philips Res. Rept. 8, 441-31.
- Martin, R.L., R.S. Nyholm, and N.C. Stephenson (1956). Antiferromagnetism in complex fluorides with perovskite structure, Chem. Ind.(London) 1956, 83-85.

Internal standard W, a = 3.16504 Å CuK α_1 λ = 1.5405 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
4.331	65	020,101	20.49
3.062	100	200,121	29.14
2.733	1	102	32.74
2.609	2	031,211	34.34
2.499	2	220	35.90
2.403	2	131	37.39
2.314	1	221	38.89
2.167	25	040	41.64
2.162	35	202	41.75
2.100	1	230	43.03
1.986 1.936 1.933 1.7669 1.7638	1 } 20 30 30	231,132 141,301 222 321,042 123	45.65 46.90 46.96 51.69 51.79
1.5299	12	400,242	60.46
1.4634	1	411,152,+	63.52
1.4435	6	420,341	64.50
1.4407	7	143,303	64.64
1.3702	7	161	68.41
1.3674	8	323	68.57
1.3056	2	062,422	72.31
1.3027	2	224	72.50
1.2503	2	440	76.06
1.2474	3	044	76.27
1.2002	3	343	79.85
1.1975	2	105	80.07
1.1567	7	442,163	83.51
1.1542	6	125	83.73
1.0830	, 2	080	90.67
1.0808 1.0508 1.0485 1.0209 1.0182	2 3 4 5	404 181,460,+ 064,424 082,600 325	90.91 94.28 94.55 97.97 98.31
.9932 .9685 .9673 .9449 .9431	1 2 3 3	462 282 444 622,183 345	101.71 105.38 105.56 109.22 109.52
.9229	2	561,640	113.16
.9216	2	165	113.40

Additional patterns

1. Brisi [1952]

The sample was prepared by melting an equimolar mixture of $K_2 CO_3$ and $CaCO_3$ at about 900 °C. The sample was slightly unstable.

Color

Colorless

Optical data

Uniaxial (-) $N_0 = 1.532$, $N_e = 1.478$

Structure

Hexagonal, $P6_3$ /mmc (194), $P6_3$ mc (186) or $P\overline{6}2c$ (190), Z=2, [Mrose et al., 1967]

Lattice constants

	$a(\overset{{}_\circ}{A})$	c(Å)
Baptista and Baptista		
[1962]	5.280	13.276
Mrose et al.[1967]	5.29	13.32
NBS, sample at 25°C	5.294	13.355
	±.001	±.002

Density

(calculated) 2.441 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 1.5$

Polymorphism

At room temperature, in the presence of moisture, fairchildite converts to buet-schliite, K_2 Ca (CO₂)₂ [Mrose, 1969].

Additional patterns

- 1. PDF card 3-0504 [Dow Chemical Co.]
- 2. PDF card 6-0321 [Milton & Axelrod, 1947]
- 3. Baptista and Baptista [1962].

Internal standard Ag, a = 4.08641 Å CuKa ₁ λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
6.67	14	002	13.26
4.586	12	100	19.34
4.339	10	101	20.45
3.338	7	004	26.68
3.192	100	103	27.93
2.699	30	104	33.17
2.646	70	110	33.85
2.309	2	105	38.97
2.292	5	200	39.27
2.259	5	201	39.88
2.225	15	006	40.51
2.168	20	202	41.63
2.073	1	114	43.63
2.039	14	203	44.39
1.891	13	204	48.08
1.762	2	107	51.85
1.719	4	211	53.26
1.703	9	116	53.77
1.677	2	212	54.67
1.669	1	008	54.96
1.615	2	213	56.96
1.5966	<1	206	57.69
1.5375	2	214	60.13
1.5279	2	300	60.55
1.4667	1	207	63.36
1.4120	2	118,109	66.12
1.3234	2	220	71.19
1.2826	2	217,1.0.10	73.82
1.2597	1	306	75.39

References

- Baptista, A. and N.R. Baptista (1962). The determination of Bragg's angle from x-ray precession photographs and the applications of the expressions derived, Anais Acad. Brasil. Cienc. 34, 181-199.
- Milton, C. and J. Axelrod (1947). Fused wood-ash stones: fairchildite (n. sp.) K₂CO₃ • CaCO₃, buetschliite(n.sp.) 3K₂CO₃. 2CaCO₃ • 6H₂O and calcite, CaCO₃, their essential components, Am. Mineralogist, 32, 607-624.

Mrose, M.E., H.J. Rose, Jr., and J.W. Marinkenko, (1967). Fairchildite and buetschliite, Am. Mineralogist 52, 929. Mrose, M.E. (1969). Private communication.

The material was prepared by heating KF and CaF_2 for several hours at 900 °C, followed by grinding, and reheating at 900 °C overnight.

Color

Colorless

Optical data

Almost isotropic, N≈1.390

Structure

Orthorhombic, distorted perovskite, Pnma (62), Z=4, by analogy with NaMnF₃ and CaZrO₃. KCaF₃ has been reported as cubic [Brisi, 1952], as pseudocubic [Klasens et al., 1953] and as monoclinic [Lude-kens and Welch, 1952].

Lattice constants

	$a(\mathring{A})$	b(Å)	c(Å)
Brisi [1952]	8.742*		
Welch [1952]	8.82**	8.82**	8.82**
[1953]	4.37		
NBS, sample at 25 °C	6.209 ±.001	8.757 ±.001	6.164 ±.001
* as published ** from kX and with	n β=92°3	б ′	J
Density (calculated) 2.699 g/cm ³ at 25° C.			
Reference intensity I/I _{corundum} = 1.9			
Additional patterns 1. Brisi [1952]			
2. PDF card 3-0567 [Dow Chemical Co.]			
References			
Brisi, C. (1952). Sulla struttura cristal- lina dei composti KCdF ₃ e KCaF ₃ , Ann.			
Chim. Kome 42, 356-360. Ludekens, W.L.W. and A.J.E. Welch (1952). Reactions between metal oxides and fluo- rides: some new double - fluoride struc- tures of type ABF ₃ , Acta Cryst. 5, 841.			

Klasens, H. A., P. Zalm, and F. O. Huysman (1953). The manganese emission in ABF compounds, Philips Res. Rept. 8,441-451.

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
4.38	16	020,101	20.28
3.914	3	111,200	22.70
3.095	100	121	28.82
2.772	4	201	32.28
2.758	5	102	32.43
2.637	12	031	33.97
2.531	12	220	35.43
2.520	1	022	35.60
2.428	5	131	36.99
2.342	5	221	38.41
2.335	5	122	38.53
2.183	75	040,202	41.22
2.127	2	230	42.46
2.122	3	212	42.56
2.010	1	231	45.05
2.005	2	132	45.18
1.963	4	301	46.21
1.958	6	141,222	46.34
1.916	4	311	47.42
1.791	25	321,240	50.96
1.782	30	123	51.23
1.719	1	241,302	53.23
1.712	2	203	53.47
1.683	2	213	54.48
1.628	1	331	56.46
1.552	8	400	59.52
1.548	18	242	59.69
1.541	5	004	59.96
1.506	1	401	61.51
1.495	, 1	104	62.02
1.4810	2	251,332	62.68
1.4778	3	233	62.83
1.4615	1	341	63.61
1.4384	1	313	64.75
1.4152	1	124	65.96
1.3866	4	402	67.49
1.3847	8	161	67.60
1.3315	1	134	70.69
1.3061	2	351	72.28
1.3036	2	153	72.44
1.2269	3	440	74.88
1.260	2	044	75.35
1.1715	5	442,361	82.22
1.1685	6	163	82.48
1.1656	5	125	82.73

The sample was obtained by using the first crystals formed by evaporation of a water solution of KCl and an excess of MgCl₂.

Color

Colorless

Optical data

Biaxial(+) $\mathrm{N}_{\alpha}{=}1.468,$ $\mathrm{N}_{\beta}{=}1.47,$ $\mathrm{N}_{\gamma}{=}1.495,$ 2V is large.

Structure

Orthorhombic, Pnna (52), Z=12, structure determined by Fischer [1965].

Lattice constants

	a(Å)	b(A)	c(Å)
Leonhardt [1928]-	16.08	22.25	9.53
[1939] Fischer [1965]	16.02 16.141	22.52 22.519	9.54 9.598
NBS, sample at 25 °C	16.154 ±.003	22.508 ±.005	9.575 ±.002

Density

(calculated) 1.590 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 0.6$

Additional patterns

1. PDF card 8-75, [Armstrong et al., 1951]

Internal standard W, a = 3.16516 Å			
CuK	$a_1 \lambda = 1$.54056 Å; temp. 2	25 °C
d (Å)	Ι	hkl	20(°)
7.76 5.56 5.49 4.79 4.691	7 5 4 17 30	111 131 230 002 301	11.40 15.93 16.12 18.49 18.90
4.650 4.616 4.057 3.980 3.954	20 14 8 8 8	141 240 212 331,410 151	19.07 19.21 21.89 22.32 22.47
3.865 3.800 3.751 3.614 3.603	40 35 70 } 65 {	222 420 060 232 341	22.99 23.39 23.70 24.61 24.69
3.562 3.553 3.324 3.281 3.229	<pre>70 { 100 70 3</pre>	142 430 242 440 332	24.98 25.04 26.80 27.16 27.60
3.103 3.061 3.049 3.038 3.013	3 8 12 65 25	441,113 501,412 071 252 123	28.75 29.15 29.27 29.38 29.62
3.004 2.977 2.935 2.929 2.887	30 25 } 80 { 8	450 422 033 361 133	29.72 29.99 30.43 30.49 30.95
2.855 2.837 2.747 2.736 2.728	30 8 12 12 10	432,271 531 460,303 143 313	31.30 31.51 32.57 32.70 32.80
2.694 2.663 2.643 2.633	35 11 6 8	600 181 461 172	33.23 33.63 33.89 34.02 34.77

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C				
$d(A)$ I hkl $2\theta(\circ)$				
2.570	5	153	34.88	
2.547	5	452	35.20	
2.534	14	272,630	35.39	
2.518	2	470	35.62	
2.477	4	253	36.23	
2.426 2.399 2.393 2.346 2.324	8 25 35 20	082 182 191,372,+ 602,353 282	37.03 37.45 37.56 38.34 38.72	
2.308	10	650,480	38.99	
2.259	8	513,134	39.87	
2.242	9	701,173,+	40.19	
2.225	9	472,523	40.50	
2.215	7	363	40.70	
2.188	11	453,660	41.23	
2.173	6	533,1.10.1	41.53	
2.149	5	731,324	42.01	
2.138	25	292	42.23	
2.125	11	490,244	42.50	
2.099	6	334	43.06	
2.084	9	741,463	43.38	
2.064	4	670	43.83	
2.058	3	404,572	43.95	
2.024	5	424,623	44.74	
2.018 2.011 1.990 1.985 1.974	18 18 } 40 { 13	671,064 810 662 434,633,+ 473,2°10°2	44.89 45.04 45.55 45.67 45.94	
1.964	2	383	46.19	
1.954	1	193	46.43	
1.950	9	742,830	46.53	
1.933	11	444,643	46.98	
1.906	4	681,3 • 10 • 2,+	47.68	
1.900	10	105,840	47.84	
1.887	4	752	48.19	
1.875	20	3•11•1,0•12•0	48.50	

References

Andress, K. R., and O. Saffe (1939). Röntgenographische Untersuchung der Mischkristallreihe Karnallit – Bromkarnallit, Z. Krist. 101, 451-469.

Armstrong, G., K. C. Dunham, C. O. Harvey, P.A. Sabine, and W.F. Waters (1951). The paragenesis of sylvine, carnallite, polyhalite, and kieserite in Eskdale borings nos. 3, 4, and 6, north-east Yorkshire, Min. Mag. 29, 667-689.

- Fischer, W. (1965). Struktur des Carnallit KCl·MgCl₂·6H₂O, Deut. Mineral. Ges. Sektion für Kristallk., Marburg Program, October 1965.
- Leonhardt, J. (1928). Das Raumgitter des Carnallits, Z. Krist. 66, 506-507.

The sample was made by heating a mixture of $K_2\,CrO_4\,$ and $MgCrO_4\,$ at 510 $^\circ C$ for one half hour in nitrogen.

Color

Vivid yellow

Optical data

Isotropic, N=1.864

Structure

Cubic, $P2_1 3$ (198), Z=4, langbeinite type by analogy with langbeinite, $K_2 Mg_2 (SO_4)_3$, and similar sulfates. The structure of langbeinite was determined by Zemann and Zemann [1957].

Lattice constants

					a(Å)
NBS, sa	ample	at	25	°C	10.3684 ±.0002

Density

(calculated) 2.829 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 1.4$

Referen	ces	
7	7	222

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, K₂ Mg₂ (SO₄)₃, Acta Cryst. 10, 409-413.

Internal standard W, a = 3.16516 Å				
CuK	$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. } 25 \text{ °C}$			
d (Å)	Ι	hkl	20(°)	
5.99	9	111	14.78	
4.64	3	210	19.12	
4.23	35	211	20.96	
3.66	7	220	24.24	
3.46	9	221	25.73	
3.279	100	310	27.17	
3.127	20	311	28.52	
2.992	9	222	29.84	
2.876	25	320	31.07	
2.771	40	321	32.27	
2.592	6	400	34.57	
2.515	11	410	35.67	
2.444	2	411	36.74	
2.379	5	331	37.79	
2.319	5	420	38.80	
2.262	5	421	39.81	
2.211	6	332	40.78	
2.117	8	422	42.68	
2.075	2	430	43.60	
2.034	9	510	44.51	
1.996 1.926 1.893 1.8051 1.7778	5 5 11 3	511 420 521 522 530	45.40 47.15 48.03 50.52 51.35	
1.7524 1.7278 1.7046 1.6820 1.6394	6 6 16 4	531 600 610 611 620	52.15 52.95 53.73 54.51 56.05	
1.6193	6	621	56.81	
1.5999	6	541	57.56	
1.5631	2	622	59.05	
1.5455	9	630	59.79	
1.5290	5	631	60.50	
1.4967	3	444	61.95	
1.4812	4	632	62.67	
1.4665	3	710	63.37	
1.4376	3	640	64.79	
1.4239	3	720	65.50	

Internal standard W, a = 3.16516 Å CuKa, λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	2⊎(°)
1.4111	5	721	66.17
1.3856	3	642	67.55
1.3736	3	722	68.22
1.3510	4	731	69.58
1.3276	4	650	70.92
1.3168	4	732	71.60
1.2862	4	810	73.58
1.2761	3	811	74.26
1.2665	3	733	74.92
1.2574	3	820	75.55
1.2482	4	821	76.21
1.2391	3	653	76.87
1.2219	3	822	78.16
1.2053	3	831	79.45
1.1972	4	751	80.09
1.1815	2	832	81.38
1.1740	3	752	82.10
1.1521	2	841	83.92
1.1381	4	911	85.19
1.1311	3	842	85.84
1.0990	4	922	89.00
1.0928	4	930	89.64

The material was prepared by slow evaporation at room temperature of a 1:3 aqueous solution of K_2SO_4 and $MgSO_4$. The first crystals formed were used. The material also has the mineral name schoenite.

Color

Colorless

Optical data

Biaxial (+) ${\rm N}_{\alpha}{=}1.460$, ${\rm N}_{\beta}{=}1.462$, ${\rm N}_{\gamma}{=}1.472$ 2V is medium

Structure

Monoclinic, $P2_1/a$ (14),Z=2,structure determined by Kannan and Viswamitra[1965], isostructural with other "Tutton salts", [Tutton, 1893].

	a(Å)	b (Å)	c(Å)	β(°)
Hofmann [1931] Kannan and	9.04*	12.24*	6.095*	104°48′
Viswami- tra [1965] NBS,	9.072	12.212	6.113	104°50 ′
at 25 °C	9.096 ±.001	12.254 ±.002	6.128 ±.001	104°47′ ±1′

Lattice constants

* as published

Density

(calculated) 2.025 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 0.7$

Internal standard Ag, a = 4.08641 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
7.14	25	110	12.39
6.13	1	020	14.43
5.339	18	011	16.59
5.026	6	120	17.63
4.397	16	200	20.18
4.261	11	021	20.83
4.156	85	111	21.36
4.064	95	201	21.85
3.859	7	211	23.03
3.706	100	130	23.99
3.583	9	121	24.83
3.383	5	221	26.32
3.362	12	031	26.49
3.307	12	I31	26.94
3.164	40	201	28.18
3.063	70	211,040	29.13
2.995	20	230	29.81
2.964	60	I12,002	30.13
2.895	7	140	30.86
2.882	10	231,012	31.00
2.863 2.853 2.813 2.740 2.733	30 11 40 25 12	311 310 221,202 212 122 122	31.22 31.33 31.78 32.65 32.74
2.690	9	141	33.28
2.668	4	022	33.56
2.654	9	321	33.75
2.555	2	222,112	35.09
2.516	8	141,240	35.66
2.503	15	$ \begin{array}{r} 231\\ \overline{2}41,\overline{1}32\\ 032\\ \overline{3}31\\ 051 \end{array} $	35.85
2.446	12		36.71
2.398	10		37.47
2.388	45		37.64
2.265	8		39.77
2.248	6	Ī51,322	40.07
2.220	5	411	40.61
2.199	25	132,400	41.00
2.175	5	212	41.49
2.165	4	410,Ī42	41.68

Internal standard Ag, a = 4.08641 Å CuKa ₁ λ = 1.54056 Å; temp. 25 °C				
d (Å)	$d(A)$ I hkl $2\theta(\circ)$			
2.129	12	$ \begin{array}{r} 042 \\ \overline{3}41 \\ \overline{4}21,340 \\ \overline{2}51 \\ \overline{2}42,420 \\ \end{array} $	42.42	
2.122	11		42.56	
2.118	11		42.66	
2.098	5		43.07	
2.070	19		43.69	
2.015	2	113	44.96	
2.004	3	412,203	45.22	
1.987	3	142	45.62	
1.975	11	431,003	45.90	
1.936	8	123,430	46.89	
1.912	2	152	47.52	
1.896	4	342	47.95	
1.888	9	052,341	48.17	
1.883	9	351	48.30	
1.879	7	.350,023	48.41	
1.854 1.824 1.799 1.786 1.753	9 10 9 3	161,313 261 233,511 440 123	49.09 49.95 50.70 51.09 52.13	
1.741	8	510	52.53	
1.729	2	431	52.91	
1.717	3	170,261	53.32	

Additional patterns

 PDF card 20-839 (natural mineral) Dept. of Geology and Mineralogy, University of Oxford, England.

- Hofmann, W. (1931). Die Struktur der Tuttonschen Salze, Z. Krist. 78, 279 - 333.
- Kannan, K. K. and M. A. Viswamitra (1965). Crystal structure of magnesium potassium sulfate hexahydrate MgK₂ (SO₄)₂ • 6H₂O, Z. Krist. 122, 161-174.
- Tutton, A.E.(1893). Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_2 M(SO_4)_2 \cdot 6H_2O$, J. Chem. Soc.,63, 337-423.

The sample was prepared by H.T. Evans of U.S. Geological Survey by acidification of the metavanadate solution at temperatures of about 60-80 °C as described by Kelmers [1961].

Color

Deep orange

Optical data

Biaxial (-) $N_{\alpha}=$ 1.77, $N_{\beta}=$ 2.27, $N_{\gamma}=$ 2.34 2V= 26 $^{\circ}$ [Evans and Block, 1966]

Structure

Monoclinic, $P2_1/m$ (11), Z=2, structure determined by Evans and Block [1966].

	a(Å)	b (Å)	c(Å)	β(°)
Evans &	7.640	8.380	4.979	96°57′
Block	7.644	8.395	4.980	96°59′
NBS	±.001	±.002	±.001	±1′

Density

(calculated) 3.349 g/cm³ at 25° C.

Additional patterns

1. PDF card 14-333, [Kelmers, 1961]

- Evans, H. T. Jr., and S. Block (1966). The crystal structures of potassium and cesium trivanadates, Inorg. Chem. 5, 1808-1814.
- Kelmers, A.D. (1961). Ammonium, potassium, rubidium and cesium hexavanadates, J. Inorg. Nucl. Chem. 21, 45 - 48.

Internal standard W, a = 3.16516 Å CuK a, λ = 1.54056 Å; temp. 25 °C					
$\begin{array}{c c} \hline \\ \\ \hline \\ \\ \hline \\ \\ \hline \\ \\ \\ \\ \hline \\ \\ \\ \\ \hline \\ \\ \\ \\ \hline \\$					
7.58	45	100	11.67		
5.64	30	110	15.70		
3.795	8	200	23.42		
3.556	10	111	25.02		
3.458	30	210	25.74		
3.200 100 201,021 27.86					
2.993	14	211	29.83		

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
2.868	20	121	31.16
2.850	25	201	31.36
2.815	20	220	31.76
2.696	4	211	33.20
2.626	9	130	34.12
2.547	2	221	35.20
2.529	5	300	35.46
2.471	14	002	36.33
2.435	12	031	36.88
2.422	8	310	37.09
2.371	7	301,012	37.91
2.356	9	221	38.16
2.281	5	311,131	39.47
2.251	4	230	40.03
2.197	17	202	41.05
2.166	5	320	41.67
2.149	5	301	42.01
2.124	7	212	42.53
2.064	7	321	43.83
1.996	20	122,231	45.41
1.946	7	222	46.64
1.913	4	212,321	47.50
1.897	4	400	47.91
1.886	5	302	48.22
1.848	7	401	49.27
1.804	6	411	50.54
1.778	7	222	51.33
1.728	4	420,232	52.95
1.704	4	331,401	53.76
1.690	7	241	54.24
1.669	4	302,411	54.97
1.637	5	312	56.13
1.571	9	103,430	58.74
1.551	7	322	59.54
1.5341	9	023	60.28
1.5175 1.5028 1.4934 1.4797 1.4270	3 5 5 7	500,242 501 510 511 213,520	61.01 61.67 62.10 62.74 65.34
1.4037	7	501,412	66.56
1.3870	8	441	67.47
1.3706	5	351,133	68.39
1.3476	4	422	69.72
1.3310	5	521	70.72

The sample was made from a mixture of Rb_2CO_3 and $CaCO_3$ that was reacted with an excess of hydrofluoric acid, dried, and heated to 750 °C overnight.

Color

Colorless

Optical data

Isotropic, N=1.420

Structure

Cubic, perovskite type, Pm3m (221), Z=1 [Ludekens and Welch, 1952].

Lattice constants

	a(Å)
Ludekens and Welch [1952] Klasens el al. [1953] NBS, sample at 25 °C	4.452* 4.46 4.4560 ±.0001

* from kX

Density

(calculated) 3.426 g/cm³ at 25° C.

Reference intensity

 $I/I_{conundum} = 4.5$

0				
Internal standard Ag, $a = 4.08641$ A				
$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. } 25 \text{ °C}$				
d (Å)	I	hkl	20(°)	
4.45	5	100	19.92	
3.154	100	110	28.27	
2.572	30	111	34.85	
2.229	55	200	40.43	
1.993	2	210	45.48	
1.819	35	211	50.10	
1.576	20	220	58.51	
1.485	2	300	62.50	
1.4094	11	310	66.26	
1.3434	4	311	69.97	
1.2865	6	222	73.56	
1.2357	3	320	77.12	
1.1907	10	321	80.62	
1.1139	2	400	87.50	
1.0502	5	411	94.35	
1.0222	<1	331	97.80	
0.9964	5	420	101.26	
.9501	3	332	108.33	
.9095	4	422	115.75	
.8739	6	510	123.64	
.8576	1	511	127.85	
.8136	4	521	142.45	

References

Ludekens, W.L.W., and A.J.E. Welch (1952). Reactions between metal oxides and fluorides: Some new doublefluoride structures of type ABF₃, Acta Cryst. 5, 841. Klasens, H. A., P. Zalm and F. O. Huysman (1953). The manganese emission in ABF₃ compounds, Philips Res. Rept. 8, 441-451.

The sample was prepared by adding an aqueous solution of CoCl₂ to one of RbF. The precipitate was washed with water.

Color

Light purplish pink

Optical data

Isotropic, N=1.504

Structure

Cubic, Pm3m (221), Z=1, perovskite type [Rüdorff et al., 1959].

Lattice constants

	a(Å)
Rüdorff et al. [1959] Crocket and Haendler [1960] NBS, sample at 25 °C	4.062 4.141 4.1331 ±.0001

Density

(calculated) 4.736 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 5.8$

Internal standard W, a = 3.16504 Å				
$(1, K) = 1.5405$ Å, terms 25°				
Cur	$CuKa_1 \lambda = 1.5405 A; temp. 25 °C$			
d (Å)	Ι	hkl	20(°)	
4 1 2 2	1	100	21.49	
4.132	100	110	21.49	
2,922	100	110	30.57	
2.387	25	111	37.66	
2.067	45	200	43.77	
1.847	1	210	49.29	
1.6872	35	211	54.33	
1.4609	19	220	63.64	
1.3070	11	310	72.22	
1.2461	4	311	76.36	
1.1930	6	222	80.43	
1.1047	11	321	88.42	
1.0333	2	400	96.40	
0.9743	4	330	104.49	
.9482	1	331	108.64	
.9242	5	420	112.91	
	J			
8812	2	332	121.88	
.0012	2	332		

References

Crocket, D. S., and H. M. Haendler (1960). Synthesis of fluorometallates in methanol. Some structure relationships, J. Am. Chem. Soc. 82, 4158-62.

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

The sample was prepared by heating a 1:2 mixture of Rb_2SO_4 and $CoSO_4$ for 10 hours at 540 °C in dry nitrogen.

Color

Strong reddish purple

Optical data

Isotropic, N=1.602

Structure

Cubic, $P_{2_1}3$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The structure of langbeinite, K_2Mg_2 (SO₄)₃ was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
Gattow and Zemann [1958]	10.026 ±.007
NBS, sample at 25 °C	10.0204 ±.0002

Density

(calculated) 3.807 g/cm³ at 25° C.

Reference intensity

 $I/I_{conundum} = 3.4$

- Gattow,G. and J.Zemann(1958). Über Doppelsulfate vom Langbeinit-typ, A⁺₂B²⁺₂ (SO₄)₃, Z. Anorg. Allgem. Chem. 293, 233-240.
- Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, K₂Mg₂ (SO₄)₃, Acta Cryst. 10, 409-413.

Internal standard Ag, a = 4.08641 Å CuKa, λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
5.77	2	111	15.32
4.09	7	211	21.73
3.54	5	220	25.15
3.337	3	221	26.69
3.171	100	310	28.12
3.020	19	311	29.55
2.891	1	222	30.91
2.778	13	320	32.20
2.678	50	321	33.43
2.504	1	400	35.83
2.430	13	410	36.96
2.299	5	331	39.16
2.240	2	420	40.22
2.186	3	421	41.27
2.136	6	332	42.27
2.045	15	422	44.26
2.004	2	430	45.21
1.966	20	510	46.13
1.930	1	511	47.05
1.8607	8	520	48.91
1.8291	1	521	49.81
1.7712	1	440	51.56
1.7444	6	522	52.41
1.7182	2	530	53.27
1.6935	1	531	54.11
1.6701	1	600	54.93
1.6475	4	610	55.75
1.6256	16	611	56.57
1.5843	.4	620	58.18
1.5647	7	621	58.98
1.5462	7	541	59.76
1.5281	2	533	60.54
1.5105	1	622	61.32
1.4936	7	630	62.10
1.4772	5	631	62.86
1.4465 1.4313 1.4168 1.4030 1.3894	2 2 1 1	444 632 710 711 640	64.35 65.12 65.87 66.60 67.34

Internal standard Ag, a = 4.08641 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	I	hkl	20(°)
1.3764	2	720	68.06
1.3636	5	721	68.79
1.3389	2	642	70.24
1.3273	1	722	70.95
1.3159	2	730	71.66
1.3044	4	731	72.39
1.2829	1	650	73.80
1.2724	3	651	74.51
1.2525	1	800	75.90
1.2428	2	810	76.60
1.2336 1.2243 1.2150 1.2063 1.1976	1 1 3 2	811 733 820 821 653	77.28 77.98 78.69 79.37 80.06
1.1810	2	822	81.42
1.1728	<1	830	82.08
1.1648	4	831	82.80
1.1570	1	751	83.48
1.1493	<1	662	84.19
1.1419	1	832	84.83
1.1344	3	752	85.53
1.1134	1	841	87.55
1.1066	<1	910	88.23
1.1000	3	911	88.89
1.0933	1	842	89.59
1.0869	1	920	90.26
1.0805	2	761	90.94
1.0681	1	664	92.30
1.0622	3	922	92.97
1.0562 1.0505 1.0391 1.0336 1.0174	2 <1 1 <1	930 931 852 932 940	93.65 94.30 95.68 96.36 98.42
1.0125	1	941	99.07
1.0073	1	933	99.76

The sample was prepared at room temperature by slow evaporation of an equimolar solution of Rb_2SO_4 and $CuSO_4$.

Color

Brilliant greenish blue

Optical data

Biaxial (+) ${\rm N}_{\alpha}{=}1.488$, ${\rm N}_{\beta}{=}1.491$, ${\rm N}_{\gamma}{=}1.506$ 2V is medium

Structure

Monoclinic, $P2_1/a$ (14), Z=2. $Rb_2Cu(SO_4)_2 \cdot 6H_2O$ is a "Tutton Salt"[Tutton, 1893]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.267 ±.001	12.366 ±.002	6.228 ±.001	105° 19′ ±1′

Density

(calculated) 2.580 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 1.6$

- Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. **117**, 334-357.
- Tutton, A. E. (1893). Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_2 M(SO_4)_2 \cdot 6H_2O$, J. Chem. Soc. 63, 337-423.

Internal standard Ag, a = 4.08641 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	I	hkl	20(°)
7.24	5	110	12.21
6.18	2	020	14.31
5.21	3	111	17.00
4.47	13	200	19.86
4.31	25	021	20.58
4.20	100	111,210,+	21.12
4.149	95	201	21.40
3.928	5	211	22.62
3.745	100	130	23.74
3.625	10	121,220	24.54
3.350	18	Ī31	26.59
3.205	35	201	27.81
3.094	40	040	28.83
3.029	40	131,230	29.46
3.013	50	Ī12	29.62
2.920	12	012,311,+	30.59
2.895	15	310	30.86
2.869	25	202	31.15
2.845	25	221	31.42
2.792	6	212	32.03
2.775	20	$ \begin{array}{r} \bar{1}22 \\ 041 \\ \bar{1}41 \\ 022, \bar{3}21 \\ 320 \\ \end{array} $	32.23
2.749	4		32.54
2.723	12		32.87
2.702	12		33.13
2.683	6		33.37
2.603	6	222	34.43
2.542	7	141,240	35.28
2.531	8	231	35.44
2.480	12	132,241	36.19
2.426	45	331,032	37.03
2.301	7	401	39.11
2.288	16	322,051	39.34
2.265	5	411	39.76
2.258	9	321	39.90
2.233	15	400,202	40.35
2.224 2.197 2.163 2.155 2.123	30 3 5 10 10	$132,241410,212250,151\overline{3}41,042\overline{2}51$	40.52 41.04 41.73 41.88 42.54

Internal standard Ag, a = 4.08641 Å			
$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. } 25 \text{ °C}$			
d (Å)	Ι	hkl	20(°)
2.100	25	420,222	43.03
2.074	<2	402	43.61
2.061	2	060	43.90
2.047	5	412,113	44.21
2.039	5	203	44.39
2.009	6	$142,160,+ \\003 \\013 \\\overline{4}22,\overline{1}23 \\251$	45.09
2.002	13		45.26
1.976	<2		45.89
1.966	3		46.13
1.957	3		46.36
1.928	3	342	47.11
1.909	12	351,052,+	47.59
1.903	8	350,023	47.74
1.889	8	313	48.13
1.874	2	252	48.54
1.854	10	432,133	49.11
1.847	10	441,261,+	49.31
1.827	5	233,323	49.87
1.810	10	440,242	50.36
1.800	4	033,322	50.67
1.775	8	521,123	51.44
1.770	10	510	51.60
1.745	2	352	52.38
1.7315	3	351	52.83
1.7111	7	332	53.51
1.6895	3	531,133,+	54.25
1.6866	5	522,451	54.35
1.6730	2	262,423	54.83
1.6552	< 2	213	55.47
1.6438	6	270,171	55.89
1.6394	2	530,441	56.05
1.6256	<2	162,271	56.57
1.6131	3	532,223	57.05

The sample was furnished by Dr. Charles S. Smith of the Univ. of North Carolina. The material was grown as a single crystal by Semi-Elements, Inc., Saxonburg, Pa. Since RbF is hygroscopic, it was necessary to prepare the pattern with the sample in a dry mount.

Color

colorless

Optical data

Isotropic, N=1.396

Structure

Cubic, Fm3m (225), Z=4, NaCl type [Gold-schmidt, 1926].

Lattice constants

		a(Å)
Goldschmidt NBS, sample	[1926] at 25 °C	5.64* 5.6516 ±.0001

Internal standard W, a = 3.16516 A			
$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. } 25 \text{ °C}$			
$d(\overset{\circ}{A})$	Ι	hkl	28(°)
3.262 2.823 1.998 1.703 1.6311 1.4130 1.2967 1.2637 1.1536	65 100 25 13 6 7 11 6	111 200 220 311 222 400 331 420 422 511	27.32 31.67 45.36 53.77 56.36 66.07 72.89 75.11 83.78
0.9990 .9553 .9420 .8937 .8619 .8520 .8156 .7914 .7837	4 1 4 2 2 3 1 2 <1	440 531 600 620 533 622 444 551 640	100.90 107.47 109.72 119.07 126.69 129.39 141.60 153.48 158.73

References

Goldschmidt, V. M. (1926). Researches on the structure and properties of crystals, Skrifter Norske Videnskaps-Akad. Oslo,I: Mat.-Naturv. Kl. No. 8, 145.

Density

*as published.

(calculated) $3.844 \text{ g/cm}^3 \text{ at } 25^\circ \text{ C}$.

The sample was prepared at room temperature by slow evaporation of a 1:3 molar solution of $Rb_2\,SO_4$ and $FeSO_4$. The first crystals formed were used.

Color

Pale green

Optical data

Biaxial (+) ${\tt N}_{\alpha}{=}1.480$, ${\tt N}_{\beta}{=}1.489$, ${\tt N}_{\gamma}{=}1.501$ 2V is large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2 $Rb_2 Fe(SO_4)_2 \circ 6H_2O$ is a "Tutton Salt"[Tutton, 1893]. The structure of a "Tutton Salt", $(NH_4)_2 Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

		b (Å)	c(Å)	β(°)
NBS, sample at 25°C	9.218 ±.001	12.497 ±.002	6.256 ±.001	105°45 ′ ±1′

Density

(calculated) 2.523 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 1.7$

the second se			
Internal standard Ag, a = 4.08641 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
7.21 6.25 6.02 5.24 5.11	8 2 2 2 2 2	110 020 001 111 120	12.26 14.17 14.71 16.90 17.35
4.44	10	200	19.99
4.33	15	021	20.49
4.19	85	111,210	21.20
4.15	100	201	21.40
3.771	80	130	23.57
3.616	7	220	24.60
3.424	2	031	26.00
3.374	14	131	26.39
3.182	25	201	28.02
3.124	25	040	28.55
3.082 3.040 3.027 2.945 2.913	20 } 50 { 2 13	211 131,230 112 140 311	28.95 29.36 29.48 30.33 30.67
2.877	30	310	31.06
2.837	17	221	31.51
2.806	13	212	31.87
2.794	18	122	32.01
2.747	8	141	32.57
2.701	2	321	33.14
2.674	2	320	33.48
2.614	3	222	34.28
2.556	6	141,240	35.08
2.528	6	231	35.48
2.495	12	241,132	35.96
2.434	45	122,331	36.90
2.308	10	051	38.99
2.300	12	322	39.14
2.255	9	411	39.95
Internal standard Ag, a = 4.08641 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
---	----	-----------	-------
d (Å)	I	hkl	20(°)
2.248	8	321	40.08
2.230	25	132,241	40.42
2.178	7	151,250	41.43
2.168	9	042	41.62
2.142	6	251	42.16
2.117	11	242	42.67
2.089	11	420	43.27
2.049	4	203	44.16
2.008	10	431,003	45.12
1.967	5	251	46.12
1.938	3	342	46.84
1.923	10	052	47.23
1.912	5	023	47.52
1.897	7	313,411	47.91
1.863	13	133,261	48.85
1.835	2	323,421	49.64
1.824	3	511	49.96
1.8088	10	440,033	50.41
1.7922	1	322	50.91
1.7756	4	123	51.42
1.7575	6	352,510	51.99
1.7437	3	333,431,+	52.43
1.7345	5	351,512	52.73
1.7072	7	520,332	53.64
1.6923	4	133	54.15

- Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.
- Tutton, A. E. (1893). Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_{2}M(SO_{4})_{2} \cdot 6H_{2}O$, J. Chem. Soc. 63, 337-423.

The sample was made by heating a 1:2 mixture of $Rb_{2}\,CrO_{4}$ and $MgCrO_{4}$ at 500 $^{\circ}C$ for 45 minutes in nitrogen.

Color

Vivid greenish yellow

Optical data

Isotropic, N=1.885

Structure

Cubic, $P2_1 3$ (198), Z=4, langbeinite type by analogy with langbeinite, $K_2 Mg_2$ (SO₄)₃, and similar sulfates. The structure of langbeinite was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
NBS, sample at 25 °C	10.4520 ±.0002

Density

(calculated) 3.301 g/cm³ at 25° C:

Reference intensity

 $I/I_{corundum} = 3.7$

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	<i>2θ</i> (°)
6.03	3	111	14.69
4.67	7	210	18.99
4.27	11	211	20.80
3.696	2	220	24.06
3.484	7	221	25.54
3.304	100	310	26.96
3.150	20	311	28.31
3.016	4	222	29.59
2.898	30	320	30.83
2.791	45	321	32.04
2.612	3	400	34.30
2.535	19	410	35.38
2.398	9	331	37.48
2.338	5	420	38.48
2.281	6	421	39.47
2.229	6	332	40.44
2.133	9	422	42.35
2.090	3	430	43.25
2.049	15	510	44.16
2.011	4	511	45.04
1.940	7	520	46.78
1.908	3	521	47.61
1.819	8	522	50.10
1.793	3	530	50.89
1.767	4	531	51.70
1.743	3	600	52.47
1.719	8	610	53.26
1.695	19	611	54.05
1.653	5	620	55.56
1.632	11	621	56.32
1.613	7	541	57.06
1.594	3	533	57.79
1.576	2	622	58.53
1.558	8	630	59.26
1.541	5	631	59.98
1.508	3	444	61.43
1.4930	4	632	62.12
1.4784	3	710	62.80
1.4493	2	640	64.21
1.4356	2	720	64.90

Internal standard W, a = 3.16516 Å CuKa, λ = 1.54056 Å ; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
1.4223	5	721	65.58
1.3963	3	642	66.96
1.3843	2	722	67.62
1.3725	2	730	68.28
1.3606	5	731	68.96
1.3383	3	650	70.28
1.3271	4	732	70.96
1.2964	5	810	72.91
1.2862	1	811	73.58
1.2770	2	733	74.20
1.2679	2	820	74.84
1.2585	4	821	75.48
1.2496	3	653	76.11
1.2320	4	822	77.40
1.2150	5	831	78.69
1.2070	3	751	79.31
1.1913	2	832	80.57
1.1835	3	752	81.21
1.1616	2	841	83.08
1.1471	4	911	84.37
1.1403	2	842	84.99
1.1338	2	920	85.59
1.1272	3	921	86.21
1.1141	1	664	87.48
1.1080	4	922	88.09
1.1018	2	930	88.71

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit,K₂Mg₂ (SO₄)₃, Acta Cryst. 10, 409-413.

,

The sample was prepared by slow evaporation of a 1:1 aqueous solution of Rb_2CrO_4 and $MgCrO_4$ at room temperature.

Color

Brilliant greenish yellow

Optical data

Biaxial, $N_{\rm CM}{=}1.635$, $N_{\rm \beta}{=}1.630$, $N_{\rm \gamma}{=}1.645$, 2V is very large.

Structure

Monoclinic, $P2_1/a$ (14) Z=2, isostructural with other "Tutton" salts [Tutton and Porter,1912]. The structure of a "Tutton Salt", (NH₄)₂Mg(SO₄)₂·6H₂O was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.474 ±.001	12.571 ±.001	6.256 ±.001	104°57′ ±1′

Density

(calculated) 2.470 g/cm³ at 25° C.

Internal standard Ag, a = 4.08641 Å CuKa ₁ λ = 1.54056 Å; temp. 25 °C			
d (Å)	I	hkl	20(°)
7.40	35	110	11.95
6.28	4	020	14.09
6.03	9	001	14.67
5.24	7	111	16.89
4.58	10	200	19.35
4.36	9	021	20.34
4.263	50	111	20.82
4.213	85	201	21.07
3.810	100	130	23.33
3.702	9	220	24.02
3.673 3.501 3.445 3.388 3.266	4 5 12 20	121 221 031 131 201	24.21 25.42 25.84 26.28 27.28
3.161	<pre>35 { 25 25 40</pre>	211	28.21
3.142		040	28.38
3.095		230	28.82
3.077		131	28.99
3.026		112	29.49
2.975 2.936 2.897 2.887 2.813	40 8 9 35 8	311,140 012 221 202 212 212	30.01 30.42 30.84 30.95 31.78
2.793	20	Ī22	32.02
2.761	13	Ī41	32.40
2.746	8	320	32.58
2.623	5	222	34.15
2.590	6	240	34.60
2.577	8	231	34.79
2.518	17	241	35.62
2.503	20	132	35.85
2.471	35	331	36.33
2.460	12	122	36.50
2.321	20	051	38.76
2.317	20	322	38.84
2.310	13	411	38.96
2.289	15	400	39.33
2.264	25	241	39.78

Interr	Internal standard Ag, a = 4.08641 \AA				
CuKa	$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. } 25 \text{ °C}$				
d (Å)	I	hkl	20(°)		
2.232	10	212	40.37		
2.204	12	250	40.91		
2.193	9	341	41.13		
2.180	12	042	41.39		
2.160	12	251	41.79		
2.149	19	$ \begin{array}{r} 420 \\ 331,222 \\ \overline{2}42 \\ 060 \\ \overline{4}12 \\ \end{array} $	42.00		
2.134	18		42.32		
2.126	13		42.48		
2.095	5		43.14		
2.076	5		43.55		
2.050	6	431,203	44.15		
2.015	11	003	44.95		
1.992	5	251	45.50		
1.978	4	123,401	45.84		
1.953	6	411,342	46.47		
1.942	8	351	46.74		
1.933	7	052	46.98		
1.903	10	313,161	47.76		
1.876	7	261	48.49		
1.866	8	133	48.75		
1.850	12	440,113	49.21		
1.841	6	233,323	49.48		
1.812	8	521,510	50.32		
1.792	6	123	50.92		
1.764	10	261,170	51.79		
1.753	6	403	52.14		
1.742	9	332	52.49		
1.717	7	451,243	53.32		
1.707	8	133	53.64		
1.677	10	530	54.67		
1.673	12	$ \begin{array}{r} 441 \\ 171 \\ \overline{3}43, \overline{5}32 \\ \overline{5}41 \\ \overline{4}33 \\ \end{array} $	54.82		
1.669	6		54.96		
1.641	10		56.00		
1.621	6		56.76		
1.617	5		56.88		

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.

Tutton, A. E. H., and M. W. Porter (1912). Crystallographic constants and isomorphous relations of the double chromates of the alkalis and magnesium, Min. Mag. 16, 169-196.

The sample was prepared at room temperature by slow evaporation of an equimolar aqueous solution of $Rb_{\gtrsim}SO_4$ and $MgSO_4$.

Color

Colorless

Optical data

Biaxial(+) $N_{\alpha}{=}1.467$, $N_{\beta}{=}1.469$, $N_{\gamma}{=}1.476$, 2V is medium.

Structure

Monoclinic, $P2_1/a$ (14), Z=2.Isostructural with other "Tutton Salts" [Tutton,1893] The structure of a "Tutton Salt", $(NH_4)_2 -$ Mg $(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.235 ±.001	12.486 ±.001	6.224 ±.001	105°59′ ±1′

Density

(calculated) 2.385 g/cm³ at 25° C.

Reference intensity.

 $I/I_{corundum} = 1.8$

Rei	feren	ces
-----	-------	-----

- Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.
- Tutton, A.E. (1893). Connection between the atomic weight of contained metals and the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates R₂M(SO₄)₂•6H₂O J. Chem. Soc. 63, 337-423.

Internal standard Ag, $a = 4.08641$ Å			
d (Å)		hkl	23 C 2 $\theta(\circ)$
7.25 5.99 5.104 4.442 4.323	25 6 6 9	110 001 120 200 021	12.20 14.77 17.36 19.97 20.53
4.235 4.174 4.156 3.770 3.614	9 }100 { 85 3	Ī21 111 201 130 220,121	20.96 21.27 21.36 23.58 24.61
3.460	4	221	25.73
3.418	4	031	26.05
3.369	12	131	26.43
3.171	35	201	28.12
3.123	40	040	28.56
3.074	25	211	29.02
3.033	40	230,131	29.42
3.015	40	112	29.60
2.945	6	140	30.32
2.916	25	311	30.63
2.874	30	202	31.09
2.826	13	221	31.63
2.802	8	212	31.91
2.779	20	122	32.18
2.743	7	141	32.62
2.703	4	$ \overline{321} 320 \overline{222} 112 240,141 $	33.12
2.674	4		33.49
2.611	2		34.32
2.569	2		34.90
2.552	6		35.13
2.523	8	231	35.56
2.497	16	241	35.94
2.489	18	132	36.05
2.433	35	331	36.91
2.426	19	312	37.02
2.412	8	330	37.24
2.304	13	051	39.07
2.298	11	322,401	39.17
2.259	7	411	39.88
2.242	6	321	40.19
2.225 2.219 2.182 2.177 2.159	19 17 6 7	241 132,400 212 250,151 042	40.51 40.62 41.35 41.45 41.80

Internal standard Ag, a = 4.08641 Å CuKa ₁ λ = 1.54056 Å; temp. 25 °C			
d (Å)	I	hkl	20(°)
2.142	8	251	42.16
2.114	9	242	42.73
2.092	9	420	43.22
2.083	5	060,331	43.40
2.049	3	412	44.17
2.026	2	160	44.69
2.012	4	431	45.02
1.994	8	003	45.45
1.968	4	013,123	46.09
1.961	6	251	46.26
1.945	2	Ī52	46.65
1.938	4	342	46.84
1.916	9	052,401	47.40
1.908	5	350	47.61
1.894	6	313,411	47.99
1.884	2	260,161,+	48.26
1.860	8	261	48.93
1.855	8	133	49.08
1.831	4	323,421,+	49.75
1.810	7	152,440	50.37
1.807	8	242	50.47
1.785	2	322	51.14
1.765	6	123	51.74
1.757	7	510,352	51.99
1.739	6	261	52.58
1.729	5	\$\overline{442}, \overline{162} \$062, 520 \$332 \$522, \$\overline{531} \$133	52.91
1.708	3		53.62
1.700	5		53.87
1.688	3		54.31
1.683	4		54.49
1.676	3	423	54.71
1.658	3	450,252	55.37
1.654	5	270,171	55.50
1.639	3	271	56.08
1.633	4	530,343,+	56.28
1.616	5	532	56.95
1.598	2	452	57.65
1.580	3	253	58.35

The sample was made by heating $Rb_2\,SO_4$ and $NiSO_4$ in nitrogen at 540 $^\circ C$ for 10 minutes. It was then ground and reheated at 450 $^\circ C$ for 15 minutes.

Color

Light yellow

Optical data

Isotropic, N=1.636

Structure

Cubic, P2₁3 (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The langbeinite structure was determined by Zemann and Zemann [1957].

Lattice constants

		a(Å)
Gattow and Zemann	[1958]	9.930 ±.003
NBS, sample at 25	°C	9.9217 ±.0002

Density

(calculated) 3.921 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 3.6$

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C							
d (Å)	Ι	hkl	2∂(°)				
5.73	3	111	15.44				
4.05	6	211	21.95				
3.51	6	220	25.39				
3.30	4	221	26.96				
3.14	100	310	28.43				
2.992	20	311	29.84				
2.863	2	222	31.22				
2.750	13	320	32.53				
2.651	55	321	33.78				
2.480	1	400	36.18				
2.406	13	410	37.34				
2.276	5	331	39.56				
2.219	2	420	40.63				
2.165	5	421	41.68				
2.116	7	332	42.70				
2.026	17	422	44.70				
1.984	3	430	45.69				
1.946	20	510	46.64				
1.909	2	511	47.59				
1.842	9	520	49.43				
1.811	2	521	50.34				
1.754	2	440	52.09				
1.727	7	522	52.98				
1.702	2	530	53.82				
1.677	2	531	54.67				
1.654	1	600	55.53				
1.631	6	610	56.37				
1.610	17	611	57.18				
1.569	6	620	58.81				
1.550	8	621	59.61				
1.532 1.513 1.495 1.479 1.463	7 2 8 5	541 533 622 630 631	60.39 61.19 62.01 62.77 63.55				
1.432 1.418 1.402 1.3894 1.3757	4 3 1 1	444 632 710 711 640	65.09 65.83 66.63 67.35 68.10				

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C						
d (Å)	Å) I hkl					
1.3624	2	720	68.86			
1.3498	5	721	69.59			
1.3258	3	642	71.04			
1.3141	2	722	71.77			
1.3025	3	730	72.51			
1.2917	4	731	73.20			
1.2700	2	650	74.68			
1.2597	3	732	75.39			
1.2404	2	800	76.78			
1.2306	3	810	77.50			
1.2214 1.2123 1.2034 1.1945 1.1859	2 2 4 1	811 733 820 821 653	78.20 78.90 79.60 80.31 81.01			
1.1693	3	822	82.41			
1.1610	2	830	83.12			
1.1535	5	831	83.79			
1.1458	2	751	84.48			
1.1307	1	832	85.88			
1.1234	3	752	86.58			
1.1025	2	841	88.64			
1.0957	3	910	89.34			
1.0892	2	911	90.01			

Gattow,G.and J.Zemann (1958). Über Doppelsulfate vom Langbeinit-typ, A⁺₂ B²⁺₂ (SO₄)₃, Z. Anorg. Allgem. Chem. 293, 233 - 240. Zemann,A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit,K₂Mg₂ (SO₄)₃, Acta Cryst. 10, 409 - 413.

The sample was prepared at room temperature by slow evaporation of an equimolar aqueous solution of Rb_2SO_4 and $NiSO_4$.

Color

Strong bluish green

Optical data

Biaxial(+) $N_{\rm C}{=}1.488,~N_{\rm \beta}{=}1.496,~N_{\rm \gamma}{=}1.505,$ 2V is very large

Structure

Monoclinic, $P2_1/a$ (14), Z=2.Isostructural with other "Tutton Salts" [Tutton, 1893] The structure of a "Tutton Salt", (NH_4)₂ -Mg(SO₄)₂·6H₂O, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.138 ±.001	12.416 ±.001	6.223 ±.001	106°3.7′ ±.5′

Density

(calculated) 2.594 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 2.0$

References

- Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.
- Tutton, A.E.(1893). Connection between the atomic weight of contained metals and the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates R₂M(SO₄)₂·6H₂O J. Chem. Soc. 63, 337-423.

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C							
d (Å)	Ι	hkl	20(°)				
7.18	6	110	12.31				
6.20	1	020	14.27				
5.98	1	001	14.81				
5.21	2	111	16.99				
5.072	3	120	17.47				
4.390 4.310 4.209 4.151 4.122	9 16 6 }100 {	200 021 121 111 201	20.21 20.59 21.09 21.39 21.54				
3.745	85	130	23.74				
3.586	6	220	24.81				
3.400	2	031	26.19				
3.356	15	Ī31	26.54				
3.148	20	201	28.33				
3.104	25	040	28.74				
3.052	20	211	29.24				
3.013	65	112,230	29.62				
2.992	12	002	29.84				
2.925	4	140,231	30.54				
2.906	7	012	30.74				
2.893	12	311	30.88				
2.868	19	202	31.16				
2.849	13	310	31.37				
2.807	18	221	31.85				
2.796	13	212	31.98				
2.778	18	122	32.20				
2.755	4	041	32.47				
2.730	9	141	32.78				
2.695	1	022	33.22				
2.682	2	321	33.38				
2.649	2	320	33.81				
2.603	3	222	34.42				
2.536	7	141,240	35.36				
2.506	6	231	35.80				
2.483 2.422 2.414 2.390 2.358	$ \begin{array}{c} 14\\ 45\left(\begin{array}{c} 2\\ 1\end{array}\right) $	$ \begin{bmatrix} 132, \overline{2}41 \\ 032 \\ \overline{3}31, \overline{3}12, + \\ 330, 150 \\ \overline{2}32 $	36.14 37.09 37.21 37.61 38.13				

Rubidium Nickel Sulfate Hydrate, $Rb_2Ni(SO_4)_2 \cdot 6H_2O$ (monoclinic) – continued

Inte CuK	rnal stan $a_1 \lambda = 1.$	dard W, a = 3.165 .54056 Å; temp. 2	16 Å 5 °C	Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			516 Å 25 °C	
d (Å)	I	hkl	20(°)		d (Å)	Ι	hkl	20(°)
d (Å) 2.339 2.293 2.286 2.237 2.225 2.210 2.197 2.170 2.163 2.154 2.128 2.106 2.069 2.062 2.040 2.034 2.013 1.994 1.965 1.949 1.927 1.910 1.906 1.895 1.890	<i>I</i> 1 14 13 7 6 20 6 2 8 10 7 10 12 7 2 3 2 10 1 5 3 8 7 6 10	$\begin{array}{c} hkl \\ 311 \\ 051 \\ 322 \\ 411 \\ 321 \\ 241 \\ 400, \overline{1}42 \\ 212 \\ 151, 410, + \\ 042 \\ 340, \overline{2}51 \\ \overline{2}42 \\ 420, 060 \\ \overline{4}02 \\ \overline{2}03 \\ \overline{4}12 \\ 160, \overline{2}13 \\ 003, \overline{4}31 \\ \overline{1}23 \\ 251 \\ \overline{3}42 \\ 052 \\ \overline{3}51 \\ 350 \\ \overline{3}13, 341 \\ \end{array}$	$2\theta(\circ)$ 38.46 39.26 39.38 40.29 40.51 40.79 41.05 41.59 41.73 41.91 42.45 42.91 43.72 43.88 44.37 44.51 45.00 45.46 46.15 46.55 47.11 47.56 47.68 47.98 48.09		d (Å) 1.775 1.761 1.753 1.748 1.739 1.7248 1.7188 1.7049 1.6900 1.6792 1.6750 1.6699 1.6451 1.6293 1.6195 1.6030 1.5988 1.5954 1.5762 1.5616 1.5530 1.5401 1.5279 1.5231 1.5163	I 2 3 2 6 3 5 1 5 4 3 2 6 1 2 7 5 3 2 4 3 2 4 5 4 3 2 4 5 4 3	$\begin{array}{c} hkl \\ 322 \\ 123 \\ 521 \\ 352 \\ 510, 170 \\ 431 \\ 351, 442 \\ 243 \\ 332, 520, + \\ 133, 262 \\ 522 \\ 423 \\ 450, 270, + \\ 271 \\ 530 \\ 532 \\ 433 \\ 223 \\ 253 \\ 361, 412 \\ \hline 204, 080 \\ 214, 172 \\ 540, 180 \\ 521, 371 \\ 542, 370 \\ \end{array}$	$2\theta(\circ)$ 51.45 51.87 52.13 52.29 52.57 53.05 53.25 53.72 54.23 54.62 54.76 54.94 55.84 56.43 56.90 57.44 57.61 57.74 58.51 59.11 59.47 60.02 60.55 60.76 61.06
1.854 1.849 1.829 1.807 1.793	} 14 { 2 2 9	133 261 233 511 440	49.11 49.24 49.82 50.45 50.90		1.5052 1.5013 1.4869	3 3 1 ,	224,460 523,314,+ 602	61.56 61.74 62.40

The sample was prepared from a 1:1 molar mixture of KCl and RbCl by melting, quenching, and annealing for 3 days at 400 $^{\circ}$ C.

Color

Colorless

Optical data

Isotropic, N=1.492.

Structure

Cubic, Fm3m (225) NaCl type, Z=4. This 1:1 composition is the midpoint in the complete solid solution series between KCl and RbCl.

Lattice constants

					$a(\mathring{A})$
NBS,	sample	at	25	°C	6.4481 ±.0002

Density

(calculated) 2.421 g/cm³ at 25° C.

Reference intensity

 $1/I_{corundum} = 5.3$

r							
Internal standard W, a = 3.16504 Å CuK α_1 λ = 1.5405 Å; temp. 25 °C							
d (Å)	l (Å) I hkl						
3.725	13	111	23.87				
3.225	100	200	27.64				
2.280	60	220	39.49				
1.945	6	311	46.67				
1.862	18	222	48.87				
1,6117	8	400	57.10				
1.4793	3	331	62.76				
1 4419	16	420	64.58				
1 3160	10	420	71 65				
1 2/10	1	422	76 73				
1.2410		JII	10.15				
1.1397	3	440	85.04				
1.0899	1	531	89.94				
1.0745	4	600	91.59				
1.0195	3	620	98.15				
0.9833	1	533	103.14				
.9720	2	622	104.83				
.9309	1	444	111.68				
.9029	1	711	117.10				
.8942	2	640	118.96				
.8615	3	642	126.79				
	-						

The sample was prepared by heating a mixture of Sm_2O_3 and SnO_2 at 1200 °C overnight. It was then ground and reheated overnight at 1200 °C followed by two hours at 1400 °C.

Color

Colorless

Optical data

Isotropic, N≅1.98

Structure

Cubic, pyrochlore type, Fd3m (227), Z=8, [Whinfrey et al., 1960].

Lattice constants

	a(Å)
Whinfrey et al. [1960] NBS, sample at 25 °C	10.507 10.5083 ±.0002

Density

(calculated) 7.442 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 7.9$

References

Whinfrey, C.G., D.W. Eckart, and A. Tauber (1960). Preparation and x-ray diffraction data for some rare earth stannates, J. Am. Chem. Soc. 82, 2695-7.

Internal standard Ag, a = 4.08641 Å								
CuKa	$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. } 25 \text{ °C}$							
d (Å)	20(°)							
6.07	4	111	14.59					
3.71	2	220	23.97					
3.166	3	311	28.16					
3.032	100	222	29.43					
2.627	35	400	34.10					
2.410	4	331	37.28					
2.146	2	422	42.08					
2.021	3	511	44.80					
1.857	60	440	49.00					
1.777	2	531	51.39					
1.585	55	622	58.17					
1.5170	13	444	61.03					
1.4711	3	551	63.15					
1.4043	2	642	66.53					
1.3681	2	731	68.53					
1.3136	11	800	71.80					
1.2839	3	733	73.73					
1.2054	20	662	79.44					
1.1749	18	840	81.93					
1.0727	19	844	91.79					
1.0156	3	951	98.65					
1.0113	19	10·2·2	99.22					
.9289	9	880	112.05					
.8881	30	10·6·2	120.31					
.8757	19	12·0·0	123.20					
.8307	20	$12 \cdot 4 \cdot 0$ $10 \cdot 6 \cdot 6$	136.01					
.8013	20		148.03					

Additional patterns

 PDF card 13-181, [A. Tauber, U.S. Army Signal Corps Laboratory, Monmouth, New Jersey]

The sample was crystallized at room temperature by slow evaporation of an equimolar aqueous solution of AgCN and KCN.

Color

Colorless

Optical data

Uniaxial (+), $N_0 = 1.492$, $N_p = 1.602$

Structure

Hexagonal, P3lc (159), Z=6 [Staritzky, 1956]. The structure was determined by Hoard [1933], assuming P3lc to be the space group.

Lattice constants

	a(Å)	c(Å)
Hoard [1933] Staritzky [1956] NBS, sample at 25 °C	7.399* 7.40 7.390 ±.001	17.589* 17.59 17.607 ±.002

*from kX units.

Density

(calculated) 2.381 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 2.1$

Additional patterns

1. PDF card 9-337 [Staritzky, 1956]

R	e	f	e	r	e	n	С	e	S	

Hoard,	J.L.	(1933).	The	crysta	l sti	cuct	ure
of	potass	ium silv	er cy	/anide,	z.	Kri	st.
84,	231-25	5,					
Starit	zky, E	(1956)	. Pot	assium	silv	ver	di-
cyan	ide KA	$g(CN)_2$,	Anal	Chem.	28, 4	419 -	20.

Internal standard W, a = 3.16516 A CuK a_1 λ = 1.54056 Å; temp. 25 °C				
d (Å)	I	hkl	20(°)	
8.803	50	002	10.04	
6.398	5	100	13.83	
6.013	35	101	14.73	
5.178	6	102	17.11	
4.397	70	004	20.18	
4.323	18	103	20.53	
3.691	5	110	24.09	
3.402	100	112	26.17	
3.199	16	200	27.87	
3.145	75	201	28.35	
3.085	<1	105	28.92	
3.007	11	202	29.68	
2.935	15	006	30.43	
2.827	20	114	31.62	
2.808	35	203	31.84	
2.588	5	204	34.63	
2.396	8	211	37.51	
2.368	20	205	37.96	
2.340	8	107	38.43	
2.333	7	212	38.56	
2.299	30	116	39.16	
2.237	5	213	40.29	
2.201	15	008	40.98	
2.133	5	300	42.34	
2.072	16	302	43.64	
1.994	4	215	45.45	
1.977	9	207	45.86	
1.920	2	304	47.31	
1.871	2	109	48.61	
1.848	10	220	49.27	
1.808	6	222	50.42	
1.766	3	311	51.71	
1.762	4	0.0.10	51.85	
1.743	3	217	52.45	
1.725	5	306	53.03	
1.704	18	224	53.76	
1.669	6	209	54.97	
1.594	5	401	57.79	
1.589	7	1.1.10	57.99	
1.564	3	226	59.02	
1.543	4	403,2.0.10		

A 1:1 molar mixture of NaCl and AgCl was melted, ground, and then annealed at 400 $^{\circ}$ C overnight.It was reground and annealed at 400 $^{\circ}$ C for an additional hour.

Color

Colorless, becoming gray with prolonged exposure to light.

Optical data

Isotropic, N≈1.780

Structure

Cubic, Fm3m (225), Z=4, NaCl type. This composition is the midpoint in the complete solid solution series from NaCl to AgCl.

Internal standard Ag, a = 4.08641 Å				
CuKa	$\lambda = 1.$	54056 A; temp. 2	5 °C	
d (Å)	I	hkl	20(°)	
3.24 2.807 1.984 1.692	14 100 55 4	111 200 220 311 222	27.49 31.85 45.69 54.17	
1.4028 1.2868 1.2545 1.1451 .9919	6 2 11 6 1	400 331 420 422 440	66.61 73.54 75.76 84.55 101.90	
.9483 .9351 .8870 .8457	1 3 2 2	531 600 620 622	108.63 110.93 120.55 131.23	

Lattice constants

	Ċ.				a(Å)
NBS,	sample a	at 2	25	°C	5.6102 ±.0002

Density

(calculated) 3.795 g/cm³ at 25° C.

Reference intensity

 $I/I_{commutum} = 3.3$

The sample was prepared by heating $SrCO_3$ and SnO_2 together at 1200 °C, followed by grinding and reheating at 1000 °C for 16 hours.

Color

Colorless

Optical data

Isotropic, $N \approx 1.90$, material was very fine grained.

Structure

Cubic, $P2_1 3(198)$ or $P4_2 32(208)$, Z=8 [Smith and Welch, 1960]. Structure is a doubled perovskite type. Samples which have been heated to 800-1000 °C and examined immediately on cooling give only lines of of the monomolecular cubic perovskite cell. Lines of the doubled cell appear after an hour or two at room temperature. No indications of symmetry lower than cubic could be detected in the diffraction pattern.

Lattice constants

	a(Å)
Hoffman [1934]	4.025* 4.033 7* *
Naray-Szabo [1947]	8.05***
Smith and Welch [1960] NBS, sample at 25 °C	8.070 8.0682
	±.0001

* as published

** from kX

*** as published, and considered to be monoclinic

Internal standard W, a = 3.16516 Å					
$CuKa_1 \lambda = 1.54056 A; temp. 25 °C$					
d (Å)	Ι	hkl	20(°)		
4.033	9	200	22.02		
3.608	2	210	24.65		
2.853	100	220	31.33		
2.689	2	221	33.29		
2.550	2	310	35.17		
2.431	2	311	36.94		
2.348	2	222	38.65		
2.237	1	320	40.28		
2.156	1	321	41.86		
2.018	30	400	44.89		
1.957	2	410	46.37		
1.851	1	331	49.17		
1.803	4	420	50.57		
1.760	2	421	51.90		
1.647	40	422	55.76		
1.614	1	430	57.03		
1.582	1	510	58.26		
1.498	2	520	61.91		
1.4262	17	440	65.38		
1.4043	<1	522	66.53		
1.3656	2	531	68.79		
1.3448	2	600	69.89		
1.2758	14	620	74.28		
1.2599	2	621	75.38		
1.2306	<1	533	77.50		
1.2164	2	622	78.58		
1.2025	1	630	79.67		
1.1648	5	444	82.80		
1.1528	2	632	83.85		
1.1298	<1	711	85.96		
1.1189	1	640	87.01		
1.1081	2	720	88.08		
1.0781	17	642	91.20		
1.0688	<1	722	92.22		
1.0503	<1	731	94.35		

Internal standard W, a = 3.16516 Å				
$CuKa_1 \ \lambda = 1.54056 \ \text{\AA}; \text{ temp. 25 °C}$				
d (Å)	Ι	hkl	20(°)	
1.0330 1.0086 1.0008 0.9784 .9713 .9509 .9317 .9255 .9195 .9022 .8965 .8803 .8601 .8551 .8567	1 3 1 2 1 9 <1 1 1 5 1 2 4 1 1	650 800 810 820 821 822 751 662 832 840 841 842 664 922 852	96.43 99.59 100.63 103.87 104.92 108.21 111.53 112.65 113.79 117.26 118.46 122.09 127.15 128.48 134.03	
.8235 .8068 .8028 .7912	6 2 1 11	10.0.0 10.1.0 10.2.0	138.59 145.40 147.28 153.61	

Density

(calculated) $6.432 \text{ g/cm}^3 \text{ at } 25^\circ \text{ C}$.

Reference intensity

 $I/I_{corundum} = 11.0$

Additional patterns

1.PDF card 2-1448,[Hoffman, 1934].
2.PDF card 3-0715,[Philip Lamps Ltd].

References

- Hoffman, A. (1934). Untersuchungen über Verbindungen mit Perowskitstruktur, Z. Phy. Chem. B28, 65-74.
- Megaw, H.D. (1964). Crystal structure of double oxides of the perovskite type, Proc. Phy. Soc. 58 part 2, 133-152.
- Naray-Szabo, I. (1947). The perovskite structure family, Müegg. Kozl. No.1, 30-41.
- Smith, A.J., and A.J.E. Welch (1960). Some mixed metal oxides of perovskite structure, Acta Cryst. 13, 653-66.

The sample of $\text{Tl}N_{\scriptscriptstyle 3}$ was obtained from Picatinny Arsenal, Dover, N.J.

Color

Yellowish white

Structure

Tetragonal, I4/mcm (140), Z=4. Isostructural with KN₃ [Krause, 1963]

Lattice constants

	a(Å)	c(Å)
Krause [1963] NBS, sample at 25 °C	6.22 6.2037 ±.0003	7.37 7.379 ±.001

Density

(calculated) 5.763 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 3.2$

Additional patterns

 PDF card 15-699 [Hendricks and Krause, Fort Belvoir, Virginia, 1963].

References

Krause, B.H. (1963). Diffraction studies of photochemical decomposition of azides I. X-ray and UV-induced lattice constant changes in TlN₃,J.Chem.Phys. 39,1706-13.

Internal standard W, a = 3.16516 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C				
d (Å)	Ι	hkl	20(°)	
4.386	80	110	20.23	
3.690	40	002	24.10	
3.102	50	200	28.76	
2.826	100	112	31.63	
2.598	3	211	34.50	
2.375	40	202	37.85	
2.1928	17	220	41.13	
1.9621	19	310	46.23	
1.8857	17	222	48.22	
1.8455	8	004	49.34	
1.7321	30	312	52.81	
1.7005	12	114	53.87	
1.5859	10	204	58.12	
1.5514	4	400	59.54	
1.4620	2	330	63.59	
1.4295 1.4118 1.3872 1.3593 1.3441 \	5 5 4 6	402 224 420 332 314	65.21 66.13 67.46 69.04 69.93	
1.2982	5	422	72.79	
1.2296	1	006	77.58	
1.2168	2	510	78.55	
1.1870	3	404	80.92	
1.1841	2	116	81.16	
1.1553	3	512	83.63	
1.1460	2	334	84.47	
1.1430	2	206	84.74	
1.1087	4	424	88.02	

The sample was made by heating a mixture of Tl_2SO_4 and $CdSO_4$ for 100 hours at 470 °C.

Color

Colorless

Optical data

Isotropic, N=1.730

Structure

Cubic, $P2_1 3$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The structure of langbeinite, $K_2 Mg_2 (SO_4)_3$ was determined by Zemann and Zemann [1957].

Lattice	constants
---------	-----------

	a(Å)
Gattow and Zemann [1958]	10.385 ±.007
NBS, sample at 25 °C	10.3841 ±.0002

Density

(calculated) 5.467 g/cm³ at 25° C.

Reference intensity

 $1/1_{corundum} = 6.0$

Internal standard Ag, $a = 4.08641$ Å				
$CuKa_1 = 1.54056 \text{ A}; \text{ temp. } 25 \text{ °C}$				
d (Å)	Ι	hkl	20(°)	
5.99	6	111	14.78	
5.20	2	200	17.05	
4.64	1	210	19.12	
4.24	30	211	20.94	
3.67	18	220	24.22	
3.46	3	221	25.72	
3.283	100	310	27.14	
3.128	13	311	28.51	
2.999	1	222	29.77	
2.880	9	320	31.03	
2.776	65	321	32.22	
2.598	1	400	34.49	
2.519	10	410	35.61	
2.382	3	331	37.73	
2.322	1	420	38.75	
2.266	4	421	39.74	
2.214	5	332	40.71	
2.120	25	422	42.61	
2.077	2	430	43.53	
2.037	40	510	44.44	
1.999	1	511	45.33	
1.9286	6	520	47.08	
1.8964	2	521	47.93	
1.8354	1	440	49.63	
1.8081	4	522	50.43	
1.7808 1.7556 1.7303 1.7072 1.6846	2 1 3 16	530 531 600 610 611	51.26 52.05 52.87 53.64 54.42	
1.6418	7	620	55.96	
1.6219	5	621	56.71	
1.6022	10	541	57.47	
1.5833	1	533	58.22	
1.5481	4	630	59.68	
1.5311	6	631	60.41	
1.4986	4	444	61.86	
1.4833	1	632	62.57	
1.4684	2	710	63.28	
1.4540	1	711	63.98	

Internal standard Ag, a = 4.08641 Å					
CuKa	$CuKa_1 \lambda = 1.54056 \text{ Å}; \text{ temp. } 25 \text{ °C}$				
d (Å)	Ι	hkl	20(°)		
1.4260	2	720	65.39		
1.4128	5	721	66.08		
1.3877	3	642	67.43		
1.3757	1	722	68.10		
1.3636	3	730	68.79		
1.3519	2	731	69.47		
1.3296	2	650	70.81		
1.3187	4	732	71.48		
1.2980	2	800	72.80		
1.2880	2	810	73.46		
1.2782	1	811	74.12		
1.2685	1	733	74.78		
1.2503	3	821	76.06		
1.2412	3	653	76.72		
1.2236	4	822	78.03		
1.2152	1	830	78.67		
1.2070	5	831	79.31		
1.1990	2	751	79.95		
1.1910	1	662	80.59		
1.1833	<1	832	81.23		
1.1758 1.1537 1.1467 1.1398 1.1331	2 1 1 1	752 841 910 911 842	81.86 83.77 84.40 85.03 85.66		
1.1264	1	920	86.29		
1.1197	2	921	86.93		
1.1070	1	664	88.19		
1.1008	2	922	88.81		
1.0945	2	930	89.46		
1.0887	1	931	90.07		

Gattow,G.and J.Zemann (1958). Über Doppel-sulfate vom Langbeinit-typ, A⁺₂ B²⁺₂ (SO₄)₃, Z. Anorg. Allgem. Chem. 293, 233 - 240.
Zemann,A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, K₂Mg₂ (SO₄)₃, Acta Cryst. 10, 409 - 413.

The sample was prepared by heating a 1:2 mixture of Tl_2SO_4 and $CoSO_4$ at 500 °C for several hours in N_2 .

Color

Strong reddish purple

Optical data

Isotropic, N=1.775

Structure

Cubic, $P2_1 3$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The structure of langbeinite, $K_2 Mg_2$ (SO₄)₃ was determined by Zemann and Zemann [1957].

Lattice constants

		a(Å)
Gattow and Zemann NBS, sample at 25	[1958] °C	10.033 ±.005 10.0312 ±.0002

Density

(calculated) 5.361 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 4.5$

Internal standard Ag, $a = 4.08641 \text{ Å}$					
$CuKa_1 = 1.54056 \text{ A}; \text{ temp. } 25 \text{ °C}$					
d (Å)	Ι	hkl	20(°)		
5.79	25	111	15.30		
5.01	1	200	17.68		
4.48	11	210	19.80		
4.09	19	211	21.70		
3.55	19	220	25.09		
3.34	12	221	26.65		
3.171	100	310	28.12		
3.024	20	311	29.51		
2.894	2	222	30.87		
2.782	20	320	32.15		
2.681	55	321	33.40		
2.509	<1	400	35.76		
2.433	25	410	36.92		
2.30 2	10	331	39.10		
2.244	4	420	40.16		
2.189	10	421	41.20		
2.139	8	332	42.21		
2.048	19	422	44.18		
2.006	4	430	45.15		
1.967	35	510	46.11		
1.931	3	511	47.02		
1.863	10	520	48.85		
1.832	4	521	49.73		
1.773	1	440	51.49		
1.747	6	522	52.34		
1.721 1.696 1.672 1.649 1.628	2 2 6 17	530 531 600 610 611	53.17 54.02 54.85 55.69 56.49		
1.587	5	620	58.09		
1.567	13	621	58.90		
1.548	11	541	59.69		
1.530	3	533	60.46		
1.513	1	622	61.23		
1.496	8	630	61.99		
1.479	6	631	62.77		
1.448	4	444	64.28		
1.434	3	632	65.00		
1.4187	2	710	- 65.77		

Thallium Coba	ilt Sulfate	$, TI_2CO_2(SO_4)_3$	(cubic) - continu	ied
---------------	-------------	----------------------	-------------------	-----

Internal standard Ag, a = 4.08641 Å				
CuKa	$\lambda = 1.5$	54056 Å; temp. 25	5 °C	
d (Å)	Ι	hkl	20(°)	
1.4049 1.3910 1.3780 1.3653 1.3404 1.3286 1.3173	1 1 3 8 1 4 3 4	711 640 720 721 642 722 730 731	66.50 67.25 67.97 68.69 70.15 70.87 71.57 72.28	
1.3061 1.2844 1.2737	4 3 4	650 732	72.28 73.70 74.42	
1.2539 1.2442 1.2347 1.2252 1.2167	1 3 2 1 1	800 810 811 733 820	75.80 76.50 77.20 77.91 78.56	
1.2077 1.1991 1.1820 1.1741 1.1660	5 2 1 7	821 653 822 830 831	79.26 79.94 81.34 82.00 82.69	
1.1583 1.1509 1.1431 1.1358 1.1144	2 <1 1 3 2	751 662 832 752 841	83.37 84.02 84.73 85.40 87.45	
1.1076 1.1010 1.0945 1.0878	1 3 2 1	910 911 842 920	88.13 88.79 89.46 90.16	

- Gattow,G. and J.Zemann(1958). Über Doppelsulfate vom Langbeinit-typ, A⁺₂B²⁺₂ (SO₄)₃, Z. Anorg. Allgem. Chem. 293, 233-240.
- Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, K₂Mg₂ (SO₄)₃, Acta Cryst. 10, 409-413.

The sample was prepared at room temperature by slowly evaporating a 1:4 aqueous solution of Tl_2SO_4 and $FeSO_4$. Only the first crystals formed were used.

Color

Unground: very pale green Ground: colorless

Optical data

Biaxial(-) $\rm N_{\alpha}{=}1.590$, $\rm N_{\beta}{=}1.605$, $\rm N_{\gamma}{=}1.615$, 2V is large

Structure

Monoclinic, P_{2_1}/a (14), Z=2. Isostructural with other "Tutton" salts [Tutton, 1928]. The structure of a "Tutton" salt, (NH₄)₂Mg(SO₄)₂.6H₂O was determined by Margulis and Templeton, [1962].

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.264 ±.001	12.499 ±.002	6.236 ±.001	106°9′ ±1′

Density

(calculated) 3.662 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 3.0$

Internal standard Ag, $a = 4.08641 \text{ Å}$ CuK $a_1 \lambda = 1.54056 \text{ Å}$; temp. 25 °C				
d (Å)	Ι	hkl	2 <i>θ</i> (°)	
7.25	20	110	12.20	
5.99	9	001	14.77	
5.40	14	011	16.40	
5.110	20	120	17.34	
4.454	3	200	19.92	
4.325	7	021	20.52	
4.235	35	ī21	20.96	
4.174	100	111,201	21.27	
3.959	6	211	22.44	
3.771	50	130	23.57	
3.623	2	220	24.55	
3.469	1	221	25.66	
3.377	6	131	26.37	
3.173	17	201	28.10	
3.125	25	040	28.54	
3.074	17	211	29.02	
3.033	30	131	29.42	
3.021	35	112	29.54	
2.927	16	311	30.52	
2.883	30	202,310	30.99	
2.828	7	221	31.61	
2.809	5	212	31.83	
2.784	13	122	32.12	
2.773	8	041	32.25	
2.745	7	141	32.59	
2.678	6	320	33.43	
2.617	3	222	34.23	
2.558	2	240	35.05	
2.525	4	231	35.52	
2.495	1,4	I32	35.96	
2.440	30	331	36.80	
2.418	12	330	37.15	
2.307	25	051,322	39.01	
2.268	7	411	39.70	
2.244	9	321	40.15	

Internal standard Ag, a = 4.08641 Å CuK a_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	Ι	hkl	20(°)
2.225	18	241,400	40.50
2.180	10	250	41.39
2.145	6	251	42.10
2.119	11	242	42.63
2.095	5	420	43.14
2.056 2.020 1.997 1.963 1.959	5 5 6 6	412 213 003 251,430 161	44.00 44.84 45.38 46.21 46.31
1.942	2	$ \begin{array}{r} 342 \\ 052,401 \\ 341 \\ 313 \\ \overline{4}32,261 \end{array} $	46.73
1.9190	10		47.33
1.9061	2		47.67
1.8993	5		47.85
1.8635	6		48.83
1.8578	10	$ \begin{bmatrix} 1_{33} \\ \overline{323}, \overline{233} \\ 152 \\ \overline{521} \\ 510, \overline{352} $	48.99
1.8364	4		49.60
1.8111	9		50.34
1.7762	5		51.40
1.7616	6		51.86

- Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.
- Tutton, A. E.(1928). The hexahydrated double sulphates containing thallium, Proc. Roy. Soc. London, Ser. A 118, 367-392.

The sample was prepared by heating a 1:2 mixture of Tl_2CrO_4 and $MgCrO_4$ for one hour at 350 °C in air.

Color

Strong orange yellow

Optical data

Isotropic, N > 2.0

Structure

Cubic, $P2_13$ (198), Z=4, langbeinite type by analogy with langbeinite, K_2Mg_2 (SO₄)₃, and similar sulfates. The structure of langbeinite was determined by Zemann and Zemann [1957].

Lattice constants

					$a(\mathring{A})$
NBS,	sample	at	25	°C	10.4174 ±.0003

Density

(calculated) 4.731 g/cm³ at 25° C.

Reference intensity

 $I/I_{corundum} = 4.5$

Internal standard W, a = 3.16516 Å CuK a, λ = 1.54056 Å; temp. 25 °C				
$d(\overset{\circ}{A})$	I	hkl	20(°)	
7.35	3	110	12.02	
6.01	25	111	14.72	
5.20	2	200	17.03	
4.660	30	210	19.03	
4.257	10	211	20.85	
3.684	10	220	24.14	
3.473	17	221	25.63	
3.292	100	310	27.06	
3.141	15	311	28.39	
3.007	5	222	29.68	
2.889	40	320	30.93	
2.783	55	321	32.14	
2.526	25	410	35.51	
2.455	2	411	36.58	
2.389	14	331	37.62	
2.331	5	420	38.60	
2.273	8	421	39.62	
2.220	7	332	40.60	
2.126	15	422	42.49	
2.0833	3	430	43.40	
2.0430 2.0052 1.9341 1.9016 1.8135	25 8 3 5	510 511 520 521 522	44.30 45.18 46.94 47.79 50.27	
1.7869	3	530	51.07	
1.7606	3	531	51.89	
1.7362	1	600	52.68	
1.7122	7	610	53.47	
1.6897	19	611	54.24	
1.6470	5	620	55.77	
1.6266	16	621	56.53	
1.6073	10	541	57.27	
1.5881	4	533	58.03	
1.5701	2	622	58.76	
1.5526	7	630	59.49	
1.5359	6	631	60.20	
1.5032	4	444	61.65	
1.4880	3	632	62.35	
1.4730	3	710	63.06	

Internal standard W, a = 3.16516 Å				
CuK	$a_1 \lambda = 1$.54056 Å; temp. 2	25 °C	
d (Å)	I	hkl	20(°)	
1.4587	2	711	63.75	
1.4446	2	640	64.45	
1.4309	4	720	65.14	
1.4173	5	721	65.84	
1.3921	3	642	67.19	
1.3681	2	730	68.53	
1.3567	4	731	69.19	
1.3338	4	650	70.55	
1.3232	4	732	71.20	
1.3017	3	800	72.56	
1.2921	4	810	73.19	
1.2826	3	811	73.82	
1.2726	2	733	74.50	
1.2634	3	820	75.12	
1.2541	5	821	75.79	
1.2449	4	653	76.45	
1.2277	3	822	77.72	
1.2110	5	831	79.00	
1.2030	3	751	79.63	
1.1873	2	832	80.90	
1.1794	2	752	81.55	
1.1577	2	841	83.42	
1.1504	1	910	84.07	
1.1435	4	911	84.69	
1.1369	3	842	85.30	
1.1300	2	920	85.95	
1.1235	2	921	86.57	
1.1043	3	922	88.46	
1.0983	2	930	89.07	

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit,K₂Mg₂ (SO₄)₃, Acta Cryst. 10, 409 - 413.

Monoclinic, $P2_1/c$ (14) Z=4 [Young et al., 1968]

Lattice parameters

a=13.687 \pm 0.005Å, b=5.971 \pm 0.003Å, c=14.767 \pm 0.005Å, β =116°10′ \pm 5′, (published value, c=14.766) [ibid.]

Density

(calculated) 1.313 g/cm³ [ibid.]

Thermal parameters

Anisotropic values for F,O,C; isotropic value B=8.0 for H(12),H(13),H(14)[ibid.] isotropic value B=0.0 for remaining H's.

Scattering factors

 F^{-1} , O° , C° , H° [3.3.1A]

Scale factor

(integrated intensities) 3.465 \times 10⁴

Reference

Young, D.W., P.Tollin, and H.H. Sutherland (1968). The crystal structure of 4-Acetyl-2'-fluorobiphenyl, Acta Cryst. B24, 161-167.

Calculated Pattern (Peak heights)					
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$		
12.27	5	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	7.20		
6.62	50		13.36		
6.14	14		14.42		
6.01	6		14.72		
5.44	71		16.28		
5.35	9	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	16.56		
4.98	7		17.78		
4.63	51		19.14		
4.50	4		19.72		
4.48	6		19.82		
4.44	6	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	23.00		
4.28	6		20.74		
4.10	8		21.68		
3.828	3		23.22		
3.693	7 0		24.08		
3.669	100	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	24.24		
3.627	6		24.52		
3.601	5		24.70		
3.581	8		24.84		
3.550	16		25.06		

Calculated Pattern (Peak heights)					
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$		
3.419	3	-4 0 2	26.04		
3.129	3	1 1 3	28.50		
3.099	28	-1 1 4	28.78		
3.070	4	4 0 0	29.05		
3.009	1	-4 0 4	29.66		
2.965	26	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	30 • 1 2		
2.910	2		30 • 7 0		
2.897	11		30 • 8 4		
2.884	6		30 • 9 8		
2.766	1		32 • 34		
2.736 2.730 2.685 2.647 2.605	2 2 5 2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32.70 32.78 33.34 33.84 34.40		
2.596	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	34 • 5 2		
2.583	1		34 • 7 0		
2.490	2		36 • 0 4		
2.473	1		36 • 3 0		
2.457	5		36 • 5 4		
2.439 2.423 2.412 2.309 2.272	1 3 1 4	-4 1 5 G 1 5 3 2 0 3 1 3 3 2 1	36 • 8 2 37 • 0 8 37 • 2 4 36 • 9 8 39 • 6 4		
2.249	1	-4 2 2	40.06		
2.209	1	0 0 6	40.82		
2.111	1	-6 1 2	42.80		
2.101	1	5 1 1	43.02		
2.078	1	1 2 4	43.52		
2.058	1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	43.96		
2.030	3		44.60		
2.009	2		45.10		
1.982	2,		45.74		
1.956	4		. 46.38		
1.945	1	-7 0 4	46.64		
1.936	1	6 1 0	46.88		
1.919	1	-7 0 2	47.34		
1.893	1	2 3 0	48.02		
1.847	1	-4 2 6	49.30		
1.840	1	2 3 1	49.50		
1.791	2	3 1 5 +	50.96		
1.762	1	-3 1 8	51.84		
1.758	2	2 3 2	51.96		
1.723	2	-3 2 7	53.12		
1.711	2	-5 1 8 +	53.50		
1.640	1	1 3 4	56.02		

C	alculated	d Pattern (Integr	ated)	C	alculate	d Pattern (Integr	ated)
d (Å)	I	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$
12.28 6.63 5.14 6.02 5.44	4 44 13 5 58	1 0 0 0 2 2 0 0 -2 0 2 0 1 1	7.19 13.35 14.41 14.71 16.27	2.647 2.645 2.604 2.596 2.583	4 2 3 3 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	33.63 33.67 34.41 34.52 34.70
5.37 5.35 4.99 4.63 4.50	2 6 51 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	16.49 16.56 17.78 19.15 19.72	2.490 2.474 2.472 2.457 2.439	2 1 1 5 1	-3 2 1 0 2 3 -5 1 3 5 0 0 -4 1 5	36 • 0 4 36 • 2 9 36 • 3 2 36 • 5 4 36 • 8 1
4 • 4 8 4 • 4 4 4 • 2 8 4 • 0 9 3 • 82 7	5 6 9 3	-3 0 2 0 1 2 2 1 0 3 0 0 1 1 2	19.82 20.00 20.73 21.69 23.22	2 • 423 2 • 412 2 • 308 2 • 272 2 • 24 9	1 4 1 4 1	0 1 5 3 2 0 3 1 3 3 2 1 -4 2 2	37.08 37.24 38.39 39.64 40.05
3.694 3.670 3.626 3.601 3.582	69 100 3 3 7	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	24 • 0 7 24 • 2 3 24 • 5 3 24 • 7 0 24 • 8 4	2.209 2.111 2.101 2.078 2.058	1 2 1 2 1	0 C 6 -6 1 2 5 1 1 1 2 4 -5 1 6	40.82 42.80 43.01 43.51 43.96
3.551 3.421 3.129 3.099 3.071	17 3 30 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	25.05 26.03 28.51 28.78 29.05	2.030 2.009 1.982 1.956 1.946	4 3 2 4 1	5 0 2 -5 2 3 0 2 5 -4 1 7 -7 0 4	44.59 45.10 45.74 46.38 46.64
3.009 2.986 2.968 2.965 2.950	1 1 27 5	-4 0 4 0 2 0 -4 1 2 -3 1 4 3 0 2	29.66 29.30 30.08 30.12 30.27	1.937 1.919 1.893 1.847 1.840	1 2 1 1 1	6 1 C -7 D 2 2 3 D -4 2 6 . 2 3 1	46.87 47.34 48.01 49.30 49.51
2.910 2.898 2.897 2.894 2.883	1 5 7 1 5	-4 1 1 -1 2 1 G 1 4 1 0 4 -4 1 3	30.70 30.83 30.84 30.87 30.99	1.792 1.791 1.790 1.762 1.753	1 1 2 2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	50.90 56.95 50.97 51.84 51.96
2.765 2.736 2.729 2.687 2.685	1 2 1 1 1	$\begin{array}{cccc} -1 & 2 & 2 \\ -2 & 2 & 1 \\ -5 & 0 & 2 \\ -4 & 1 & 4 \\ 2 & 2 & 0 \end{array}$	32.35 32.70 32.79 33.32 33.34	1.723 1.712 1.710 1.640	2 2 1 1	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	53•13 53•49 53•53 56•03

Orthorhombic, $P2_1 2_1 2_1$ (19), Z=4 [Simpson and Marsh, 1966]

Lattice parameters

a=6.032±0.001, b=12.343±0.001, c=5.784± 0.001Å [ibid.]

Density

(calculated) 1.374 g/cm³ [ibid.]

Thermal parameters

Anisotropic for carbon,oxygen,and nitrogen. Isotropic for hydrogen. [ibid.]

Polymorphism

The <u>d</u> form has the same powder pattern given here, but the <u> $d\ell$ </u> form has a different orthorhombic structure and powder pattern. [ibid.]

Scattering factors

 N° , O° , and C° [Berghuis et al.,1955] H° [McWeeny, 1951]

Scale factor

(integrated intensities) 1.251×10^4

Additional patterns

- PDF 5-0306 [Institute of Physics, University College, Cardiff]
- PDF 11-993 [P. Cherin, Polytechnic Inst. of Brooklyn, N.Y., 1959]

Reference

- Berghuis, J., IJ. M. Haanapel, M. Potters, B.O. Loopstra, C.H. MacGillavry, and A. L. Veenendahl (1955). New calculations of atomic scattering factors, Acta Cryst. 8, 478-483
- McWeeny,R. (1951). X-ray scattering by aggregates of bonded atoms. I. Analytical approximations in single-atom scattering Acta Cryst. 4, 513-519.
- Simpson, H.J. and R.E. Marsh (1966). The crystal structure of *l*-alanine, Acta Cryst. 20, 550-555.

Ca	lculated	Patter	n (P	Peak he	eights)
d (Å)	I		hkl		$\frac{2\theta(°)}{\lambda = 1.54056 \text{ A}}$
6 • 1 71 5 • 4 20 5 • 2 36 4 • 3 12 4 • 2 19	5 11 22 100 3	0 1 0 1 0	2 1 1 2 2	0 0 1 0 1	14.34 16.34 16.92 20.58 21.04
3.955 3.458 3.399 3.353 3.085	4 3 2 6 20	1 1 1 0	1 2 3 3 4	1 1 0 1	22.46 25.74 26.20 26.56 28.92
2.930 2.891 2.815 2.748 2.709	14 10 3 9 9	1 1 1 2	3 0 1 4 2	1 2 0 0	30.48 30.90 31.76 32.56 33.04
2 •6 08 2 • 4 82 2 • 4 5 3 2 • 4 5 3 2 • 4 03	16 1 2 2 5	1 1 2 2 1	D 4 2 3 2	2 1 1 0 2	34.36 35.16 35.60 35.92 37.40
2 • 2 85 1 2 • 2 42 5 2 • 2 02 6 2 • 1 25 3 2 • 0 58 0	1 3 1 2 2	1 2 1 1 2	5 3 3 5 1	0 1 2 1 2	39.40 40.18 40.94 42.50 43.96
2.0205 1.9919 1.9771 1.9380 1.8776	1 5 4 1 2	2 1 2 0	4 4 2 6 5	1 2 2 1 2 +	44.87 45.50 45.86 46.84 48.44
1.8138 1.7245 1.6996 1.6846 1.6354	2 1 2 1 1	2 3 3 0	53644	1 + 1 0 3	50.26 53.06 53.90 54.42 56.20
1.6242 1.5711	1 1	1 7	7 2	1 र	56.62 58.72

С	alculated	Calculated Pattern (Integrated)					
d (Å)	Ι	hkl	$2\theta(°)$ $\lambda = 1.54056 \stackrel{\circ}{A}$				
6 •1 72	4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	14.34				
5 •4 19	10		16.34				
5 •2 37	21		16.91				
4 •3 14	100		20.57				
4 •2 20	3		21.03				
3.955	4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	22.46				
3.458	3		25.74				
3.393	2		26.20				
3.353	2		26.57				
3.086	2		28.91				
2.930	15	1 3 1	30.48				
2.892	11	0 0 2	30.89				
2.816	4	0 1 2	31.75				
2.747	10	1 4 0	32.57				
2.710	10	2 2 0	33.03				
2.619	1	n 2 2	34.21				
2.608	17	1 0 2	34.35				
2.481	1	1 4 1	36.17				
2.454	3	2 2 1	36.59				
2.432	2	2 3 0	36.92				
2 •4 02	6	1 2 2	37.41				
2 •2 84 7	1	1 5 0	39.41				
2 •2 42 2	3	2 3 1	40.18				
2 •2 02 6	1	1 3 2	40.94				
2 •1 24 9	3	1 5 1	42.51				
2 •1 10 1	1	n 4 2	42.82				
2 •0 58 2	2	2 1 2	43.96				
2 •0 20 9	1	2 4 1	44.81				
1 •9 91 8	6	1 4 2	45.50				
1 •9 77 4	5	2 2 2	45.85				
1 •9382 1 • 8992 1 • 8776 1 • 8771 1 • 8165	1 1 1 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	46.83 47.86 48.44 48.45 50.18				
1 • 8 13 9	2	2 5 1	5 N • 26				
1 • 7 6 0 2	1	1 2 3	5 1 • 90				
1 • 7 24 3	1	3 3 1	5 3 • 07				
1 • 6 9 9 5	3	2 6 0	5 3 • 90				
1 • 6 8 4 6	1	3 4 0	5 4 • 42				
1 •6 35 1 1 •6 24 3 1 •5 70 9 1 •5 10 9 1 •2 87 6	1 1 1 1	1 7 1 2 2 3 2 3 3 3 6 2	56.21 56.62 58.72 61.30 73.49				

Monoclinic, P2₁/c (14), Z=4 [Nahringbauer, 1967]

Lattice parameters

a=4.787 \pm 0.001, b=7.742 \pm 0.001, c=12.015 \pm 0.004Å, β =100.76 \pm 0.02° [ibid.]

Density

(calculated) 1.169 g/cm³ [ibid.]

Thermal parameters

Isotropic				
H 7.0 [ibid.	.]			
0(1) 4.20	N	3.66	C(1)	3.49
0(2) 4.28			C(2)	5.41

Atomic positions

The parameters used were those derived from data around the a-axis. [ibid.]

Scattering factors

 H° , C° , N° , O° [3.3.1A]

Scale factor

(integrated intensities) 0.3776 \times 10⁴

Reference

Nahringbauer, I. (1967). Hydrogen bond studies. XIV. The crystal structure of ammonium acetate, Acta Cryst. 23, 956-965.

Calculated Pattern (Peak heights)							
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ A}}$				
6.468 5.971 4.691 4.066	28 3 65 100	0 1 1 n 0 2 n 1 2 -1 0 2	13.68 15.00 16.90 21.84				
4 • n 19 3 • 8 70 3 • 6 78 3 • 6 30 3 • 5 99 3 • 5 96	94 94 14 33 19	1 1 n n 2 0 n 2 1 1 1 1 -1 1 2 C 1 3	+ 22.10 22.96 24.18 24.50 24.72 25.38				
3 • 3 8 3 3 • 2 3 6 3 • 0 9 9 3 • 0 6 6 2 • 9 8 2	1 8 9 25 29 6	1 0 2 0 2 2 1 1 2 -1 1 3 -1 2 1	25.38 26.32 27.54 28.78 29.10 29.94				

Calculated Pattern (Peak heights)					
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$		
2 • 951	8	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	30.25		
2 • 8 03	46		31.90		
2 • 7 58	22		32.44		
2 • 7 41	4		32.64		
2 • 5 11	8		34.32		
2.583	3	-1 1 4	34.70		
2.528	7	-1 2 3	35.48		
2.521	17	n 3 1	35.58		
2.365	2	n 3 2	38.02		
2.352	3	2 0 0	38.24		
2.340	2	-2 0 2	38.44		
2.313	3	1 0 4	38.90		
2.286	2	-2 1 1	39.38		
2.262	8	1 3 0	39.82		
2.255	6	1 2 3	39.94		
2.250	6	2 1 0	40.04		
2.239	19	-2 1 2 +	40.24		
2.216	5	1 1 4	40.68		
2.185	7	1 3 1	41.26		
2.179	6	-1 3 2	41.40		
2.141 2.042 2.036 1.987 1.967	1 6 3 3	2 1 1 -1 3 3 -2 2 1 2 1 2 + 0 0 6 +	42.18 44.32 44.46 45.62 45.10		
1.949	1	-1 0 6	46.56		
1.943	1	0 3 4	46.72		
1.918	3	-2 2 3	47.36		
1.9103	1	0 4 1	47.56		
1.9065	2	0 1 6	47.66		
1.8901	8	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	48.10		
1.8791	2		48.40		
1.8392	1		49.57		
1.7998	2		50.68		
1.7899	1		50.98		
1.7540	4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	52.10		
1.7478	2		52.30		
1.7336	3		52.76		
1.6915	1		54.18		
1.6863	2		54.36		
1 •6749 1 •6671 1 •5495 1 •5457 1 •5355	1 1 1 1	-1 4 3 -2 2 5 -1 2 7 0 2 7 0 5 1	54.76 55.04 59.62 59.78 60.22		
1 • 4 94 3	1	2 4 0	62.05		
1 • 4 78 0	2	-3 1 4	62.82		
1 • 4 55 6	1	-2 4 3	63.90		
1 • 4 4 9 5	2	3 0 2	64.20		

Ca	alculated	l Pattern (Integra	ated)	C	alculated	l Pattern (Integra	ated)
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 ^{\alpha}}$
6 •4 74 5 •3 02 4 •6 94 4 •0 67 4 •0 19	26 2 54 100 92	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	13.67 15.00 18.89 21.84 22.10	2 • 0 42 2 • 0 36 1 • 9 87 1 • 9 85 1 • 9 67	8 4 3 2 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	44.32 44.47 45.51 45.66 46.10
4 •0 05 3 •8 71 3 •6 78 3 •6 32 3 •6 00	8 97 14 37 19	-1 1 1 0 2 0 0 2 1 1 1 1 -1 1 2	22.18 22.96 24.18 24.49 24.49	1.967 1.949 1.943 1.918 1.9100	1 1 4 1	-2 1 4 -1 0 6 0 3 4 -2 2 3 0 4 1	4 6 • 1 2 4 6 • 5 6 4 6 • 7 2 4 7 • 3 6 4 7 • 5 7
3 •5 08 3 •3 83 3 •2 37 3 •1 00 3 •0 67	1 9 10 28 33	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2 5 • 37 2 6 • 32 2 7 • 5 3 2 8 • 78 2 9 • 0 9	1.9067 1.8901 1.8833 1.8788 1.8788	1 7 5 2 1	∩ 1 6 −1 1 6 1 3 3 −1 3 4 ∩ 4 2	47.66 48.10 48.12 48.41 49.52
2 •9 83 2 •9 51 2 •8 19 2 •8 14 2 •7 59	7 9 2 54 12	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	29.93 30.26 31.72 31.89 32.42	1 •8 00 1 1 •7 89 8 1 •7 54 1 1 •7 53 8 1 •7 47 6	3 1 4 1 2	-224 140 125 026 -142	50.67 50.98 52.10 52.11 52.30
2 •7 57 2 •7 41 2 •F 11 2 •5 83 2 •5 29	15 3 10 4 6	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32.44 32.65 34.32 34.69 35.47	1 .7 334 1 .6 91 5 1 .6 86 4 1 .6 74 7 1 .6 67 2	4 1 3 1 2	-232 204 231 -143 -225	52.77 54.18 54.36 54.77 55.03
2 •5 21 2 •3 64 2 •3 51 2 •3 40 2 •3 13	17 2 3 2 3	n 3 1 n 3 2 2 0 0 - 2 0 2 1 n 4	35.58 38.02 38.24 38.44 38.44 38.91	1 •6 32 5 1 •5 49 4 1 •5 45 9 1 •5 35 3 1 •4 94 4	1 1 1 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	56.31 59.62 59.77 60.23 62.06
2 •2 87 2 •2 62 2 •2 55 2 •2 50 2 •2 40	2 10 - 3 4 23	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	39.37 39.81 39.95 40.04 40.23	1 •4 78 1 1 •4 55 5 1 •4 49 4 1 •4 01 9 1 • 3 79 8	3 1 1 1	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	62.82 63.91 64.21 66.66 67.87
2 • 2 37 2 • 2 16 2 • 1 86 2 • 1 79 2 • 1 41	3 5 8 5 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	40.29 40.68 41.27 41.40 42.17	1 •2 71 4 1 •1 43 7	1 1	n 4 7 2 1 8	74.58 84.68

Monoclinic, P2/n (13), Z=2 [McDonald and Spink, 1967]

Lattice parameters

 $a=9.18\pm0.01$, $b=6.09\pm0.01$, $c=7.89\pm0.01$ Å, $\beta=90.2\pm0.1^{\circ}$ [ibid.]

Density

(calculated) 2.27 g/cm³ [ibid.]

Thermal parameters

Anisotropic [ibid.]

Scattering factors

 N° , O° , C° [Berghuis et al., 1955] Y° [3.3.1B]

Scale factor

(integrated intensities) 3.049×10^4

Additional patterns

1. PDF card 19-1441 [Barrett et al., 1964]

Reference

- Barrett,M.F., T.R.R.McDonald, and N.E.Topp (1964). Double ammonium oxalates of the rare earths and yttrium, J. Inorg. Nucl. Chem. 26, 931-936.
- Berghuis, J., IJ. M. Haanapel, M. Potters, B.O. Loopstra, C.H. MacGillavry, and A. L. Veenendaal (1955). New. calculations of atomic scattering factors, Acta Cryst. 8, 478-483.

McDonald, T.R.R. and J.M. Spink(1967). The crystal structure of a double oxalate of yttrium and ammonium, NH₄Y(C₂O₄)₂·H₂O, Acta Cryst. 23, 944-949.

Ca	Calculated Pattern (Peak heights)							
d (Å)	Ι	hkl			$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$			
6.09 5.97 5.08 4.82 4.59	100 93 16 17 3	n 1 1 2	1 0 1 1 0	0 1 + 0 1 0	14.54 14.82 17.46 18.40 19.32			
4.26 3.94 3.32 3.12 3.00	3.8 2 1.6 1.8 9	-1 2 -1 -2	1 0 1 1 0	1 + 2 1 2 2	20.82 22.52 26.82 28.62 29.80			
2.99 2.89 2.86 2.85 2.85 2.84	14 3 3 4 5	2 1 - 3 3 n	0 2 0 0 2	2 0 1 1 1	29.88 30.92 31.30 31.36 31.46			

Calculated Pattern (Peak heights)					
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$		
2.73	2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32.72		
2.72	1		32.96		
2.69	2		33.30		
2.68	4		33.38		
2.59	6		34.66		
2 • 5 8	4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	34.74		
2 • 5 4	6		35.34		
2 • 5 3	7		35.44		
2 • 5 3	5		35.50		
2 • 4 14	14		37.22		
2.333	19	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	38.55		
2.295	5		39.22		
2.244	9		40.16		
2.158	6		41.82		
2.147	3		42.04		
2.140	10	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42.20		
2.134	7		42.32		
2.083	3		43.40		
2.071	4		43.68		
2.030	4		44.60		
1.998 1.990 1.987 1.981 1.972	1 5 4 3	-3 0 3 0 2 3 + -4 0 2 4 0 2 0 0 4	45.36 45.54 45.62 45.76 45.98		
1.967	3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	46.68		
1.944	1		46.68		
1.922	2		47.24		
1.892	5		48.06		
1.876	2		48.48		
1.840	1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	49.50		
1.833	2		49.70		
1.828	5		49.84		
1.814	2		50.24		
1.807	' 6		50.46		
1 • 7 89 1 • 7 85 1 • 7 71 1 • 7 35 1 • 7 17	4 5 1 2	$\begin{array}{ccccc} -5 & 0 & 1 \\ 4 & 2 & 1 & + \\ 1 & 3 & 2 & + \\ 2 & 1 & 4 \\ -5 & 1 & 1 \end{array}$	51.00 51.14 51.56 52.72 53.32		
1.714	1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	53.40		
1.691	3		54.18		
1.561	1		55.26		
1.630	1		56.40		
1.607	2		57.28		
1.556 1.554 1.518 1.516 1.508	1 1 1 1	-3 3 2 1 7 5 -2 3 3 2 3 3 -5 0 3	59.36 59.42 61.00 61.08 61.44		
1.506	1	-4 2 3	61.54		

Ca	alculated	Pattern (Integro	ated)	C	alculated	d Pattern (Integra	ated)
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 ^{\alpha}}$
6.09 5.99 5.97 5.07 4.82	100 58 62 17 20	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1 4.53 1 4.77 1 4.82 1 7.46 1 8.39	1 •981 1 •972 1 •966 1 •944 1 •923	3 4 2 2 1	4 0 2 0 0 4 0 3 1 1 2 3 -1 3 1	45.77 45.97 46.13 46.68 47.23
4.59 4.27 4.26 3.94 3.32	3 28 23 20	2 0 0 -1 1 1 1 1 1 0 0 2 2 1 1	1 9.32 20.78 20.81 22.52 26.83	1 .922 1 .898 1 .896 1 .893 1 .893	2 1 2 2 6	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	47.25 47.88 47.95 48.03 48.06
3 • 1 2 3 • 0 0 2 • 9 9 2 • 8 9 2 • 8 6	23 10 15 4 3	-1 1 2 -2 0 2 2 0 2 1 2 0 -3 0 1	28.61 29.79 29.89 30.91 31.29	1.889 1.877 1.840 1.833 1.828	2 2 1 7	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	48.14 48.47 49.51 49.7) 49.85
2 .85 2 .84 2 .73 2 .71 2 .69	2 5 3 1 2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	31.37 31.47 32.73 32.97 33.29	1 .815 1 .810 1 .808 1 .807 1 .790	3 3 4 5 5	-2 0 4 2 0 4 -2 3 1 2 3 1 -5 0 1	50.24 50.37 50.44 50.47 50.99
2 • 6 8 2 • 5 9 2 • 5 8 2 • 5 4 2 • 5 3	4 7 1 8 4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	33.39 34.66 34.73 35.34 35.44	1 • 7 87 1 • 7 86 1 • 7 84 1 • 7 72 1 • 7 71	1 2 3 5 5	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	51.07 51.09 51.16 51.54 51.58
2.53 2.417 2.414 2.414 2.414 2.410	3 4 1 15 3	1 0 3 -2 2 1 0 1 3 2 2 1 0 2 2	35.51 37.17 37.21 37.21 37.27	1 .7 35 1 .7 17 1 .7 15 1 .6 92 1 .6 79	1 2 1 4 1	2 1 4 -5 1 1 5 1 1 3 3 0 2 3 2	52.72 53.31 53.39 54.18 54.62
2 • 3 37 2 • 3 33 2 • 3 33 2 • 3 30 2 • 2 95	2 6 19 3 6	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	38.49 38.55 38.56 38.61 39.22	1 .661 1 .630 1 .628 1 .608 1 .607	1 1 1 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	55.27 56.40 56.46 57.26 57.28
2 • 2 51 2 • 2 44 2 • 1 58 2 • 1 48 2 • 1 40	1 12 8 2 13	- 3 1 2 3 1 2 3 2 0 4 1 0 - 2 1 3	4 0. 03 4 0. 15 4 1. 82 4 2. 04 4 2. 20	1 •5 72 1 •5 56 1 •5 54 1 •5 18 1 •5 16	1 1 1 1	5 2 0 - 3 3 2 1 0 5 - 2 3 3 2 3 3	58.67 59.35 59.42 61.00 61.09
2 •1 36 2 •1 32 2 •1 83 2 •1 74 2 •0 70	2 2 4 2 4	-2 2 2 2 2 2 -3 2 1 -4 1 1 4 1 1	42.28 42.36 43.40 43.61 43.68	1 •5 08 1 •5 06 1 •5 03 1 •5 02 1 •4 94	1 1 1 1	-503 -423 503 423 -431	61.44 61.54 61.66 61.72 62.09
2.030 1.998 1.991 1.990 1.987	5 1 3 5 6	0 3 0 - 3 0 3 3 0 3 0 2 3 - 4 0 2	44.60 45.35 45.52 45.54 45.62	1 • 4 92 1 • 4 76 1 • 4 75 1 • 4 64 1 • 4 62	1 1 1 1 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	62.15 62.93 62.95 63.50 63.58

Monoclinic, P2, (4), Z=4, [Hvoslef, 1968]

Lattice parameters

 $a=17.300\pm.008, b=6.353\pm.003, c=6.411\pm.003Å$ $\beta=102^{11'\pm08'}, (published value, a=17.299)$ [ibid.]

Density

(calculated) 1.699 g/cm³ [ibid.]

Thermal parameters

Isotropic:0(1) 1.94;0(2) 1.70;0(3) 1.85; 0(4) 1.85;0(5) 2.04;0(6) 2.38;0(1)*1.98; 0(2)*1.77;0(3)*2.16;0(4)*1.55;0(5)*1.80; 0(6)*1.92;C(1) 1.51;C(2) 1.37;C(3) 1.41; C(4) 1.59;C(5) 1.60;C(6) 1.96;C(1)*1.45; C(2)*1.53;C(3)*1.62;C(4)*1.56;C(5)*1.57; C(6)*1.72; Hydrogen parameters as given [ibid.] for the Stewart, Davidson, and Simpson form factors.

Scattering factors

C°, O° [3.3.1A] H° [Stewart, Davidson, and Simpson, 1965]

Scale factor

(integrated intensities) 1.773 \times 10⁴

Additional patterns

 PDF card 4-0308 [Inst. of Physics, Univ. College, Cardiff]

Reference

- Hvoslef, J. (1968). The crystal structure of *l*-ascorbic acid, "vitamin C". I. The x-ray analysis, Acta Cryst. B24, 23-35.
- Stewart, R.F., E.R.Davidson, and W.T.Simpson (1965). Coherent x-ray scattering for the hydrogen atom in the hydrogen molecule, J. Chem. Phys. 42, 3175-3187.

Ca	Calculated Pattern (Peak heights)						
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 ^{\circ}A}$				
8.45	40	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	10.46				
6.32	8		14.00				
6.27	14		14.12				
5.63	17		15.72				
5.51	15		16.08				
5.08	40	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	17.46				
4.480	65		19.80				
4.462	68		19.88				
4.215	18		21.06				
4.160	7		21.34				
3.786	12	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	23.48				
3.720	1		23.90				
3.520	38		25.28				
3.329	15		26.76				
3.281	10		27.16				
3.204	6	-1 0 2 +	27.82				
3.177	100	0 2 0	28.06				
3.023	8	-3 0 2	29.52				
2.972	64	2 2 0 +	30.04				
2.914	1	-5 1 1	30.66				
2.861 2.838 2.832 2.819 2.801	2 2 1 3	$ \begin{array}{cccccc} -1 & 1 & 2 \\ -1 & 2 & 1 \\ 0 & 2 & 1 \\ 6 & 0 & 0 \\ -6 & 0 & 1 \end{array} $	31.24 31.50 31.56 31.72 31.92				
2.768 2.751 2.730 2.692 2.635	1 2 5 3	$\begin{array}{ccccc} -2 & 2 & 1 \\ 1 & 2 & 1 \\ -3 & 1 & 2 \\ 1 & 1 & 2 \\ -3 & 2 & 1 \end{array}$	32.32 32.52 32.78 33.26 34.00				
2.612	2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	34 • 30				
2.586	10		34 • 6 6				
2.576	10		34 • 80				
2.563	4		34 • 98				
2.539	8		35 • 32				
2.523	22	3 0 2 +	35.56				
2.439	1	3 2 1	36.82				
2.433	2	-7 0 1	36.92				
2.395	10	-5 1 2	37.52				
2.272	3	-7 1 1	39.64				
2.256	3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	39.92				
2.236	9		40.30				
2.169	11		41.60				
2.136	3		42.28				
2.109	7		42.84				
2.103 2.089 2.054 2.032 2.018	5 4 2 2	$ \begin{array}{cccccc} -6 & 2 & 1 \\ 5 & 0 & 2 \\ 2 & 3 & 0 \\ -7 & 1 & 2 \\ -1 & 1 & 3 \end{array} $	42.98 43.28 44.04 44.56 44.88				

Calculated Pattern (Peak heights)							
d (Å)	Ι	hkl			$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$		
2.005 2.002 1.975 1.953 1.932	5 9 6 1 2	8 -3 3 -4 -7	1 1 2 1 2	0 3 2 3 1	+ +	45.18 45.26 45.90 46.46 47.00	
1.893 1.886 1.879 1.851 1.808	2 2 2 1 1	4 8 -6 2 8	3 0 0 1 1	0 1 3 3 1	+	48.02 48.22 48.40 49.18 50.44	
1.802 1.786 1.778 1.772 1.764	1 1 3 2 1	-6 -9 -7 -2 3	1 0 2 2 1	3 2 2 3 3	+	50.62 51.10 51.36 51.52 51.78	
1.757 1.745 1.693 1.689 1.681	1 2 3 1	7 0 6 -6 7	2 2 3 3 1	1 3 0 1 2	+	52.00 52.38 54.14 54.26 54.54	
1.639 1.634 1.588 1.584 1.582	1 2 3 3 2	-5 10 0 6 -4	3 1 4 3 0	2 0 1 4		56.08 56.24 58.02 58.18 58.28	
1.561 1.557 1.535 1.501 1.494	4 3 1 1 1	2 -9 -4 9 -3	4 2 1 2 3	0 2 4 1 3		59.14 59.30 60.24 61.74 62.06	
1.441 1.437 1.409 1.401 1.395	1 1 2 1 1	9 -10 -9 1 10	1 1 2 4 2	2 3 3 2 1	+	64.62 64.82 66.30 66.72 67.04	
Ca	Calculated Pattern (Integrated) Calculated Pattern (Integrated)						
---	---	---	---	--	-----------------------	---	--
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$
8.46 6.33 6.27 5.64 5.51	29 6 10 13 12	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	10.45 13.99 14.12 15.71 16.07	2.101 2.089 2.054 2.032 2.022	3 4 4 1 1	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	43.02 43.27 44.05 44.56 44.79
5.08 4.483 4.461 4.216 4.162	35 52 46 15 6	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	17.45 19.79 19.88 21.06 21.33	2.018 2.008 2.006 2.006 2.006	2 2 1 2 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	44.87 45.11 45.16 45.17 45.17
3.786 3.722 3.520 3.329 3.280	11 1 36 14 9	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	23.48 23.89 25.28 26.76 27.17	2.002 2.002 1.975 1.953 1.932	2 6 6 1 2	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	45.25 45.26 45.91 46.45 47.01
3.205 3.204 3.176 3.023 2.974	1 2 100 7 51	4 0 1 -1 0 2 0 2 0 -3 0 2 2 2 0	27.81 27.82 28.07 29.53 30.03	1.893 1.886 1.884 1.879 1.851	2 2 1 1 1	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	48.01 48.21 48.26 48.42 49.18
2.971 2.914 2.861 2.839 2.833	19 1 2 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	30.06 30.65 31.24 31.49 31.55	1.808 1.801 1.786 1.779 1.777	1 1 1 2 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	50.43 50.63 51.09 51.31 51.37
2.818 2.801 2.767 2.752 2.730	1 2 1 2 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	31.72 31.92 32.32 32.51 32.78	1.772 1.764 1.757 1.745 1.693	1 1 1 1 2	-2 2 3 3 1 3 7 2 1 0 2 3 6 3 0	51.52 51.77 51.99 52.38 54.13
2.691 2.634 2.612 2.587 2.576	5 3 1 10 8	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	33.27 34.00 34.30 34.65 34.79	1.691 1.689 1.681 1.639 1.634	1 2 1 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	54.20 54.26 54.53 56.08 56.25
2.563 2.540 2.522 2.519 2.440	3 7 23 1 1	$\begin{array}{cccc} -6 & 1 & 1 \\ 4 & 2 & 0 \\ 3 & 0 & 2 \\ 5 & 1 & 1 \\ 3 & 2 & 1 \end{array}$	34.98 35.31 35.57 35.61 36.81	1.588 1.585 1.582 1.561 1.557	3 2 1 5 1	0 4 0 6 3 1 -4 0 4 2 4 0 -9 2 2	58.02 58.17 58.28 59.14 59.30
2.433 2.396 2.272 2.256 2.256	1 11 3 1 2	$\begin{array}{cccc} -7 & 0 & 1 \\ -5 & 1 & 2 \\ -7 & 1 & 1 \\ 4 & 2 & 1 \\ -1 & 2 & 2 \end{array}$	36.91 37.51 39.63 39.93 39.93	$1 \cdot 5 35 \\ 1 \cdot 5 01 \\ 1 \cdot 4 94 \\ 1 \cdot 4 41 \\ 1 \cdot 4 37$	1 1 1 1	-4 1 4 9 2 1 -3 3 3 9 1 2 -10 1 3	60.24 61.74 62.05 64.63 64.82
2.236 2.170 2.136 2.110 2.108	9 13 4 4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	40.30 41.59 42.29 42.83 42.85	1.409 1.408 1.401 1.395	1 1 1 1	-9 2 3 8 3 1 1 4 2 10 2 1	66.30 56.31 66.73 67.05

Monoclinic, $P2_1/c$ (14), Z=2, [Calleri et al., 1966]

Lattice parameters

a=3.868±.011,b=4.414±.015,c=10.949±.035Å β=91°10′ [ibid.]

Density

(calculated) 1.555 g/cm³ [ibid.]

Thermal parameters

Isotropic: C(l) 1.704; N(l) 1.625; O(l) 2.248; H(l) 1.50; H(l') 3.0

Scattering factors

 H° , C° , N° , O° [3.3.1A]

Scale factor

(integrated intensities) 0.1436 \times 10⁴

Reference

Calleri, M., G. Ferraris, and D. Viterbo (1966). The crystal and molecular structure of glyoxime, Acta Cryst. 20 73-80.

Calculated Pattern (Peak heights)				
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$	
5.47	1	0 0 2	16.18	
4.09	2	0 1 1	21.70	
3.87	75	1 0 0	22.98	
3.43	100	0 1 2	25.32	
3.19	82	-1 0 2	27.96	
3.13	19	1 0 2	28.50	
2.91	35	1 1 0	30.72	
2.81	50	0 1 3	31.80	
2.80	58	1 1 1	31.92	
2.74	7	0 0 4	32.70	
2.58	10	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	34.68	
2.55	20		35.14	
2.26	5		39.94	
2.21	1		40.74	
2.05	2		44.22	
1.92	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	47.38	
1.89	2		48.16	
1.88	3		48.24	
1.84	3		49.64	
1.82	6		49.94	
1.82 1.77 1.76 1.75 1.74	2 3 5 2	$ \begin{array}{cccccc} -1 & 2 & 2 \\ 2 & 1 & 0 \\ -1 & 1 & 5 \\ -2 & 1 & 1 \\ 1 & 1 & 5 \end{array} $	50.22 51.56 51.84 52.12 52.66	
1.69	4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	54.24	
1.68	12		54.72	
1.61	1		57.36	
1.58	3		58.28	
1.56	4		59.06	
1.56 1.458 1.454 1.439 1.400	2 2 3 3	-1 1 6 0 3 1 2 2 0 2 2 1 2 2 2	59.32 63.78 63.96 64.74 66.74	
1.369	1	1 1 7	68.50	
1.366	3	-1 3 1	68.68	
1.307	1	0 1 8	72.22	
1.298	2	-1 0 8	72.78	
1.293	1	-2 2 4	73.15	
1.227	1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	77.78	
1.148	1		84.30	
1.095	1		89.46	

Calculated Pattern (Integrated)				
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$	
5.47	1	0 0 2	16.18	
4.09	2	0 1 1	21.69	
3.87	69	1 0 0	22.98	
3.44	100	0 1 2	25.91	
3.19	31	-1 0 2	27.95	
3.13	19	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	28.51	
2.91	35		30.71	
2.82	2		31.68	
2.81	47		31.79	
2.80	62		31.93	
2.74	6	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	32.70	
2.59	10		34.67	
2.55	22		35.13	
2.26	5		39.93	
2.21	1		40.74	
2.05	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	44.21	
1.92	4		47.33	
1.89	2		48.14	
1.88	3		48.24	
1.88	3		43.54	
1.82 1.81 1.77 1.76 1.75	8 1 4 5	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	49.95 50.23 51.56 51.84 52.11	
1.74	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	52.67	
1.63	6		54.23	
1.68	2		54.72	
1.61	1		57.38	
1.58	4		58.28	
1.56 1.56 1.458 1.454 1.439	5 3 3 4	1 2 4 -1 1 6 0 3 1 2 2 0 2 2 1	59.07 59.33 53.77 63.96 54.74	
1.409	2	2 2 2	56.75	
1.375	1	1 3 0	58.13	
1.369	1	1 1 7	68.50	
1.366	3	-1 3 1	68.67	
1.307	1	0 1 8	72.22	
1.298	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	72 • 7 8	
1.293	1		73 • 1 6	
1.227	1		77 • 7 8	
1.183	1		91 • 2 3	
1.148	1		84 • 2 9	
1.129	1 1 1 1 1	2 2 6	86.06	
1.098		0 4 1	89.11	
1.095		-3 2 2	89.46	
1.094		1 3 6	89.48	

Monoclinic, $P2_1/n$ (14), Z=4 [Feikema and Vos, 1966]

Lattice parameters

a= 7.548±0.01, b= 7.680±0.01, c= 11.402± $0.015\text{\AA}, \beta = 90.1\pm0.1^{\circ}$ [ibid.]

Density

(calculated) 5.04 g/cm³ [ibid.]

Thermal parameters

Isotropic: O(1) through O(8) [ibid.] I(1) .557 I(2) .528 I(3) .565

Scattering factors

0° [3.3.1A] I° [3.3.1B]

Scale factor

(integrated intensities) 25.00 \times 10^4

Reference

Feikema, Y.D. and A.Vos(1966). The crystal structures of two oxy-acids of iodine. II. An x-ray diffraction study of anhydro-iodic acid, HI₃O₈, Acta Cryst. 20, 769-777.

Calculated Pattern (Peak heights)				
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$	
6 • 3 7 6 • 2 8 4 • 8 7 4 • 5 8 3 • 9 1	12 11 11 1 1 1 3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	13.90 14.08 18.22 19.38 22.70	
3 • 8 4	15	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	23.14	
3 • 7 7	60		23.56	
3 • 6 4	7		24.44	
3 • 3 9	62		26.24	
3 • 2 8	100		27.18	
3 • 2 5	8	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	27.44	
3 • 1 8	20		28.00	
3 • 1 4	11		28.36	
3 • 1 0	6		28.74	
2 • 9 34	3		30.44	
2 •9 14	7	-2 1 2 +	30.66	
2 •8 50	10	0 0 4	31.36	
2 •7 01	1	0 2 3	33.14	
2 •6 92	3	2 2 0	33.26	
2 •6 20	4	2 2 1 +	34.20	
2 •5 43	14	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	75.26	
2 •5 31	5		35.44	
2 •5 20	10		75.60	
2 •4 57	2		36.54	
2 •4 35	15		36.88	
2 •4 28	9	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	37.00	
2 •3 71	1		37.92	
2 •3 39	7		38.46	
2 •2 88	7		39.34	
2 •2 73	4		39.62	
2 • 2 31	1	-1 3 2	40.40	
2 • 2 04	2	3 1 2 +	40.92	
2 • 1 83	10	-2 1 4 +	41.32	
2 • 1 79	10	2 1 4	41.40	
2 • 1 23	1	n 3 3	42.54	
2 •1 19	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	42.54	
2 •0 99	5		43.06	
2 •0 82	1		43.42	
2 •0 69	1 3		43.72	
2 •0 45	4		44.26	
2.025 2.022 1.975 1.956 1.920	к к 7 5	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	44.72 44.78 45.90 46.38 47.30	
1 •9 04 1 •9 00 1 •8 93 1 •8 90 1 •8 87	2 3 3 3 3 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	47.72 47.84 48.02 48.10 48.18	

					and the second se
Ca	lculated	Pattern (Pe	ak he	ights)	Calc
d (Å)	Ι	hkl		$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$	d (Å)
1 •8 61 1 •8 50 1 •8 45 1 •8 42 1 •8 36	F 7 3 4	1 4 2 3 0 1 - 3 2 1 4	0 3 6 + 3 = 1	4 P . 90 4 9 . 77 4 9 . 36 4 9 . 44 4 9 . 60	6 • 3 7 6 • 3 0 6 • 2 9 5 • 7 0 4 • 8 7
1 •8 32 1 •8 09 1 •7 91 1 •7 72 1 •7 68	5 1 3 5 3	3 1 4 1 4 1 3 3 1 4	4 + 1 2 + 1 + 2	49.74 50.40 50.96 51.52 51.66	4.87 4.58 3.92 3.91 3.84
1 • 7 45 1 • 7 11 1 • 7 03 1 • 6 99 1 • 6 95	7 7 8 9 4	-4 1 2 4 0 2 2 3 -2 4	2 + N + 6 + 4 + 1	52.38 53.50 53.78 53.92 54.06	3.77 3.64 3.41 3.40 3.39
1 •6 91 1 •6 71 1 •6 62 1 •6 58 1 •5 52	3 7 3 2 4	$ \begin{array}{rrrrr} -3 & 0 \\ -1 & 4 \\ -1 & 3 \\ -2 & 1 \\ -3 & 1 \end{array} $	5 3 + 5 + 6 + 5 +	54.18 54.90 55.24 55.38 55.60	3.39 3.28 3.28 3.25 3.25 3.25
1.649 1.639 1.624 1.592 1.560	5 1 6 8 3	3 1 2 4 -3 3 -1 0 -2 4	5 + 2 + 3 + 7 + 3 +	55.70 56.06 56.64 57.86 59.18	3 •1 8 3 •1 5 3 •1 4 3 •1 0 2 •9 35
1 •5 59 1 •5 53 1 •5 49 1 •5 46 1 •5 40	3 7 4 2 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	7 + 6 + 5 5 4	59.24 59.46 59.64 59.78 60.02	2.933 2.914 2.910 2.851 2.701
1 •5 26 1 •5 19 1 •5 13 1 •4 96 1 •4 93	2 2 1 1 1	34 43 34 50 -15	0 0 1 1 + 1	60.62 61.94 61.22 61.98 62.14	2 • 6 92 2 • 6 20 2 • 6 19 2 • 5 4 4 2 • 5 4 2
1 •4 87 1 •4 74 1 •4 68 1 •4 15 1 •4 12	1 1 5 2 2	3 1 3 4 5 1 -2 3 2 5	6 7 1 + 6 + 1	62.42 63.02 63.28 65.94 65.14	2 • 5 31 2 • 5 27 2 • 5 20 2 • 5 18 2 • 4 58
1.399 1.395 1.381 1.368 1.366	3 1 2 1 1	1 5 5 2 - 2 5 - 3 0 3 0	3 1 2 7 7	66.80 67.02 67.82 68.52 68.64	2 • 4 56 2 • 4 35 2 • 4 24 2 • 3 72 2 • 3 71
1 .351 1 .345 1 .340 1 .336 1 .320	1 1 4 4 1	1 4 3 1 4 3 1 2 - 4 1	6 + 7 4 8 + 6	69.50 69.86 70.20 70.40 71.38	2.339 2.335 2.289 2.277 2.273

		1	
C	alculated	l Pattern (Integra	ited)
d (Å)	Ι	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \overset{\circ}{A}$
6 •3 7	13	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1 3.89
6 •3 0	2		1 4.05
6 •2 9	11		1 4.07
5 •7 0	1		1 5.53
4 •8 7	5		1 8.20
4.87	8	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1 8. 22
4.58	1		1 9. 37
3.92	11		22. 69
3.91	7		22. 71
3.84	18		2 3. 14
3.77	79	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	23.55
3.64	9		24.44
3.41	15		26.14
3.40	50		26.21
3.39	41		26.25
3 • 3 9	13	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	26.29
3 • 2 8	41		27.17
3 • 2 8	100		27.19
3 • 2 5	5		27.43
3 • 2 5	1		27.46
3 •1 8	27	N 2 2 -2 0 2 2 0 2 1 1 3 -1 2 2	27.99
3 •1 5	4		28.31
3 •1 4	12		28.36
3 •1 0	7		28.75
2 •9 35	2		30.43
2.933	2	1 2 2	3 N. 45
2.914	9	-2 1 2	3 N. 66
2.910	1	2 1 2	3 N. 7 N
2.851	1 4	0 0 4	3 I. 36
2.701	1	0 2 3	3 3. 1 4
2 •6 92	4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	33.26
2 •6 20	2		34.19
2 •6 19	5		34.21
2 •5 44	1, 4		35.25
2 •5 42	9		35.27
2.531	3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	35.44
2.527	3		35.50
2.520	1 0		35.59
2.518	7		35.63
2.458	3		36.53
2 • 4 56	1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	36.56
2 • 4 35	22		36.88
2 • 4 24	2		37.05
2 • 3 72	1		37.91
2 • 3 71	1		37.91
2.339	10	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	38.45
2.335	3		38.52
2.289	10		39.33
2.277	2		39.55
2.273	5		39.62

2θ(°)

 $\lambda = 1.54056 \text{ Å}$

53.42

53.47

53.50

53.78 53.79

53.90

53.94

54.14 54.19

54.76

54.88

54.90 55.22

55.24

55.27 55.35

55.43

55.59

55.60 55.67

55.70

56.05

56.08 56.62 56.65

57.84 57.86

57.89

59.14 59.18

59.24

59.24

59.46

59.48 59.53

59.54 59.70

59.79

60.01 60.62

60.94

61.23 61.97

62.02

62.15

62.42

63.01 63.19 63.24

63.27

C	alculated	l Pattern <i>(Inte</i>	grated)		Ca	alculated	l Patte	rn (Integr	rated)	
đ (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$	d	(Å)	Ι		hkl	λ =	
2 •231 2 •206 2 •204 2 •191 2 •189	2 1 2 1 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	4 N. 39 4 N. 87 4 N. 92 4 1. 16 4 1. 20	1 • 1 • 1 • 1 •	714 712 711 703 703	4 3 8 1 2 1	n -3 2 0	43 32 40 26 35		
2 • 1 86 2 • 1 84 2 • 1 83 2 • 1 79 2 • 1 23	5 4 5 8 1	0 1 5 -1 0 5 -2 1 4 2 1 4 0 3 3	41.26 41.30 41.33 41.40 42.54	1 • 1 • 1 • 1 •	7 00 6 98 6 93 6 91 6 75	9 2 1 2 2	2 -2 -3 4	3 4 0 6 4 1 0 5 2 1		
2.119 2.101 2.100 2.099 2.096	3 1 4 3 1	2 3 0 -1 1 5 -3 0 3 1 1 5 3 0 3	4 2 • 6 4 4 3 • 11 2 4 3 • 11 4 4 3 • 11 6 4 3 • 1 2		671 67) 662 662 661	8 5 2 2 1	- 1 1 - 1 - 1 1	4 3 4 3 2 6 3 5 3 5		
2.083 2.070 2.069 2.044 2.025	1 3 19 6 8	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	43.42 43.69 43.71 44.27 44.71		6 58 6 56 6 52 6 52 6 50	1 7 3 1	-2 2 -4 -3 4	1 6 1 6 1 3 1 5 1 3		
2 .022 1.985 1.975 1.958 1.956	6 1 3 1 11	3 1 3 2 3 2 -3 2 2 -2 2 4 2 2 4	44.78 45.66 45.91 46.33 46.39		649 639 639 624 623	5 1 4 8	3 - 2 2 - 4 - 3	1 5 4 2 4 2 2 2 3 3		
1.920 1.905 1.900 1.897 1.893	8 3 2 1 2	0 4 0 0 3 4 0 0 6 1 2 5 -2 1 5	47.30 47.71 47.82 47.91 48.02	1 • 1 • 1 • 1 •	5 93 5 92 5 92 5 61 5 60	7 3 6 2 2	-1 1 -2 2	07 44 07 43 43		
1 •8 90 1 •8 87 1 •861 1 •850 1 •847	2 4 10 2 1	2 1 5 4 0 0 1 4 0 2 3 3 -1 3 4	48.10 48.18 48.91 49.22 49.29	1 • 1 • 1 • 1 •	5 59 5 58 5 5 3 5 5 3 5 5 7	1 9 2 2	1 - 1 - 2 - 2 2	1 7 4 4 2 6 3 5 2 6		
1 •845 1 •842 1 •836 1 •833 1 •832	2 3 4 3 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	49.36 49.43 49.60 49.69 49.71	1 • 1 1 • 1 1 • 1 1 • 1	551 548 545 540 526	1 2 5 3	2 - 3 3 4 3	3 5 2 5 2 5 1 4 4 0		
1 •830 1 •809 1 •793 1 •791 1 •790	4 1 2 3	3 1 4 4 1 1 -1 1 6 1 1 6 4 0 2	4 9.77 5 0.41 5 0.90 5 0.94 5 0.96		519 513 495 495 492	2 1 1 1 1	4 3 5 1 - 1	3 0 4 1 0 1 3 6 5 1		
1.773 1.772 1.769 1.745 1.744	1 7 1 11 4	-331 331 142 -412 412	51.50 51.52 51.64 52.37 52.43		+ 86 + 74 + 71 + 69 + 69	1 1 2 2 5	3 3 - 5 5	1 6 4 2 2 7 1 1 1 1		
	C d(A) 2.231 2.206 2.204 2.191 2.189 2.186 2.184 2.183 2.179 2.123 2.119 2.101 2.100 2.096 2.083 2.070 2.096 2.083 2.070 2.069 2.044 2.025 2.070 2.069 2.044 2.025 2.070 2.069 2.044 2.025 2.070 1.985 1.975 1.958 1.975 1.958 1.955 1.955 1.955 1.955 1.955 1.955 1.955 1.955 1.897 1.887 1.887 1.887 1.847 1.845 1.847 1.845 1.847 1.845 1.847 1.845 1.847 1.845 1.847 1.845 1.847 1.845 1.847 1.793 1.791 1.791 1.775 1.744	Calculated $d'(A)$ I 2.23122.20612.20422.19112.18652.18442.18362.17982.17312.10112.10312.10422.09612.09612.09612.09612.09612.097032.09612.09582.02582.02582.02511.95511.95511.95511.95511.95511.89711.89711.89711.89711.89711.89711.89711.89711.89711.89711.79321.79121.79321.79121.77311.774111.745111.7444	Calculated Pattern (Integ d (Å) I hkl 2.231 2 -1 3 2 2.206 1 -3 1 2 2.191 1 -1 2 4 2.183 6 0 1 5 2.184 4 -1 0 5 2.183 6 -2 1 4 2.179 8 2 1 4 2.183 6 -2 1 4 2.179 8 2 1 4 2.100 4 -3 0 3 2.000 4 -3 0 3 2.005 1 3 0 3 2.006 1 3 0 3 2.0101 1 -1 3 2 2.0070 3 -3 2 1 2.0101 2 3 1 3 </td <td>Calculated Pattern (Integrated)$d(\hat{A})$I$hkl$$2\theta(?)$ $\lambda = 1.54056 \hat{A}$2.2312-13240.872.2061-31240.872.2061-31240.872.1911-12441.202.189312441.202.186501541.332.179821441.402.17310342.542.119323042.642.1011-11543.062.103130343.122.103130343.122.1011-11543.042.099311543.042.096130343.122.0703-32143.692.0661932143.712.0258-31344.772.0258-31344.781.956122446.391.958122446.391.958127451.956122446.391.955127349.291.96512</td> <td>Calculated Pattern (Integrated) d (Å) I hkl $2 \theta(°)$ $\lambda = 1.54056 Å$ d 2.231 2 -1 3 2 40.39 1. 2.204 2 3 1 2 40.92 1. 2.191 1 -1 2 4 1.092 1. 2.189 3 1 2 4 41.26 1. 2.184 4 -1 0 5 41.26 1. 2.185 5 0 1 5 41.26 1. 2.184 4 -1 0 5 41.30 1. 2.179 8 2 1 4 41.40 1. 2.100 4 -3 0 3 43.02 1. 2.099 3 1 1 5 43.04 1. 2.070 3 -3 2 43.69 1. 1. 2.069 <t< td=""><td>Calculated Pattern (Integrated)Calculated Pattern (Integrated)d (Å)Ihkl$2\theta(^{\circ})$ $\lambda = 1.54056Å$d (Å)2.7312-132$\theta(^{\circ})$ $\lambda = 1.54056Å$d (Å)2.7312-132$\theta(^{\circ})$ $\lambda = 1.54056Å$d (Å)2.7312-132$\theta(^{\circ})$ $\lambda = 1.54056Å$d (Å)2.1611-12$40.92$ $\lambda = 1.711$1.712 $\lambda = 1.713$2.1893124$41.261$ $\lambda = 1.703$1.7732.1865015$41.766$ $\lambda = 1.700$1.7032.1836-214$41.401$ $\lambda = 1.693$1.693 $\lambda = 1.573$2.1798214$41.401$ $\lambda = 1.6657$1.6752.11932303$43.12$2.1601-115$43.06$ $\lambda = 1.6757$2.1993115$43.06$ $\lambda = 1.6651$2.0961303$43.12$2.0691303$43.12$2.0691303$44.71$2.06919321$45.66$ <math>1.6592.06919321$45.66$ <math>1.6592.0706313$44.71$2.65278-31$44.78$ $1.65522.09263$</math></math></td></t<></td> <td>Calculated Pattern (Integrated) Calculated d (\mathring{A}) I Ikl $2\theta(?)$ $\lambda = 1.54056 \mathring{A}$ Calculated 2.231 2 -1 3 2 40.87 1.714 4 2.206 1 -3 1 2 40.87 1.711 3 2.704 2 3 1 2 40.87 1.711 8 2.191 1 -1 2 4 41.26 1.703 12 2.186 5 0 1 5 41.37 1.698 2 2.186 -1 0 5 41.407 1.693 1 2.173 1 0 3 42.64 1.671 8 2.101 1 -1 5 43.06 1.667 2 2.199 3 1 1 5 43.06 1.667 2.103 4 -3 3 42.71 1.656 2.199</td> <td>Calculated Pattern (Integrated) Calculated Pattern (Integrated) d (Å) I hkl $2\theta(7)$ $\lambda = 1.5666 Å d (Å) I 2.231 2 -1 3 2 40.39 1.714 4 0 2.206 1 -3 1 2 40.67 1.712 3 -3 2.191 1 -1 2 40.67 1.7103 1 0 2.186 5 0 1 5 41.26 1.703 1 0 2.184 4 -1 0 5 41.33 1.693 -2 2.184 4 -1 5 41.76 1.671 8 -1 2.179 8 2 1 4 41.40 1.651 1 1 2.101 1 -1 1 5 43.64 1.671 8 -1 2.006 1 3 0 3 43.12 1.658 -2<$</td> <td>Calculated Pattern (Integrated) $d(\hat{A})$ I bit of the system $d(\hat{A})$ I bit of the system Calculated Pattern (Integrated) $d(\hat{A})$ I bit of the system Calculated Pattern (Integrated) <th colspa<="" td=""></th></td>	Calculated Pattern (Integrated) $d(\hat{A})$ I hkl $2\theta(?)$ $\lambda = 1.54056 \hat{A}$ 2.2312-13240.872.2061-31240.872.2061-31240.872.1911-12441.202.189312441.202.186501541.332.179821441.402.17310342.542.119323042.642.1011-11543.062.103130343.122.103130343.122.1011-11543.042.099311543.042.096130343.122.0703-32143.692.0661932143.712.0258-31344.772.0258-31344.781.956122446.391.958122446.391.958127451.956122446.391.955127349.291.96512	Calculated Pattern (Integrated) d (Å) I hkl $2 \theta(°)$ $\lambda = 1.54056 Å$ d 2.231 2 -1 3 2 40.39 1. 2.204 2 3 1 2 40.92 1. 2.191 1 -1 2 4 1.092 1. 2.189 3 1 2 4 41.26 1. 2.184 4 -1 0 5 41.26 1. 2.185 5 0 1 5 41.26 1. 2.184 4 -1 0 5 41.30 1. 2.179 8 2 1 4 41.40 1. 2.100 4 -3 0 3 43.02 1. 2.099 3 1 1 5 43.04 1. 2.070 3 -3 2 43.69 1. 1. 2.069 <t< td=""><td>Calculated Pattern (Integrated)Calculated Pattern (Integrated)d (Å)Ihkl$2\theta(^{\circ})$ $\lambda = 1.54056Å$d (Å)2.7312-132$\theta(^{\circ})$ $\lambda = 1.54056Å$d (Å)2.7312-132$\theta(^{\circ})$ $\lambda = 1.54056Å$d (Å)2.7312-132$\theta(^{\circ})$ $\lambda = 1.54056Å$d (Å)2.1611-12$40.92$ $\lambda = 1.711$1.712 $\lambda = 1.713$2.1893124$41.261$ $\lambda = 1.703$1.7732.1865015$41.766$ $\lambda = 1.700$1.7032.1836-214$41.401$ $\lambda = 1.693$1.693 $\lambda = 1.573$2.1798214$41.401$ $\lambda = 1.6657$1.6752.11932303$43.12$2.1601-115$43.06$ $\lambda = 1.6757$2.1993115$43.06$ $\lambda = 1.6651$2.0961303$43.12$2.0691303$43.12$2.0691303$44.71$2.06919321$45.66$ <math>1.6592.06919321$45.66$ <math>1.6592.0706313$44.71$2.65278-31$44.78$ $1.65522.09263$</math></math></td></t<>	Calculated Pattern (Integrated)Calculated Pattern (Integrated)d (Å)Ihkl $2\theta(^{\circ})$ $\lambda = 1.54056Å$ d (Å)2.7312-132 $\theta(^{\circ})$ $\lambda = 1.54056Å$ d (Å)2.7312-132 $\theta(^{\circ})$ $\lambda = 1.54056Å$ d (Å)2.7312-132 $\theta(^{\circ})$ $\lambda = 1.54056Å$ d (Å)2.1611-12 40.92 $\lambda = 1.711$ 1.712 $\lambda = 1.713$ 2.1893124 41.261 $\lambda = 1.703$ 1.7732.1865015 41.766 $\lambda = 1.700$ 1.7032.1836-214 41.401 $\lambda = 1.693$ 1.693 $\lambda = 1.573$ 2.1798214 41.401 $\lambda = 1.6657$ 1.6752.11932303 43.12 2.1601-115 43.06 $\lambda = 1.6757$ 2.1993115 43.06 $\lambda = 1.6651$ 2.0961303 43.12 2.0691303 43.12 2.0691303 44.71 2.06919321 45.66 $1.6592.0691932145.661.6592.070631344.712.65278-3144.781.65522.09263$	Calculated Pattern (Integrated) Calculated d (\mathring{A}) I Ikl $2\theta(?)$ $\lambda = 1.54056 \mathring{A}$ Calculated 2.231 2 -1 3 2 40.87 1.714 4 2.206 1 -3 1 2 40.87 1.711 3 2.704 2 3 1 2 40.87 1.711 8 2.191 1 -1 2 4 41.26 1.703 12 2.186 5 0 1 5 41.37 1.698 2 2.186 -1 0 5 41.407 1.693 1 2.173 1 0 3 42.64 1.671 8 2.101 1 -1 5 43.06 1.667 2 2.199 3 1 1 5 43.06 1.667 2.103 4 -3 3 42.71 1.656 2.199	Calculated Pattern (Integrated) Calculated Pattern (Integrated) d (Å) I hkl $2\theta(7)$ $\lambda = 1.5666 Å d (Å) I 2.231 2 -1 3 2 40.39 1.714 4 0 2.206 1 -3 1 2 40.67 1.712 3 -3 2.191 1 -1 2 40.67 1.7103 1 0 2.186 5 0 1 5 41.26 1.703 1 0 2.184 4 -1 0 5 41.33 1.693 -2 2.184 4 -1 5 41.76 1.671 8 -1 2.179 8 2 1 4 41.40 1.651 1 1 2.101 1 -1 1 5 43.64 1.671 8 -1 2.006 1 3 0 3 43.12 1.658 -2<$	Calculated Pattern (Integrated) $d(\hat{A})$ I bit of the system $d(\hat{A})$ I bit of the system Calculated Pattern (Integrated) $d(\hat{A})$ I bit of the system Calculated Pattern (Integrated) Calculated Pattern (Integrated) <th colspa<="" td=""></th>	

Monoclinic, $P2_1/c$ (14), Z=4 [Maartmann-Moe, 1966]

Lattice parameters

a=8.07, b=5.20, c=13.20Å, β =107°. The cell dimensions are estimated to be accurate to within 0.5 %. [ibid.]

Density

(calculated) 1.380 g/cm³ [ibid.]

Thermal parameters

Anisotropic (ibid.)

Scattering factors

 H° , C° , O° [3.3.1A]

Scale factor

(integrated intensities) 1.294 \times 10⁴

Reference

Maartmann-Moe,K.(1966). The crystal structure of Y-hydroquinone, Acta Cryst. 21, 979-982.

Ca	Calculated Pattern (Peak heights)				
d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056 \stackrel{\circ}{A}$		
6.31	13	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	14.02		
4.30	79		20.64		
4.01	2		22.14		
3.89	54		22.P4		
3.86	100		23.04		
3.29	11	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	27.06		
3.19	2		27.96		
3.10	31		28.78		
3.08	17		28.94		
2.93	2		30.46		
2.86	2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	71.28		
2.79	7		32.02		
2.60	2		34.46		
2.55	7		35.10		
2.46	1		36.46		
2.40	14	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37.38		
2.38	5		37.74		
2.35	1		38.22		
2.29	4		39.30		
2.17	2		41.58		
2.16	6	2 2 0	41.86		
2.15	7	-2 2 2	41.98		
2.13	3	-2 0 6	42.46		
2.10	2	0 0 6	42.96		
2.02	1	-4 0 2	44.90		
1.95	2	2 2 2	46.64		
1.88	1	-4 1 2	48.36		
1.87	2	-3 2 1 +	48.78		
1.83	1	3 1 3	49.78		
1.81	1	4 1 0	50.40		
1.77	3	-1 1 7	51.60		
1.76	1	3 2 1	51.96		
1.71	1	4 0 2	53.52		
1.65	2	-3 1 7	55.84		
1.64	1	-2 0 8	56.10		
1.61	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	57.36		
1.57	1		58.58		
1.55	2		59.62		
1.54	1		60.22		
1.18	1		81.80		

C	Calculated Pattern (Integrated)				
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$		
6 • 3 1	11	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	14.02		
4 • 3 0	76		20.63		
4 • 0 1	1		22.13		
3 • 8 9	49		22.84		
3 • 8 6	100		23.03		
3 • 2 9	12	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	27.06		
3 • 1 9	2		27.97		
3 • 1 0	33		28.79		
3 • 0 8	14		28.94		
2 • 9 3	2		30.46		
2 .86	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	31.27		
2 .79	8		32.03		
2 .61	2		34.47		
2 .55	8		35.10		
2 .46	1		36.47		
2 •4 0	16	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37.38		
2 •38	6		37.75		
2 •35	1		38.22		
2 •2 9	4		39.30		
2 •1 7	2		41.58		
2 • 1 6	6	2 2 0	41.86		
2 • 1 5	6	-2 2 2	41.97		
2 • 1 3	3	-2 0 6	42.47		
2 • 1 0	3	0 0 6	42.95		
2 • 1 4	1	1 2 3	44.26		
2.02 1.95 1.88 1.87 1.86	2 2 2 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	44.89 46.65 48.35 48.77 48.82		
1 •8 3	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	4 9.78		
1 •8 1	2		5 0.41		
1 •7 7	4		5 1.60		
1 •7 6	1		5 1.95		
1 •7 1	1		5 3.53		
1.64	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	55.84		
1.64	1		56.11		
1.61	3		57.35		
1.57	1		58.57		
1.55	3		59.62		
1.54	2	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	60.22		
1.43	1		54.99		
1.23	1		77.40		
1.18	2		81.81		

Orthorhombic, Pnam (62), Z=8 [Sterns, 1967]

Lattice parameters

a=13.71±0.01,b=12.36±0.01, c=8.21±0.005Å [ibid.]

Density

(calculated) 9.124 g/cm³

Thermal parameters

Average isotropic, [ibid.] U: 0.12 Pb: 0.62 0: 0.90

Atomic positions

Positions used from table 3 [ibid.]

Scattering factors

 0° [3.3.1A] Pb^o and U^o [3.3.1B]

Scale factor

(integrated intensities) 536.6×10^4

Reference

Sterns, M. (1967). The crystal structure of Pb_3UO_6 , Acta Cryst. 23, 264-272.

Ca	Calculated Pattern (Peak heights)				
d (Å)	Ι		hk	l	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 ^{\circ}A}$
6 •1 8 6 •1 2 6 •0 0 4 •6 43 4 •0 05	2 6 2 1 2	п 1 2 1 2	2 1 1 2 2	0 1 0 1 + 1	14.32 14.46 14.76 19.10 22.18
3 •9 45 3 •5 56 3 •5 23 3 •4 27 3 •3 86	3 6 7 3 6 2	1 1 2 4 2	3 3 0 1	0 1 2 0 2	22.52 25.02 25.26 25.98 26.30
3 • 3 53 3 • 3 02 3 • 2 43 3 • 0 89 3 • 0 60	4 2 3 1 5 1 10 0	3 4 2 0 2	2 1 3 4 2	1 0 1 0 2 +	26.56 26.98 27.48 28.88 29.16
2 • 9 98 2 • 9 65 2 • 8 29 2 • 8 15 2 • 7 38	44 3 4 5 1	4 3 4 3	2 1 4 2 2	n 2 1 1 2	29.78 30.12 31.60 31.76 32.68
2 •6 77 2 •6 35 2 •6 27	22 11 7	2 4 1	3 3 1	2 + 0 3	33.44 34.00 34.10

Ca	Calculated Pattern (Peak heights)					
d (Å)	I	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$			
2 •2 45	3	5 1 1	35.24			
2 •4 90		2 1 3	35.04			
2 •4 53	1	3 3 2 2 3 1 4 1	36.60			
2 •3 50	1		38.26			
2 •3 22	5		38.74			
2 •3 06	2		39.02			
2 •2 95	2		39.22			
2 •2 42	1	5 1 2	40.18			
2 •2 02	3	6 0 1	40.96			
2 •1 63	1	2 3 3	41.72			
2 •0 53	1 6	0 0 4 +	44.08			
2 •0 40	3	3 3 3	44.36			
2 •0 23	14	2 5 2 +	44.76			
2 •0 05	4	4 5 0	45.18			
1 •9 97	20	6 0 2	45.38			
1 •9 91	12	5 4 1	45.52			
1 •9 77	1	1 6 1	45.86			
1 •922	1	3 5 2	47.26			
1 •9 nn	1	6 2 2	47.84			
1 •8 36	3	5 5 0	49.62			
1 •8 31	5	3 6 1	49.76			
1 •8 19	2	1 5 3	50.12			
1 •7 93	3	543+	50.90			
1 •7 78	13	252	51.34			
1 •7 65	7	450	51.74			
1 •7 54	4	503	52.10			
1 •7 50	5	712+	52.24			
1 •7 43	6	4 1 4	52.44			
1 •7 26	1	4 6 1	53.00			
1 •7 10	14	0 4 4 +	53.56			
1 •7 05	8	3 5 3	53.72			
1 •6 97	5	8 1 0	53.98			
1 •6 93 1 •6 77 1 •6 53 1 •6 52 1 •6 28	13 1'7 1 3	4 2 4 6 4 2 8 1 1 8 2 0 5 1 4	54.12 54.68 55.20 55.60 56.46			
1 .6 24	4	7 3 2	56.62			
1 .6 19	7	4 3 4 +	56.82			
1 .6 15	4	1 1 5	56.96			
1 .5 82	2	8 3 0	58.26			
1 .5 78	4	2 7 2 +	58.42			
1 •5 70	3	4 7 0	58.78			
1 •5 49	2	3 6 3	59.66			
1 •5 45	4	0 3 0	59.82			
1 •5 25	2	6 4 3	60.66			
1 •5 16	2	1 3 5	61.08			
1 •5 12	2	9 1 0	61.26			
1 •5 09	2	1 8 1	61.38			
1 •4 86	1	7 3 3	62.46			
1 •4 76	1	8 3 2	52.90			

	1 1		
C	alculated	l Pattern (Integra	ted)
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$
5.18	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 4. 32
6.12	5		1 4. 46
5.99	2		1 4. 76
4.841	1		1 8. 31
4.645	1		1 9. 09
4 •0 06 3 •946 3 •5 56 3 •5 22 3 •4 28	2 3 6 6 2	2 2 1 1 3 0 1 3 1 2 0 2 4 0 0	2 2. 17 2 2. 52 2 5. 02 2 5. 27 2 5. 27 2 5. 97
3 • 3 87 3 • 3 54 3 • 3 03 3 • 2 44 3 • 0 90	64 23 1 53	2 1 2 3 2 1 4 1 0 2 3 1 0 4 0	26.29 26.56 26.97 27.47 28.87
3 •064	2	4 1 1	29.12
3 •060	100	2 2 2	29.16
2 •997	46	4 2 0	29.78
2 •965	2	3 1 2	30.12
2 •830	4	1 4 1	31.59
2 •8 16	5	4 2 1	31.75
2 •7 38	1	3 2 2	32.68
2 •6 77	20	2 3 2	33.44
2 •6 77	4	5 1 0	33.45
2 •6 35	12	4 3 0	34.00
2 •6 23	3	1 1 3	34.16
2 •5 45	3	5 1 1	35.23
2 •4 90	1	2 1 3	36.05
2 •4 53	1	3 3 2	36.60
2 •3 51	1	2 2 3	38.26
2 • 3 2 3	5	2 4 2	3 A. 74
2 • 3 0 7	2	3 1 3	3 9. 02
2 • 2 95	1	4 4 0	3 9. 22
2 • 2 4 2	1	5 1 2	4 0. 18
2 • 2 0 1	4	6 0 1	4 0. 96
2 • 1 63	1	2 3 3	41.72
2 • 0 53	19	1 1 4	44.08
2 • 0 51	1	5 4 0	44.12
2 • 0 40	3	3 3 3	44.37
2 • 0 26	3	1 4 3	44.69
2 .0 23 2 .0 05 1 .9 97 1 .9 90 1 .9 77	15 4 24 1	2 5 2 4 5 0 5 0 2 5 4 1 1 5 1	44.75 45.19 45.39 45.55 45.86
1 •921	2	3 5 2	47.27
1 •900	1	6 2 2	47.84
1 •836	3	5 5 0	49.61
1 •831	4	3 6 1	49.75
1 •818	3	1 5 3	50.13

Calculated Pattern (Integrated)				
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$	
1 .7 93	2	6 4 1	50.89	
1 .7 92	2	5 5 1	50.92	
1 .7 78	1 7	2 6 2	51.34	
1 .7 66	8	4 6 D	51.73	
1 .7 54	3	6 D 3	52.10	
1 •7 51	1	1 7 0	52.19	
1 •7 50	3	7 1 2	52.23	
1 •7 43	8	4 1 4	52.44	
1 •7 26	1	4 6 1	53.00	
1 •7 13	1	1 7 1	53.45	
1 •7 10	16	n 4 4	53.56	
1 •7 08	2	3 6 2	53.52	
1 •7 02	1	3 5 3	53.80	
1 •6 98	4	8 1 0	53.97	
1 •6 93	15	4 2 4	54.11	
1 •6 77	2 2	6 4 2	54.69	
1 •6 62	1	8 1 1	55.21	
1 •6 51	3	8 2 0	55.61	
1 •6 29	1	5 1 4	56.45	
1 •6 24	4	7 3 2	56.61	
1 •6 19 1 •6 19 1 •6 16 1 •5 82 1 •5 80	6 2 2 1	4 3 4 8 2 1 1 1 5 8 3 0 7 1 3	56.81 56.82 56.92 58.26 58.37	
1 •5 78	4	2 7 2	58.42	
1 •5 70	3	4 7 0	58.78	
1 •5 48	2	3 6 3	59.66	
1 •5 45	4	0 8 0	59.81	
1 •5 25	3	6 4 3	60.66	
1 •5 16	2	1 3 5	61.08	
1 •5 12	1	9 1 0	61.26	
1 •5 09	2	1 8 1	61.38	
1 •4 86	1	7 3 3	62.46	
1 •4 76	1	8 3 2	52,69	
1 .4 40	1	4 2 5	64.67	
1 .4 34	2	4 5 4	64.97	
1 .4 29	1	9 3 0	65.25	
1 .4 11	1	3 7 3	66.16	
1 .4 08	2	8 5 0	66.31	
1 •4 00	2	5 1 5	6 6 • 78	
1 •3 88	1	8 5 1	6 7 • 41	
1 •3 68	2	5 5 4	6 8 • 51	
1 •3 39	1	1 8 3	7 N • 24	
1 •3 39	5	4 6 4	7 D • 27	
1 • 3 34	4	2 1 6	7 N. 54	
1 • 3 32	1	1 7 4	7 N. 65	

Orthorhombic, $Pna2_1$ (33), Z=4 [Burns et al., 1968]

Lattice parameters

a=9.510(1), b=8.2295(3), c=4.8762(1)Å, [ibid.]

Density

(calculated) 2.816 g/cm³

Thermal parameters

Anisotropic [ibid.]

Scattering factors

 Li^+ , Al^{3+} , F^- [3.3.1A]

Scale factor

(integrated intensities) 1.383 \times 10⁴

Polymorphism

Four other polymorphs form between room temperature and 783 °C, [Garton and Wan-klyn, 1965]. PDF cards 19-716 and 20-613 report data at 625 and 596 °C., respectively.

- Burns, J.H., A.C. Tennissen, and G.D.Brunton (1968). The crystal structure of a-Li₃AlF₆, Acta Cryst. B24, 225-230.
- Garton, G. and B.M. Wanklyn (1965). Polymorphism in Li₃AlF₆, J. Inorg.Nucl.Chem. 27, 2466-2469.

Calculated Pattern (Peak heights)					
d (Å)	Ι		hk	l	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$
6.223 4.195 4.115 3.837 3.404 2.959 2.623 2.529 2.4377 2.3902	6 42 100 2 21 2 17 17 1 2 4	1 2 1 2 3 2 3 0 0	1 1 1 0 1 2 1 0 3	0 1 0 + 1 1 1 2 1	14.22 21.16 21.58 23.16 26.16 30.18 34.16 35.46 36.84 37.60
2.3768 2.5130 2.1691 2.1358 2.0980 2.0687 1.9088 1.8968	18 6 97 3 2 5 5	4 1 2 2 2 4 3 4	0 3 0 3 1 1 3 2	0 + 1 2 1 + 2 1 1 1 1	37.82 38.80 41.60 42.28 43.08 43.72 47.60 47.92

Calculated Pattern (Peak heights)				
d (Å)	Ι	hkl	$2\theta(°)$ $\lambda = 1.54056 \stackrel{\circ}{A}$	
1.8813	1	3 1 2	48.34	
1.8532		5 1 0	49.12	
1.7609	1	2 4 1	51 • 8 8	
1.7019	21	4 0 2 +	53 • 8 2	
1.6857	25	4 3 1	54 • 3 8	
1.6671	3	4 1 2	55 • 0 4	
1.6269	1	3 4 1	56 • 5 2	
1.5730	6	4 2 2 +	58.64	
1.5556	7	2 5 0 +	59.36	
1.5119	1	2 1 3	61.26	
1.4930	1	2 4 7	62.12	
1.4887	2	5 3 1	62.32	
1.4818	3	4 4 1 +	62 • 6 4	
1.4463	1	4 3 2	64 • 3 6	
1.4407	6	2 2 3	64 • 6 4	
1.4154	5	6 2 1	65 • 9 4	
1.3982	13	0 3 3	66 • 8 6	
1.3836	1	1 3 3	67.66	
1.3718	5	0 6 0 +	68.32	
1.3575	2	1 6 0	69.14	
1.3287	2	6 0 2	70.86	
1.3245	2	4 1 3	71.12	
1.3210 1.3117 1.3039 1.2723 1.2320	5 6 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	71.34 71.92 72.42 74.52 77.40	
1.2159	2	6 4 1	78.62	
1.2054	1	4 3 3	79.44	
1.1959	1	6 3 2	80.20	
1.1887	2	8 0 0 +	80.78	
1.1858	2	1 6 2	81.02	
1.1807	'2	2 0 4	81.44	
1.1689	1	0 2 4 +	82.44	
1.1593	2	2 6 2	83.28	
1.1565	2	0 5 3	83.52	
1.1430	1	0 7 1 +	84.74	
1.1348 1.1186 1.1119 1.0848 1.0679	1 1 2 2	6 U 3 3 6 2 8 2 1 4 0 4 + 4 6 2	85.50 87.04 87.70 90.48 92.32	
1.059€ 1.0488 1.0339 .959€ .9448	1 2 1 1	6 1 2 0 4 4 6 5 2 6 1 4 + 10 1 0	93.26 94.52 96.32 106.78 109.24	
• 3057	2	8 3 3	116.52	
• 9022	1	2 3 5	117.24	
• 8969	1	4 1 5	118.38	

Calculated	l Pattern <i>(Integr</i> e	ated)	Ca	lculated	l Pattern (Integra	ated)
$d(\stackrel{\circ}{A})$ I	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$
6.223 4 4.195 34 4.117 73 4.115 16 3.838 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	14.22 21.16 21.57 21.58 23.15	1.3119 1.3115 1.3113 1.3040 1.2722	4 2 2 1 1	6 1 2 4 4 2 2 5 2 4 5 1 2 6 1	71.91 71.94 71.95 72.42 74.52
3.404 19 2.956 2 2.623 16 2.529 1 2.4381 2	2 D 1	26.15	1.2319	2	2 4 3	77.41
	3 1 D	30.19	1.2159	2	6 4 1	78.62
	2 2 1	34.16	1.2053	1	4 3 3	79.44
	3 1 1	35.46	1.1959	1	6 3 2	80.19
	0 J 2	36.83	1.1887	2	8 0 0	80.78
2.3908 3 2.3775 18 2.3761 1 2.3187 6 2.1695 53	0 3 1 4 0 0 2 3 0 1 3 1 2 0 2	37.59 37.81 37.83 38.81 41.59	1.1881 1.1861 1.1809 1.1689 1.1688	1 1 3 1	4 6 0 1 6 2 2 0 4 2 1 4 0 2 4	80.84 81.60 81.43 82.45 82.45
2.1370 1	4 0 1	42.25	1.1593	3	2 6 2	83.28
2.1360 100	2 3 1	42.28	1.1565	1	0 5 3	83.52
2.0978 3	2 1 2	43.08	1.1437	1	6 1 1	84.67
2.0684 2	4 1 1	43.73	1.1429	1	0 7 1	84.75
1.9088 5	3 3 1	47.60	1.1348	1	6 D 3	85.50
1.8965 6 1.8814 1 1.8531 1 1.7608 1 1.7022 22	4 2 1	47.93	1.1185	1	3 6 2	87.05
	3 1 2	48.34	1.1120	1	8 2 1	87.69
	5 1 0	49.12	1.0848	2	4 0 4	30.48
	2 4 1	51.88	1.0846	1	2 3 4	90.50
	4 0 2	53.81	1.0846	3	4 6 2	92.31
1.7017 2	2 3 2	53 • 8 3	1.0596	1	8 1 2	93.26
1.6858 29	4 3 1	54 • 3 6	1.0488	1	0 4 4	94.52
1.5669 3	4 1 2	55 • 0 5	1.0339	2	6 5 2	96.32
1.6269 1	3 4 1	56 • 5 2	1.0121	1	5 6 2	93.12
1.5729 F	4 2 2	58 • 6 4	1.0071	1	8 4 1	99.79
1.5724 1 1.5595 1 1.5557 3 1.5554 6 1.5118 2	0 4 2 0 5 1 4 4 0 2 5 0 2 1 3	58.67 59.20 59.36 59.37 61.26	.9663 .9597 .9595 .9544 .9447	1 1 1 2	6 0 4 6 1 4 2 5 4 6 6 2 10 1 0	1 05 . 7 2 1 06 . 7 6 1 06 . 8 0 1 07 . 6 2 1 09 . 2 5
1.4323 1 1.4884 2 1.4821 2 1.4821 1 1.4818 1 1.4463 1	2 4 2	52.13	• 93 06	1	2 2 5	111.73
	5 3 1	52.33	• 90 57	3	8 3 3	116.53
	4 4 1	52.63	• 90 22	1	2 3 5	117.25
	2 5 1	62.64	• 89 83	1	8 6 0	118.07
	4 3 2	64.36	• 896 9	1	4 1 5	118.37
1.4407 7 1.4154 7 1.3984 18 1.3835 2 1.3724 2	2 2 3	64.F4	.8949	1	2 6 4	1 18 .8 0
	6 2 1	65.94	.8843	2	4 7 3	1 21 .1 8
	0 3 3	66.85	.8631	1	2 9 1	1 21 .4 4
	1 3 3	67.67	.8805	1	6 7 2	1 22 .0 4
	6 3 0	68.29	.3804	1	4 8 2	1 22 .0 7
1.3716 F 1.3575 2 1.3289 3 1.3243 2 1.3211 6	0 6 0 1 6 0 6 0 2 4 1 3 6 3 1	68.33 69.14 70.85 71.13 71.37	.8743	1	6 6 3	123.53

Monoclinic, C2/m (12), Z=2 [Pringle and Noakes, 1968]

Lattice parameters

a=5.627,b=3.319, c=4.979Å, B=107.4°[ibid.]

Density

(calculated) 1.832 g/cm³

Thermal parameters

Anisotropic [ibid.]

Scattering factors

Li⁰ [3.3.1A] N^{-0+8} and N^{+0+6} calculated from N^{-} and N^{0} [3.3.1A]

Scale factor

(integrated intensities) 0.04698×10^4

Calculated Pattern (Peak heights)				
d (Å)	Ι	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \stackrel{\circ}{A}$	
4.75	31	0 0 1	18.66	
2.82	92	1 1 0	31.66	
2.71	61	-2 0 1	33.02	
2.69	28	2 0 0	33.34	
2.61	100	-1 1 1	34.28	
2.38	2	0 0 2	37.84	
2.12	4	-2 0 2	42.58	
2.09	3	2 0 1	43.36	
1.977	2	-1 1 2	45.86	
1.691	2	1 1 2	54.18	
1.659	8	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	55.32	
1.629	15		56.44	
1.587	1		58.06	
1.508	3		61.42	
1.415	4		65.96	
1.412	4	2 2 0	66.14	
1.407	1	-4 0 1	6F.40	
1.355	3	-4 0 2	69.28	
1.297	1	1 1 3	72.86	
1.188	1	0 0 4	80.86	
1.162 1.070 1.054 1.050 .994	1 1 1 1	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	63.04 92.04 93.94 94.42 101.62	

Calculated Pattern (Integrated)				
d (Å)	Ι	hkl		$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$
4.75 2.82 2.71 2.68 2.61	25 91 60 26 100	0 0 1 1 -2 0 2 0 -1 1	1 0 1 0 1	18.66 31.67 33.02 33.35 34.27
2.38 2.12 2.09 1.977 1.691	2 4 2 2	0 0 -2 0 2 0 -1 1 1 1	2 2 1 2 2	37.84 42.58 43.35 45.85 54.18
1.660 1.629 1.588 1.567 1.508	10 18 1 1 4	$ \begin{array}{cccc} 0 & 2 \\ -3 & 1 \\ -2 & 0 \\ 0 & 2 \\ -3 & 1 \end{array} $	0 1 3 1 2	55.31 56.44 58.05 58.90 61.41
1.415 1.412 1.407 1.355 1.307	5 3 1 4 1	-2 2 2 2 -4 0 -4 0 -2 2	1 0 1 2 2	65.95 66.14 66.41 69.28 72.21
1.297 1.214 1.188 1.162 1.084	2 1 1 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 4 4 0	72.87 78.74 80.86 83.03 90.61
1.071 1.054 1.050 1.038 .998	1 2 1 1	$ \begin{array}{rrrr} -1 & 3 \\ -5 & 1 \\ -4 & 2 \\ 1 & 1 \\ -5 & 1 \end{array} $	1 2 2 4 3	92.03 93.94 94.42 95.81 101.10
•994 •994 •966 •952 •947	1 1 1 . 1	-2 0 3 1 0 2 -3 3 -1 1	5 3 4 1 5	101.58 101.63 105.78 108.00 108.91
•929 •903	1 1	-3 1 -6 0	5	112.03 117.00

Reference

Pringle, G.E. and D.E. Noakes (1968). The crystal structures of lithium, sodium, and strontium azides, Acta Cryst. B24, 262-269.

Tetragonal, I41cd (110), Z=8 [Krogh-Moe, 1968]

Lattice parameters

a=9.479±.003, c=10.280±.004 Å [ibid.]

Density

(calculated) 2.432 g/cm³

Thermal parameters Isotropic [ibid.]

Scattering factors

 Li^{+} , O° , B° [3.3.1A]

Scale factor

(integrated intensities) 7.114 \times 10⁴

Reference

Krogh-Moe, J. (1968). Refinement of the crystal structure of lithium diborate, Li₂O·2B₂O₃, Acta Cryst. B24, 179-181.

Calculated Pattern (Peak heights)					
d (Å)	Ι		hk	l	$\frac{2\theta(^{\circ})}{\lambda = 1.54056} \stackrel{\circ}{A}$
4.736	5	2	σ	C	18.72
4.077	100	1	1	2	21.78
3.917	12	- 2	1	1	- 22.68
3.485	30	2	ū.	2	25.54
2.665	35	2	1	3	33.60
2.589	34	3	1	2	34.62
2.570	7	- 0	0	4	34.88
2.547	4	3	2	1	35.20
2.370	3	4	Ο	0	37.94
2.259	1	2	0	4	39.88
2.244	7	4	1	1	40.16
2.152	i	4	0	2	41.94
2.120	2	4	2	C	42.62
2.086	6	3	2	3	43.34
2.049	14	3	3	2	44.16

Calculated Pattern (Peak heights)					
d (Å)	Ι		hk	1	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$
2.040 1.959 1.951 1.909 1.865	9 6 5 1	2 4 3 4	2 2 1 1 3	ц 2 4 3 1	44.38 46.30 46.50 47.60 48.80
1.350 1.748 1.742 1.735 1.659	3 2 6 7	2 5 4 5 4	1 1 2 3	5 2 4 1 3 +	49.22 52.28 52.48 52.72 55.32
1.635 1.620 1.611 1.566 1.550	4 3 1 1 1	4 3 5 5	2 2 0 2 3	4 5 6 3 2	56.20 56.80 57.12 58.94 59.60
1.541 1.533 1.493 1.487 1.465	2 1 2 1 1	6 4 6 3 5	1 1 2 1 4	1 5 0 6 1	60.00 60.34 61.86 62.38 63.44
1.400 1.388 1.337 1.295 1.260	1 2 1 2 1	6 4 5 5 5	3 0 2 2 1	1 6 5 4 6	66.76 67.40 70.34 73.02 75.38
1.2420 1.2376 1.2097 1.2054 1.1680	1 2 1 1	6 4 7 6 7	1 3 5 4	5 7 2 1 1	76.66 76.98 79.10 79.44 82.52
1.1616 1.1275 1.0988 1.0774 1.0761	1 1 1 1	6 5 4 7 8	0 2 2 5 3	6 7 8 2 4	83.08 86.18 89.02 91.28 91.42
1.0598 1.0570 1.0258 1.0245 1.0230	1 1 1 2	හ හ හ හ අ	4 1 1 6 1	11 8 2 4 9	93.24 93.56 97.34 97.50 97.70

Calculated Pattern (Integrated)				
d (Å)	Ι	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 ^{\circ}$	
4.739	5	2 0 0	18.71	
4.079	100	1 1 2	21.77	
3.919	12	2 1 1	22.67	
3.484	31	2 0 2	25.54	
2.665	39	2 1 3	33.60	
2.589	39	3 1 2 0 0 4 3 2 1 4 0 0 2 0 4	34.61	
2.570	6		34.88	
2.547	4		35.21	
2.370	3		37.94	
2.259	1		39.87	
2.244 2.152 2.120 2.086 2.049	8 2 8 1 7	4 1 1 4 0 2 4 2 0 3 2 3 3 3 2	40.16 41.95 42.62 43.34 44.16	
2.039	10	2 2 4	44.38	
1.959	8	4 2 2	46.30	
1.951	7	3 1 4	46.51	
1.909	7	4 1 3	47.59	
1.864	1	4 3 1	48.81	
1.850	3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	49.21	
1.748	2		52.29	
1.742	2		52.48	
1.735	8		52.72	
1.660	5		55.30	
1.659 1.635 1.620 1.611 1.580	6 5 1 1	4 3 3 4 2 4 3 2 5 2 J 6 6 U 0	55.34 56.21 56.80 57.12 58.36	
1.566	1	5 2 3	58.94	
1.550	1	5 3 2	59.60	
1.541	2	6 1 1	59.99	
1.533	1	4 1 5	60.35	
1.499	3	6 2 0	61.85	
1.487	2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	62.37	
1.465	1		63.43	
1.400	1		66.77	
1.388	3		67.39	
1.374	1		68.20	
1.341 1.337 1.315 1.295 1.260	1 1 3 2	$\begin{array}{cccccc} 7 & 1 & 0 \\ 5 & 2 & 5 \\ 6 & 4 & 0 \\ 6 & 2 & 4 \\ 5 & 1 & 6 \end{array}$	70.14 70.35 71.75 73.02 75.38	
1.2419	2	6 1 5	76.67	
1.2376	1	4 1 7	76.98	
1.2097	3	7 3 2	79.10	
1.2053	1	6 5 1	79.45	
1.1886	1	7 1 4	80.79	

Calculated Pattern (Integrated)			
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$
1.1811 1.1793 1.1703 1.1681 1.1645 1.1614 1.1276 1.1202 1.1121	1 1 1 1 1 2 1 1	3 1 8 5 3 6 6 4 4 7 4 1 6 3 5 6 0 6 5 2 7 7 3 4 7 4 3	81.42 81.56 82.32 32.51 82.82 83.09 86.17 86.89 87.68
1.0988 1.0774 1.0760 1.0598 1.0571 1.9257	1 2 1 1 3	4 2 8 7 5 2 8 0 4 6 4 0 5 1 8 9 1 2	89.01 91.27 91.43 93.24 93.56 97.35
1.0245 1.0229 1.0070 .8806 .8616	1 2 1 1 1	6 6 4 4 1 9 7 3 6 3 2 11 6 0 10	97.50 97.70 99.80 122.03 126.75
.8431 .8294 .8237 .8230 .8207	1 1 1 1	6 6 8 8 6 6 3 1 12 10 5 3 11 3 2	1 32 . D 3 1 36 . 4 6 1 38 . 5 1 1 38 . 7 6 1 39 . 6 2
.7926 .7888 .7838	1 1 1	7 3 10 9 3 8 10 5 5	152.74 155.13 158.68

Hexagonal, R3 (146), Z=3 [Weiss et al., 1966]

Lattice parameters

a=8.944±0.008, c=8.936±0.008Å [ibid.]

Density

(calculated) 2.090 g/cm³ [ibid.]

Thermal parameters

Isotropic [ibid.]

Scattering factors

 Mg° and O^{-1} [3.3.1A] Se° [3.3.1B]

Scale factor

(integrated intensities) 6.841 imes 10^4

Additional patterns

 PDF card 20-687 [Leshchinskaya and Selivanova, 1966]

- Leshchinskaya, Z.L. and N.M Selivanova, (1966). Thermodynamic properties of magnesium selenites, Russ. J. Inorg. Chem. (English Transl.) 11, 143-145.
- Weiss, R., J.-P. Wendling, and D. Grandjean (1966). Structure cristalline précise du Sélénite de magnesium à six molécules d'eau, Acta Cryst. 20, 563-566.

Calculated Pattern (Peak heights)				
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$	
5.85	28	1 0 1	15.12	
4.47	100	1 1 0	19.84	
3.870	66	0 1 2	22.96	
3.553	11	0 2 1	25.04	
2.978	17	0 3	29.98	
2 •927	29	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	30.52	
2 •783	32		32.14	
2 •582	6		34.72	
2 •479	9		35.20	
2 •449	21		35.66	
2.236	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	40.30	
2.146	1		42.06	
2.089	5		43.28	
1.951	4		46.50	
1.936	1 7		46.90	
1.892	1	4 0 1	48.04	
1.788	4	2 2 3 +	51.04	
1.776	15	2 1 4 +	51.40	
1.743	3	3 2 1 +	52.46	
1.690	9	1 4 0 +	54.22	
1.651	4	2 3 2 +	55.62	
1.623	1	2 0 5	56.68	
1.549	4	1 3 4 +	59.66	
1.525	2	2 1 -5 +	60.66	
1.491	1	3 3 0	62.22	
1.470	4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	63.20	
1.463	3		63.52	
1.445	1		64.44	
1.413	2		66.06	
1.391	5		67.26	
1.374 1.328 .290 1.260 1.240	1 2 1 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	68.20 70.88 73.30 75.34 76.84	
1 •225	2	3 4 2 +	77.96	
1 •1 85	1	0 6 3	81.12	
1 •1 70	1	1 2 -7	82.32	
1 •1 42	1	1 6 -2	84.82	
1 •1 17	1	4 1 6 +	87.16	
1.106	1	3 4 - 4	88.26	
1.098	1	3 1 - 7	89.14	
1.044	1	6 2 - 2	95.06	

Cá	Calculated Pattern (Integrated)				
d (Å)	I	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$		
5 • 8 5	27	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	15.12		
4 • 4 7	100		19.84		
3 • 8 70	69		22.96		
3 • 5 5 3	12		25.04		
2 • 9 7 9	19		29.97		
2 •926	34	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	30.52		
2 •782	38		32.15		
2 •582	7		34.72		
2 •479	10		36.20		
2 •479	1		36.20		
2 •4 49	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	36.67		
2 •4 49	24		36.67		
2 •2 36	3		40.30		
2 •1 47	2		42.06		
2 •0 89	6		43.28		
1 •951	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	46.51		
1 •951	4		46.51		
1 •936	5		46.89		
1 •936	1 3		46.89		
1 •935	6		46.91		
1 • 8 93 1 • 7 88 1 • 7 88 1 • 7 78 1 • 7 77 1 • 7 76	2 4 1 2 1 3	4 0 1 2 2 3 2 2 - 3 0 4 2 2 1 4	4 8.03 5 1.03 5 1.03 5 1.38 5 1.41		
1 •776	6	1 2 - 4	51.41		
1 •743	3	3 2 1	52.46		
1 •743	1	2 3 - 1	52.46		
1 •741	1	0 1 5	52.50		
1 •690	5	4 1 0	54.22		
1.690 1.651 1.651 1.523 1.548	8 3 1 3	1 4 0 2 3 2 3 2 - 2 2 0 5 1 3 4	54.22 55.61 55.61 56.68 59.66		
1.548	7	3 1 -4	59.65		
1.525	1	1 2 5	60.66		
1.525	2	2 1 -5	60.66		
1.491	2	3 3 0	62.23		
1.470	2	4 1 3	63.20		
1 •4 70 1 •4 70 1 •4 70 1 •4 64 1 •4 63	1 1 2 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	53.20 63.20 63.20 63.51 63.53		
1 •445 1 •445 1 •413 1 •413 1 •391	1 1 2 1 2	2 4 1 4 2 -1 1 1 6 1 1 -6 4 2 2	64.45 64.45 66.07 65.25		

Calculated Pattern (Integrated)						
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$			
d(A) 1.391 1.391 1.391 1.391 1.374 1.328 1.328 1.291 1.290 1.290 1.290 1.261 1.240 1.240 1.240 1.240 1.225 1.224 1.184 1.170 1.142 1.117	I 2 3 2 1 2 1 3 1 2 1 2 1 2 1 2 1 1 2 2 1 1 2 2 1 1 2 1 1 2 1 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 2 1 2 2 2 1 2 2 2 1 2 2 2 2 1 2 2 2 1 2 2 2 1 2 2 2 1 2 2 2 1 2 2 2 1 2 2 2 1 2 2 2 1 2 2 2 1 1 2 2 2 1 1 2 2 2 1 1 2 2 2 1 1 2 2 2 1 1 2 2 1 1 2 2 1 1 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1	hkl $2 4 -2$ $3 2 4$ $2 3 -4$ $1 3 -5$ $1 5 2$ $5 1 -2$ $6 0 0$ $7 3 6$ $3 0 6$ $3 0 6$ $3 4 -1$ $5 2 0$ $2 5 0$ $2 2 6$ $3 4 -1$ $5 2 0$ $2 2 6$ $3 4 -1$ $6 3$ $1 2 -7$ $1 6 -2$ $4 1 6$	$2\theta(°) \\ \lambda = 1.54056 \stackrel{\circ}{A}$ $67.25 \\ 67.27 \\ 67.27 \\ 67.27 \\ 68.20 \\ 70.89 \\ 71.89 \\ 73.26 \\ 73.26 \\ 73.22 \\ 73.32 \\ 75.33 \\ 76.78 \\ 76.78 \\ 76.78 \\ 76.84 \\ 77.95 \\ 77.97 \\ 81.13 \\ 82.34 \\ 84.83 \\ 87.15 \\ \end{cases}$			
1 •1 06 1 •0 97 1 •0 44 •9 26	1 1 1 1 1 1	3 4 - 4 3 1 - 7 6 2 - 2 2 7 - 2	88.26 89.16 95.05 112.62			

Cubic, $I2_13$ (199), Z=4 [Frueh and Gray, 1968]

Lattice parameters

a=8.949±.002Å [ibid.]

Density

(calculated) 6.827 g/cm³ [ibid.]

Thermal parameters

Isotropic [ibid.]

Polymorphism

This form is one of three polymorphs, [ibid.]

Scattering factors

Hg°, S°, Cl° [3.3.1A] All values were corrected for anomalous dispersion using the corrections given by Cromer [1965]

Scale factor

(integrated intensities) 120.2 \times 10⁴

Additional patterns

1. PDF card 20-737 [Carlson, 1967]

2. Aurivillius, K. [1967]

- Aurivillius, K. (1967). An x-ray single crystal study of Hg₃S₂Cl₂, Arkiv Kemi 26(6), 497-505.
- Carlson, E.H. (1967). The growth of HgS and Hg₃S₂Cl₂ single crystals by a vapor phase method,J.Crystal Growth 1,271-277.
- Cromer, D.T. (1965). Anomalous dispersion corrections computed from self-consistent field relativistic Dirac-Slater wave functions, Acta Cryst. 18, 17-23.
- Frueh, A.J. and N. Gray (1968). Confirmation and refinement of the structure of Hg₃S₂Cl₂, Acta Cryst. B24, 156-157.

Calculated Pattern (Peak heights)						
d (Å)	Ι		hk	l		$2\theta(^{\circ})$ $\lambda = 1.54056 \stackrel{\circ}{A}$
6 • 330 4 • 4 76 3 • 65 4 3 • 16 4 2 • 829	43 14 100 1 47	1 2 2 0	1 0 1 2 1	0 0 1 0 3		13.98 19.82 24.34 28.18 31.60
2.583 2.391 2.237 2.109 2.001	36 24 24 20 8	2 1 4 4 4	2 2 0 1 2	2 3 + 0 1 + 0		34.70 37.58 40.28 42.84 45.28
1.908 1.827 1.7553 1.6338 1.5819	3 1 22 10 5	3 4 1 5 4	3 2 3 2 4	2 2 4 + 1 *		47.62 49.88 52.06 56.26 58.28
1.5345 1.4917 1.4516 1.4151 1.3807	8 1 9 2 2	4 4 0 5	3 4 3 2 4	3 + 2 5 + 6 1 +		60.26 62.18 64.10 65.96 67.82
1.3490 1.3194 1.2656 1.2177 1.1959	2 2 5 2 2	6 0 6 2	2 3 1 3 4	2 1 + 7 + 3 6		69.64 71.44 74.98 78.48 80.20
1.1365 1.1015 1.0852 1.0695 1.0403	3 3 1 1 3	1 7 8 3 1	5 4 2 5 3	6 + 1 + 0 6 + 8 +		85.34 88.74 90.44 92.14 95.54
•9434 •9230 •8775 •8382 •8102	1 1 1 1	7 9 8 1 9	5 3 6 7 5	4 2 + 2 + 8 4 +		109.48 113.14 122.76 133.56 143.88
.7972	1	3	6	9 +		150.12

Calculated Pattern (Integrated)					
d (Å)	I	1	ıkl	2θ(°)	
				$\Lambda = 1.54056 A$	
6.328 4.475 3.653 3.164 2.830	38 13 100 1 53	1 2 2 0	1 0 0 0 1 1 2 0 1 3	13.98 19.83 24.34 28.18 31.59	
2.583 2.392 2.392 2.237 2.109	40 7 20 28 11	2 3 1 4 3	2 2 2 1 2 3 0 0 3 0	34.70 37.58 37.58 40.28 42.84	
2.109 2.001 1.908 1.827 1.7550	13 9 3 1 6	4 4 3 4	1 1 2 0 3 2 2 2 3 1	42 • 8 4 45 • 2 8 47 • 6 2 49 • 8 8 52 • 07	
1.7550 1.6339 1.6339 1.5820 1.5347	24 12 1 7 1	1 5 1 4 5	3 4 2 1 2 5 4 0 3 0	52.07 56.26 56.26 58.28 60.25	
1.5347 1.5347 1.4915 1.4517 1.4517	9 1 5 3	4 4 6 5	3 3 3 5 4 2 1 1 3 2	60.25 60.25 62.19 64.09 64.09	
1.4517 1.4150 1.3809 1.3809 1.3491	5 2 2 2 3	2 0 5 1 6	35 26 41 45 22	64.09 65.96 67.81 67.81 69.63	
1.3195 1.3195 1.2917 1.2656 1.2656	3 1 1 2 2	6 1 4 5 0	3 1 3 6 4 4 4 3 1 7	71.43 71.43 73.22 74.98 74.98	
1.2656 1.2656 1.2656 1.2410 1.2178	1 1 2 1 1	5 7 3 6 6	5 0 1 0 4 5 4 0 3 3	74.98 74.98 74.98 76.73 78.47	
1.1959 1.1751 1.1365 1.1365 1.1015	2 1 1 3 1	2 4 0 1 7 1 5 1	4 6 3 7 3 2 5 6 5 4	80.20 81.92 85.34 85.34 88.74	
1.1015 1.1015 1.0852 1.0696 1.0696	3 2 2 1 2	7 1 8 6 3	4 1 4 7 2 0 5 3 5 6	88.74 88.74 90.44 92.13 92.13	

Mercury Sulfide	Chloride,	alpha,	Hg ₂ S ₂ Cl ₂	(cubic) -	continued
-----------------	-----------	--------	--	-----------	-----------

Calculated Pattern (Integrated)						
d (Å)	Ĭ	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$			
1.0546 1.0403 1.0403 1.0403 .9883	1 1 2 2 1	8 2 2 7 5 0 7 4 3 1 3 8 8 3 3	93.83 95.54 95.54 95.54 102.42			
•9764 •9433 •9230 •9230 •8949	1 2 1 1 1	2 4 8 7 5 4 9 3 2 3 6 7 0 6 8	104.16 109.49 113.13 113.13 118.80			
.8775 .8775 .8382 .8309 .8169	1 2 1 1 1	0 2 10 8 6 2 1 7 8 4 6 8 2 4 10	122.75 122.75 133.57 135.96 141.09			
.8169 .8102 .8102 .7972 .7972	1 1 1 2	10 4 2 9 5 4 3 7 8 1 5 10 11 2 1	141.09 143.88 143.88 150.11 150.11			
	2	5 6 9	150.11			

Monoclinic, $P2_1/c$ (14), Z=4 [Brown and Walker, 1966]

Lattice parameters

a=5.846±.003,b=12.693±.006,c=8.515±.004Å β=90.0°±0.1° [ibid.]

Density

(calculated) 3.197 g/cm³

Thermal parameters

Isotropic:Nb 1.064;K(1) 1.916;K(2) 2.048
F(1) 1.850;F(2) 2.042;F(3) 2.008
F(4) 2.101;F(5) 3.100;F(6) 3.673
F(7) 2.344

Scattering factors

- K⁺ [3.3.1A]
- Nb⁰ [3.3.1A]
- F° [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 7.495 \times 10⁴

Additional patterns

 PDF card 18-1013 [Mukhtar and Winand, 1965]

- Brown, G.M. and L.A. Walker(1966). Refinement of the structure of potassium heptafluoroniobate, K₂NbF₇, from neutrondiffraction data,Acta Cryst.20, 220-229.
- Cromer, D.T. and J.T. Waber (1965). Scattering factors computed from relativistic Dirac-Slater wave functions, Acta Cryst. 18, 104-109.
- Mukhtar,A. and R.Winand (1965). Établissement, par analyse thermique et aux rayons X, du diagramme des phases du system KF-K₂NbF₇, Compt. Rend. 260, 3674-3676.

Calculated Pattern (Peak heights)						
d (Å)	Ι	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \stackrel{\circ}{A}$			
7.06	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	12.52			
6.35	2		13.94			
5.85	2		15.14			
5.31	58		16.68			
5.09	100		17.42			
4.50	42	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	19.70			
4.28	38		20.84			
4.04	1		22.00			
3.837	6		23.16			
3.789	5		23.46			
3.537	3	0 2 2 -1 0 2 + 1 3 0 - 1 1 2 + -1 3 1 +	25 • 1 6			
3.440	34		25 • 8 8			
3.427	67		25 • 9 8			
3.321	64		26 • 8 2			
3.180	41		28 • D 4			
3.025	1	-1 2 2	29.50			
3.002	2	0 3 2	29.74			
2.974	1	0 4 1	30.02			
2.923	15	2 0 0	30.56			
2.789	1	1 4 0	32.06			
2.701	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	33.14			
2.670	4		33.54			
2.654	2		33.74			
2.550	2		33.60			
2.590	2		34.50			
2.545	2	0 4 2	35.24			
2.535	3	-2 2 1	35.38			
2.503	8	1 1 3 +	35.84			
2.433	2	0 5 1	36.92			
2.410	6	-2 0 2 +	37.28			
2.367	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37.98			
2.328	5		38.64			
2.314	8		38.68			
2.253	12		39.98			
2.247	8		40.10			
2.186	2	1 3 3	41.26			
2.149	3	2 4 0	42.00			
2.129	2	0 0 4	42.42			
2.116	7	0 4 3 +	42.70			
2.099	14	0 1 4	43.06			
2.094	20	-2 3 2 +	43.15			
2.085	6	2 4 1 +	43.35			
2.053	16	0 6 1	44.08			
2.018	1	0 2 4	44.88			
2.000	4	1 0 4 +	45.30			
1.989 1.976 1.939 1.919	5 4 17 13 4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	45.56 45.68 46.82 47.32 47.62			

Calculated Pattern (Peak heights)			Calculated Pattern (Integrated)				
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$	d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$
1.878 1.835 1.820 1.808 1.800	2 1 2 3 4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	48.42 49.64 50.08 50.42 50.66	7.07 6.35 5.85 5.31 5.09	2 2 58 100	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12.51 13.94 15.14 16.68 17.41
1.770 1.755 1.748 1.732 1.721	9 4 2 4 5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	51.60 52.08 52.30 52.80 53.13	4.51 4.51 4.26 4.04 3.838	28 18 43 2 5	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	19.59 19.59 20.85 22.00 23.15
1.714 1.705 1.697 1.693 1.688	2 2 6 3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	53.42 53.70 53.98 54.14 54.30	3.238 3.789 3.535 3.442 3.442	1 7 3 11 21	$ \begin{array}{cccccc} -1 & 2 & 1 \\ 0 & 3 & 1 \\ 0 & 2 & 2 \\ 1 & 0 & 2 \\ -1 & 0 & 2 \end{array} $	23.15 23.46 25.17 25.87 25.87
1.680 1.645 -1.534 1.630 1.622	9 1 3 3 3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	54 • 5 8 55 • 8 4 56 • 2 4 56 • 4 2 56 • 7 2	3.428 3.322 3.322 3.180 3.180	68 45 28 18 27	1 3 0 1 1 2 -1 1 2 1 3 1 -1 3 1	25.97 26.82 26.82 28.04 28.04 28.04
1.604 1.594 1.590 1.586 1.583	1 3 2 4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	57.40 57.80 57.96 58.10 58.22	3 • 173 3 • 025 3 • 901 2 • 973 2 • 923	9 1 3 1 19	0 4 0 -1 2 2 0 3 2 0 4 1 2 0 0	28.10 29.50 29.74 30.03 30.56
1.580 1.571 1.558 1.547 1.528	3 2 1 3 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	58 • 3 6 58 • 7 2 59 • 2 8 59 • 7 2 60 • 5 4	2.789 2.701 2.701 2.570 2.555	1 1 2 5 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	32.07 33.14 33.14 33.54 33.73
1.525 1.513 1.502 1.487 1.478	2 4 1 1 4	1 3 5 + 2 4 4 + 3 3 3 0 8 2 -1 7 3 +	60.68 61.22 61.72 62.42 62.80	2.650 2.591 2.544 2.535 2.503	1 3 2 ,3 9	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	33.79 34.59 35.25 35.38 35.84
1.467 1.461 1.453 1.433 1.414	3 2 2 2	2 6 3 + 4 C 9 3 5 2 2 2 5 -3 6 1 +	63.34 63.62 64.02 65.02 66.04	2.503 2.433 2.410 2.410 2.367	1 2 5 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	35.84 36.92 37.28 37.28 37.28
1.410 1.405 1.402 1.390 1.382	2 1 2 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	65 • 2 2 66 • 5 0 65 • 6 6 67 • 3 2 67 • 7 4	2 • 33 3 2 • 32 9 2 • 31 4 2 • 31 4 2 • 25 3	1 7 2 8 7	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	38.56 30.63 38.88 38.88 38.88 39.99
1.379 1.371 1.353 1.361 1.358	4 1 1 2	$\begin{array}{cccccccc} -1 & 0 & 6 & + \\ 1 & 3 & 0 \\ -4 & 3 & 1 \\ 3 & 3 & 4 \\ 3 & 5 & 3 & + \end{array}$	67.90 68.36 68.80 68.94 69.14	2.253 2.246 2.186 2.150 2.129	10 1 2 4 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	39.53 40.11 41.26 41.93 42.43

Calculated Patter	Calculated Pattern (Integrated)			alculated	l Pattern <i>(Integr</i> u	ated)
d (Å) I	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 ^{\alpha}}$	d (Å)	Ι	hkl	λ =
2.116 5 0 2.116 3 0 2.093 18 0 2.094 4 2 2.094 13 -2	4 3 5 D 1 4 3 2 3 2	42.71 42.71 43.05 43.17 43.17	1.680 1.645 1.634 1.634 1.634	5 1 2 3 1	2 6 1 0 2 5 3 3 2 -3 3 2 -1 6 3	
2.084 4 2 2.084 2 -2 2.053 22 0 2.043 1 -1 2.018 1 0	4 1 4 1 6 1 5 2 2 4	43.37 43.37 44.07 44.30 44.87	1.622 1.622 1.604 1.594 1.594	2 3 1 1 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
2.000 3 1 2.000 2 -1 1.989 3 1 1.989 4 -1 1.976 3 1	0 4 0 4 4 3 4 3 1 4	45.30 45.30 45.56 45.56 45.89	1.590 1.587 1.583 1.583 1.583	1 2 1 2 2	2 6 2 0 8 0 1 2 5 -1 2 5 0 3 5	
1.976 2 -1 1.939 14 2 1.939 6 -2 1.937 2 1 1.937 5 -1	1 4 2 3 2 3 6 1 6 1	45.89 46.82 46.82 46.86 46.86	1,571 1.571 1.557 1.547 1.546	2 1 2 3 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
1.919 11 2 1.919 7 -2 1.908 4 1 1.908 1 -1 1.879 2 -3	4 2 4 2 2 4 2 4 1 1	47.33 47.33 47.63 47.63 47.63 48.41	1.528 1.525 1.525 1.513 1.513	1 1 5 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	6 6 6 6
1.835 1 -2 1.820 3 -3 1.808 3 1 1.800 4 1 1.772 1 3	3 3 2 1 3 4 5 3 0 2	49.64 50.08 50.42 50.67 51.54	1.502 1.487 1.478 1.478 1.478 1.467	2 2 3 3 3 3	3 3 3 0 8 2 1 7 3 -1 7 3 2 6 3	9 9 8 8 8
1.772 6 -3 1.770 9 3 1.755 3 3 1.755 2 -3 1.748 2 -2	0 2 3 0 1 2 1 2 5 2	51.54 51.60 52.07 52.97 52.30	1.467 1.462 1.453 1.433 1.433	1 4 1 2 1	-2 6 3 4 0 0 3 5 2 2 2 5 0 5 5	60 60 60 60 60 60 60 60 60 60 60 60 60 6
1.733 2 3 1.733 3 -3 1.732 3 1 1.721 4 2 1.721 2 -2	3 1 3 1 7 0 0 4 0 4	52.73 52.78 52.82 53.18 53.18	1.413 1.410 1.405 1.402 1.402	2 1 1 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	6 6 6
1.714 1 2 1.707 1 3 1.705 2 -2 1.697 6 -1 1.697 4 1	6 0 2 2 1 4 7 1 7 1	53.42 53.66 53.71 53.98 53.38	1.390 1.382 1.380 1.379 1.379	1 1 2 3	-2 3 5 4 0 2 0 7 4 1 0 6 -1 0 6	9 9 9 9
1.696 1 0 1.692 2 1 1.692 2 -1 1.688 2 0 1.680 8 -2	63 44 15 61	54.02 54.16 54.16 54.31 54.58	1 • 37 1 1 • 36 4 1 • 36 1 1 • 35 8 1 • 35 8	2 1 1 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9

	1		
d (Å)	Ι	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \stackrel{\circ}{A}$
1.680 1.645 1.634 1.634 1.634	5 1 2 3 1	2 6 1 0 2 5 3 3 2 -3 3 2 -1 6 3	54.58 55.85 56.24 56.24 56.24 56.44
1.622 1.622 1.604 1.594 1.594	2 3 1 1 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	56 • 7 2 56 • 7 2 57 • 3 9 57 • 7 9 57 • 8 0
1 • 590 1 • 587 1 • 583 1 • 583 1 • 580	1 2 1 2 2	2 5 2 0 8 0 1 2 5 -1 2 5 0 3 5	57.96 58.09 58.22 58.22 58.22 58.36
L • 571 L • 571 L • 557 L • 547 L • 546	2 1 2 3 2	1 5 4 -1 5 4 -3 2 3 -3 4 2 3 5 0	58.72 58.72 59.29 59.72 59.78
•528 •525 •525 •513 •513	1 1 5 2	0 7 3 1 3 5 -1 3 5 2 4 4 -2 4 4	60.54 60.67 60.67 61.22 61.22
•502 •487 •478 •478 •478	2 2 3 3 3 3	3 3 3 0 8 2 1 7 3 -1 7 3 2 6 3	61.71 62.41 62.80 62.80 63.34
•467 •462 •453 •433 •414	1 4 1 2 1	-2 6 3 4 0 0 3 5 2 2 2 5 0 5 5	63.34 63.61 64.03 55.01 66.00
•413 •410 •405 •402 •402	2 1 1 1 1	-3 6 1 0 1 6 4 2 1 3 2 4 -3 2 4	66.05 66.21 66.51 66.66 66.66
• 390 • 382 • 380 • 379 • 379	1 1 2 3	-2 3 5 4 0 2 0 7 4 1 0 6 -1 0 6	67.32 67.73 67.84 67.91 67.91
• 371 • 364 • 361 • 358 • 358	2 1 1 1 1	1 9 0 -4 3 1 3 3 4 3 5 7 -3 5 3	68.37 68.79 68.94 69.14 69.14

59.14

Reservine, $C_{33}H_{40}N_2O_9$ (monoclinic)

Structure

Monoclinic, $P2_1(4), Z=2$ [Karle and Karle, 1968].

Lattice parameters

a=14.45±.02, b=8.98±.02, c=13.37±.02Å, β=115°12′±15′ [ibid.]

Thermal parameters

Anisotropic [ibid.]

Density

(calculated) 1.287 g/cm³ [ibid.]

Scattering factors

C°, N°, O° [3.3.1A]

Scale factor

(integrated intensities) 4.708 \times 10⁴

Additional patterns

1. PDF card 9-718 [Rose, 1954]

Reference

Karle, I.L. and J. Karle (1968). The crystal structure of the alkaloid reserpine, C₃₃H₄₀N₂O₉, Acta Cryst. B24 81-91. Rose, H.A. (1954). Crystallographic Data. 83.Reserpine, Anal. Chem. 26 1245.

Calculated Pattern (Peak heights)					
d (Å)	Ι		hk	l	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$
13.06 12.10 11.68 7.43 7.20	47 44 10 36 100	1 0 -1 1 0	0 0 0 1	0 1 1 1 + 1 +	6.76 7.30 7.56 11.90 12.28
6.68 6.53 6.05 5.73 5.60	5 5 45 3	-1 2 0 1 -2	0 0 1 1	2 0 2 1 1	13.24 13.54 14.64 15.46 15.82
5.36 5.29 5.02 4.90 4.77	33 9 69 13 60	-1 2 0 -2 1	1 1 1 0	2 0 2 2 2	16.54 16.76 17.66 18.08 18.58
4 • 5 8 4 • 4 9 4 • 4 2 4 • 3 6 4 • 3 3	5 63 4 3 5	-3 0 -1 -2 2	0 2 0 0 1	2 0 3 3 1	19.36 19.76 20.08 20.36 20.50
4.25 4.21 4.19 4.08 4.03	38 22 35 7 13	1 0 -1 -3 0	2 2 1 0	0 + 1 + 1 2 3	20.90 21.08 21.18 21.76 22.02
3.97 3.92 3.90 3.84 3.80	1 4 3 16 16	-1 -2 -3 1 -2	1 1 2 2	3 3 1 1	22.40 22.66 22.78 23.12 23.36
3.73 3.68 3.64 3.60 3.58	27 4 2 .4 18	-1 0 3 0 -3	2 1 0 2 1	2 + 3 1 2 3 +	23.86 24.18 24.46 24.68 24.86
3.46 3.44 3.37 3.33 3.31	13 12 3 4 3	1 2 3 -4 -4	0 1 1 1 1	3 2 1 2 + 1	25.72 25.90 26.42 26.76 26.92
3.27 3.23 3.20 3.13 3.12	8 7 6 3 4	4 - 3 - 4	0 1 0 2 1	0 + 3 4 0 + 3	27.26 27.60 27.82 28.52 28.60
3.07 3.02 3.02 3.00	2 1 1 2	-1 0 -3 0 -1	1 0 1 2 3	4 4 3	29.06 29.52 29.58 29.76 30.80

Ca	lculated	Pattern	Peak he	ights)	C	alculate
d (Å)	Ι	h	ıkl	$\frac{2\theta(^{\circ})}{\lambda \approx 1.54056 ^{\circ}A}$	d (Å)	Ι
2.86 2.81 2.80 2.78 2.76	4 2 2 8	4 0 -5 0 -4 2 1 3 -2 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	31.20 31.86 31.92 32.20 32.38	13.07 12.10 11.71 7.44 7.40	41 40 9 34 3
2.74 2.73 2.72 2.70 2.68	1 2 1 6	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2 3 3 2 5 0 9 4 3 +	32.64 32.76 32.88 33.10 33.42	7.21 7.17 7.12 6.68 6.54	100 10 6 5 5
2.67 2.64 2.62 2.59 2.58	3 2 1 2 2	-2 3 -1 2 5 0 1 1 -1 0	2 2 4 0 4 0 5	33.60 33.90 34.26 34.62 34.68	6 • 0 5 5 • 7 3 5 • 6 0 5 • 3 6 5 • 2 9	5 48 3 37 8
2 • 56 2 • 4 8 2 • 4 7 2 • 3 9 2 • 3 8	1 1 1 2 4	$ \begin{array}{ccc} -2 & 1 \\ -1 & 3 \\ -2 & 3 \\ 3 & 1 \\ 4 & 1 \end{array} $	5 3 3 3 3 2	35.04 36.22 36.38 37.60 37.76	5.02 4.94 4.90 4.77 4.58	78 1 13 70 6
2 • 36 2 • 31 2 • 30 2 • 29 2 • 28	1 1 1 1	5 C 6 1 4 3 2 2 3 2	1 3 2 5 2 5	38.14 38.98 39.18 39.24 39.48	4 • 4 9 4 • 4 2 4 • 36 4 • 33 4 • 2 5	71 3 1 5 40
2.27 2.25 2.216 2.213 2.161	1 5 2 2 2	$ \begin{array}{c} -5 & 1 \\ -5 & 2 \\ 1 & 0 \\ 1 & 4 \\ -3 & 1 \end{array} $	5 4 + 5 + 0 5 + 0 6	39.76 40.04 40.68 40.74 41.76	4.24 4.21 4.21 4.19 4.08	8 8 1 D 3 4 8
2.151 2.143 2.136 2.119 2.109	2 3 2 2 3	1 1 -2 4 -1 0 -4 1 -6 2	5 1 + 6 6 2 3	41.96 42.14 42.28 42.64 42.84	4 • D 3 3 • 9 7 3 • 9 2 3 • 9 D 3 • 8 4	15 1 4 3 18
2.105 2.064 2.046 2.040 2.028	3 2 2 2 1	0 4 -6 2 3 1 5 1 -5 1	2 + 1 4 2 + 6	42.94 43.82 44.24 44.36 44.64	3 • 8 1 3 • 7 3 3 • 7 2 3 • 7 0 3 • 6 8	18 28 8 4 4
1.996 1.962 1.900 1.867 1.813	1 2 1 1 1	-2 4 -4 2 5 2 -3 1 -6 3	3 6 2 7 4	45.40 46.24 47.84 48.72 50.12	3.64 3.61 3.58 3.58 3.58 3.56	2 3 12 13 4
1.775	1	-1 5	5 1	51.44	3.56 3.46	2 16

Calculated Pattern (Integrated)						
d (Å)	Ι	hkl	$2\theta(°)$ $\lambda = 1.54056 \overset{\circ}{A}$			
13.07	41	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	6.75			
12.10	40		7.30			
11.71	9		7.55			
7.44	34		11.89			
7.40	3		11.95			
7.21	100	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	12.26			
7.17	10		12.34			
7.12	6		12.41			
6.68	5		13.24			
6.54	5		13.53			
6.05	5	0 0 2	14.63			
5.73	48	1 1 1	15.45			
5.60	3	-2 1 1	15.81			
5.36	37	-1 1 2	16.53			
5.29	8	2 1 0	16.76			
5.02	78	0 1 2	17.66			
4.94	1	2 0 1	17.95			
4.90	13	-2 1 2	18.08			
4.77	70	1 0 2	18.59			
4.58	6	-3 0 2	19.37			
4.49	71	0 2 0	19.76			
4.42	3	-1 0 3	20.07			
4.36	1	-2 0 3	20.35			
4.33	5	2 1 1	20.51			
4.25	40	1 2 0	20.90			
4.24	8	-3 1 1 1 1 2 0 2 1 -1 2 1 -3 1 2	20.95			
4.21	8		21.07			
4.21	1 D		21.09			
4.19	3 4		21.18			
4.08	8		21.77			
4 • D3	15	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	22.02			
3 • 97	1		22.40			
3 • 92	4		22.65			
3 • 9D	3		22.77			
3 • 84	18		23.12			
3.81	18	-2 2 1	23.36			
3.73	28	-1 2 2	23.86			
3.72	8	2 0 2	23.90			
3.70	4	2 2 0	24.02			
3.68	4	0 1 3	24.17			
3.64	2	3 0 1	24.46			
3.61	3	0 2 2	24.67			
3.58	12	-4 0 2	24.82			
3.58	13	-3 1 3	24.86			
3.56	4	-2 2 2	24.97			
3.56	2	-4 0 1	24.99			
3.46	16	1 0 3	25.72			
3.44	13	2 1 2	25.90			
3.37	4	3 1 1	26.42			
3.34	1	-2 0 4	26.67			

C	alculated	l Patter	n <i>(I</i>)	ntegra	ıted)
d (Å)	Ι		hkl		$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$
3.33 3.32 3.31 3.28 3.27	4 2 1 2	-4 2 -4 -3 1	1 2 1 2 2	2 1 1 1 2	26.75 26.81 26.92 27.16 27.25
3.27	5	4	0	0	27.26
3.27	2	-1	0	4	27.27
3.23	9	1	1	3	27.60
3.20	6	-3	0	4	27.82
3.13	1	-2	1	4	28.49
3.13	2	3	2	0	28.52
3.12	4	-4	1	3	28.61
3.07	2	-1	1	4	29.05
3.02	1	0	0	4	29.51
3.02	1	-3	1	4	29.57
3.00 2.91 2.90 2.87 2.86	2 2 2 1	0 -1 0 2	2 3 3 1 2	3 1 1 4 2	29.75 30.74 30.81 31.18 31.20
2.86 2.81 2.80 2.78 2.78	3 1 1 1 1	4 -5 -4 2 1	0 2 1 3	1 3 2 3 1	31.21 31.86 31.92 32.20 32.21
2.76	10	-2	3	1	32.39
2.74	1	1	2	3	32.64
2.73	2	-1	3	2	32.76
2.72	2	2	3	0	32.88
2.70	1	1	0	4	33.09
2.68	1	0	3	2	33.37
2.68	3	-2	2	4	33.41
2.68	5	-5	1	3	33.43
2.66	3	-2	3	2	33.60
2.66	2	-1	2	4	33.90
2.61	1	5	0	0	34.26
2.59	3	1	1	4	34.61
2.58	1	-1	0	5	34.69
2.56	1	-2	1	5	35.05
2.48	1	-1	3	3	36.21
2.47	1	-2	3	3	36.38
2.45	1	-4	2	4	36.62
2.41	1	4	2	1	37.21
2.39	2	3	1	3	37.60
2.39	1	-5	2	1	37.58
2.38	5	4	1	2	37.75
2.36	1	5	0	1	38.15
2.31	1	-6	1	3	38.98
2.30	1	-4	3	2	39.18
2.29	1	-2	2	5	39.24

Calculated Pattern (Integrated)					
d (Å)	Ι		hkl		$2\theta(^{\circ})$ $\lambda = 1.54056 \overset{\circ}{A}$
2.28 2.27 2.25 2.25 2.250 2.219	1 1 5 1 1	-3 -5 -6 -6	2 1 2 1 1	5 5 4 1 4	39.49 39.76 40.04 40.04 40.63
2.218 2.213 2.161 2.152 2.146	2 1 2 2 1	1 - 3 1 - 2	0 4 1 1 1	5 0 6 5 6	40.68 40.75 41.76 41.95 42.07
2.142 2.134 2.119 2.109 2.108	4 1 1 3 1	-2 -1 -4 -6 2	4 0 1 2 2	1 6 3 4	42.14 42.31 42.64 42.84 42.90
2 • 1 05 2 • 06 4 2 • 04 6 2 • 04 2 2 • 04 0	2 3 1 1 1	0 -6 3 5 -6	4 2 1 1 2	2 1 4 2 4	42.94 43.82 44.24 44.32 44.37
2.028 1.996 1.961 1.900 1.867	1 1 2 1 1	- 5 -2 -4 5 -3	1 4 2 2 1	6 3 6 2 7	44.64 45.40 46.25 47.83 48.73
1.819 1.786 1.775	1 1 1	-6 -3 -1	3 3 5	4 6 1	50.11 51.08 51.43

Monoclinic, C2/c (15),Z=8 [Engel and No-wacki, 1968]

Lattice parameters

a=12.00±.01, b=6.26±.01, c=17.08±.01Å, β =110°0′±20′ [ibid.]

Thermal parameters

Anisotropic [ibid.]

Density

(calculated) 5.53 g/cm³ [ibid.]

Atomic positions

For the given positions and anisotropic temperature factors, the R-value was 13% using 1125 reflections [ibid.].

Polymorphism

A polymorph, proustite, is hexagonal(R3c)

Scattering factors

 S° [3.3.1A] As^o, Ag^o [3.3.1B]

Scale factor

(integrated intensities) 61.68× 10⁴

Additional patterns

1. PDF card 8-134 [Peacock, 1959]

Reference

Engel, P. and W. Nowacki (1968). Die Kristallstruktur von Xanthokon, Ag₃AsS₃, Acta Cryst. B24, 77-81.

Peacock, M.A. (1950). Studies of mineral sulpho-salts:XV. Xanthoconite and pyrostilpnite, Mineral. Mag. 29, 346-358.

Calculated Pattern (Peak heights)						
d (Å)	Ι	hk	el	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$		
5.60 5.47 4.92 4.19 4.01	1 25 3 8 28	-2 0 1 1 -1 1 -1 1 0 0	2 G + 2 3 4 +	15.82 16.20 18.02 21.20 22.14		
3.54 3.53 3.35 3.22 3.13	4 25 7 55	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 4 2 + 0 0	25.12 25.22 26.60 27.66 28.50		
3.07 3.01 2.974 2.841 2.819	30 82 100 4 70	0 2 1 1 -3 1 2 0 4 0	1 4 4 0 +	29.04 29.68 30.02 31.46 31.72		
2.801 2.774 2.727 2.674 2.620	10 13 26 5 12	-4 0 -2 2 3 1 0 0 -2 2	4 2 6 3	31 • 92 32 • 24 32 • 82 33 • 48 34 • 20		
2.579 2.468 2.461 2.439 2.414	9 9 6 7 3	$ \begin{array}{cccc} -1 & 1 \\ 2 & 2 \\ -2 & 2 \\ -3 & 1 \\ 4 & 0 \end{array} $	6 2 4 6 2	34 • 76 36 • 38 36 • 48 36 • 82 37 • 22		
2.391 2.277 2.260 2.237 2.197	5 2 12 1	-4 0 -2 2 1 1 -5 1 -3 1	6 5 6 2 + 7	37.58 39.54 39.86 40.28 41.04		
2.148 2.135 2.104 2.094 2.052	22 19 2 15 2	-4 2 -2 0 2 2 4 2 -1 3	1 + 8 4 0 + 1	42.02 42.30 42.96 43.16 44.10		
2.033 2.020 2.006 2.000 1.994	2 2 12 8 7	0 2 1 3 4 0 1 1 -1 1	6 1 + 4 + 7 8	44.52 44.84 45.16 45.30 45.46		
1.987 1.982 1.957 1.922 1.912	7 8 5 1 3 4	-4 D -6 D -1 3 -2 2 4 2	8 + 4 + 3 + 7 2	45.62 45.74 46.36 47.26 47.52		
1.906 1.901 1.877 1.867	5 5 12 8 4	5 1 -4 2 1 3 -6 0 -3 3	2 6 3 + 6 2 +	47.68 47.82 48.46 48.72 49.30		

Ca	lculated	Pattern (Peak he	ights)	C	alculated	d Pattern (Integra	ated)
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 ^{\circ}A}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$
1.824 1.821 1.801 1.782 1.776	3 4 2 11 15	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	49.96 50.04 50.64 51.22 51.42	5.60 5.47 5.46 4.92 4.21	1 13 11 3 2	$\begin{array}{cccc} -2 & 0 & 2 \\ 1 & 1 & 0 \\ -1 & 1 & 1 \\ -1 & 1 & 2 \\ 1 & 1 & 2 \end{array}$	15.81 16.18 16.21 18.02 21.09
1.771 1.763 1.719 1.714 1.705	12 7 1 2 1	2 2 6 + -2 2 8 3 3 2 2 0 8 -2 0 10	51.56 51.80 53.26 53.42 53.72	4.19 4.01 4.01 3.54 3.53	7 10 15 3 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	21.19 22.13 22.14 25.11 25.23
1.690 1.686 1.675 1.667 1.660	6 4 3 1	$\begin{array}{cccc} -6 & 0 & 8 & + \\ -6 & 2 & 3 & \\ 4 & 0 & 6 & + \\ 5 & 1 & 4 & \\ -4 & 0 & 10 & \end{array}$	54 • 24 54 • 38 54 • 74 55 • 04 55 • 28	3.36 3.35 3.22 3.13 3.07	8 19 7 56 30	$ \begin{array}{ccccccc} -3 & 1 & 1 \\ -3 & 1 & 2 \\ 3 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 2 & 1 \end{array} $	26.55 26.59 27.66 28.49 29.04
1.650 1.646 1.636 1.630 1.623	3 3 6 5 1	$\begin{array}{ccccc} -7 & 1 & 4 \\ 3 & 3 & 3 & * \\ -7 & 1 & 2 \\ 2 & 2 & 7 \\ -2 & 2 & 9 \end{array}$	55.64 55.82 56.16 56.42 56.68	3.01 2.974 2.842 2.819 2.819	86 100 2 55 18	1 1 4 -3 1 4 2 0 4 4 0 0 -2 0 6	29.69 30.02 31.45 31.71 31.72
1.614 1.603 1.569 1.560 1.558	4 1 2 2	$\begin{array}{cccc} -1 & 1 & 10 \\ -6 & 2 & 6 & * \\ -4 & 2 & 9 \\ 7 & 1 & 0 \\ 6 & 2 & 1 & * \end{array}$	57.00 57.42 58.82 59.18 59.26	2.801 2.775 2.727 2.675 2.626	5 13 27 6 1	-4 0 4 -2 2 1 3 1 2 0 0 6 2 2 1	31.93 32.23 32.82 33.47 34.11
1.549 1.541 1.527 1.515 1.503	2 2 1 1 1	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	59.62 60.00 60.58 61.14 61.64	2.619 2.578 2.468 2.459 2.440	12 10 9 2 8	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	34 • 21 34 • 77 36 • 37 36 • 51 36 • 81
1.500 1.492 1.487 1.477 1.475	1 1 3 2 3	$\begin{array}{cccc} -6 & 0 & 10 \\ 5 & 3 & 1 \\ -6 & 2 & 8 & + \\ 4 & 2 & 6 \\ 1 & 1 & 10 \end{array}$	61.80 62.16 62.38 62.88 62.94	2.414 2.391 2.278 2.260 2.241	3 5 2 .1 5	4 0 2 -4 0 6 -2 2 5 1 1 6 0 2 5	37.21 37.58 39.54 39.86 40.21
1.472 1.444 1.437 1.409 1.389	3 1 2 1 2	-8 0 6 7 1 2 + -5 3 7 -4 0 12 5 3 3 +	63.12 64.46 64.82 66.26 67.34	2.237 2.197 2.149 2.148 2.135	12 1 9 17 20	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	40.29 41.05 42.01 42.02 42.30
1.383 1.368 1.343	2 2 1	-4 4 1 -7 1 10 -5 1 12	67.70 68.54 69.98	2.104 2.095 2.095 2.051 2.034	1 13 4 2 2	2 2 4 4 2 0 -2 2 6 -1 3 1 0 2 6	42.95 43.15 43.15 44.11 44.52
				2.021 2.020 2.012 2.006 2.006	1 1 10 3	5 1 1 1 3 1 4 2 1 4 0 4 0 0 8	44.82 44.84 45.01 45.15 45.16

Ca	lculated	Pattern (Integra	ited)
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$
2.000	2	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	45.31
1.994	6		45.46
1.987	2		45.62
1.987	3		45.62
1.984	1		45.69
1.982	5	$\begin{array}{ccccc} -6 & 0 & 4 \\ 1 & 3 & 2 \\ -1 & 3 & 3 \\ -2 & 2 & 7 \\ 4 & 2 & 2 \end{array}$	45.74
1.959	3		46.31
1.957	4		46.36
1.922	16		47.26
1.912	3		47.53
1.905	4	5 1 2	47.69
1.900	3	-4 2 6	47.83
1.879	2	6 0 0	48.39
1.877	14	1 3 3	48.45
1.867	9	-6 0 6	48.73
1.847	1	-3 3 1	49.28
1.846	4	-3 3 2	49.31
1.824	3	3 3 0	49.95
1.822	4	-3 3 3	50.03
1.801	2	4 2 3	50.63
1.785	2	5 1 3	51.12
1.782	12	1 3 4	51.21
1.780	2	3 3 1	51.29
1.780	2	-1 3 5	51.29
1.776	15	-3 3 4	51.42
1 • 7 72	5	2 2 6	51.55
1 • 76 9	1	-5 1 8	51.61
1 • 76 4	8	-2 2 8	51.79
1 • 718	1	3 3 2	53.26
1 • 714	1	2 0 8	53.41
1.705 1.690 1.689 1.689 1.685	1 6 1 1 4	-2 0 10 -6 0 8 4 2 4 0 2 8 -6 2 3	53.72 54.23 54.26 54.26 54.26 54.40
1.678	1	-6 2 2	54.67
1.675	4	4 0 6	54.75
1.667	3	5 1 4	55.04
1.660	1	-4 0 10	55.29
1.650	3	-7 1 4	55.65
1.647	1	-6 2 5	55.79
1.645	2	3 3 3	55.83
1.636	8	-7 1 2	56.17
1.629	6	2 2 7	56.42
1.622	1	-2 2 9	56.69
1.614	5	$ \begin{array}{cccccc} -1 & 1 & 10 \\ 0 & 0 & 10 \\ -6 & 2 & 6 \\ -4 & 2 & 9 \\ 7 & 1 & 0 \end{array} $	57.00
1.605	1		57.36
1.604	4		57.42
1.563	1		58.81
1.560	2		59.17

Calculated Pattern (Integrated)						
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$			
1.558 1.558 1.549 1.541 1.527	1 1 2 2 2	6 2 1 0 4 1 -6 2 7 -5 1 10 -5 3 5	59.24 59.28 59.63 60.00 60.59			
1.514 1.503 1.500 1.492 1.487	1 1 1 2	-2 4 1 2 2 8 -6 0 10 5 3 1 -2 4 3	61.15 61.64 61.80 62.15 62.38			
1.487 1.477 1.475 1.472 1.451	2 2 3 2 1	-6 2 8 4 2 6 1 1 10 -8 0 6 5 1 6	62.40 62.87 62.94 63.12 64.15			
1.444 1.444 1.437 1.416 1.409	1 2 1 1	7 1 2 5 3 2 -5 3 7 -2 4 5 -4 0 12	64.46 64.48 64.82 65.93 66.26			
1.390 1.388 1.383 1.368 1.343	3 1 3 2 1	5 3 3-3 1 12-4 4 1-7 1 10-5 1 12	67.33 67.43 67.70 68.55 69.99			
	L					

Monoclinic, C2/m (12), Z=2 [Pringle and Noakes, 1968]

Lattice parameters

a=6.211, b=3.658, c=5.323 Å, β=108.43°, at -90° to -100 °C. [ibid.]

Density

(calculated) 1.882 g/cm³

Thermal parameters

Anisotropic [ibid.]

Polymorphism

A hexagonal polymorph, β -NaN₃, exists at room temperature.

Scattering factors

 Na° [3.3.1A] $N^{\circ} \cdot {}^{\circ}$ and $N^{\circ} \cdot {}^{\circ}$ calculated from N° and N° [3.3.1A]

Scale factor

(integrated intensities) 0.1648 \times 10⁴

Reference

Pringle, G.E. and D.E. Noakes (1968). The crystal structures of lithium, sodium, and strontium azides, Acta Cryst. B24, 262-269.

Calculated Pattern (Peak heights)					
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$		
5.07 3.09 2.915 2.535 2.429 2.191 1.823 1.791 1.629 1.546	2 11 100 1 14 10 17 5 1 5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	17.48 28.86 30.64 35.38 36.98 41.16 49.98 50.96 56.44 59.78		
1.480 1.458 1.402 1.371 1.179 1.041	1 1 1 2 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	62 • 7 2 63 • 7 8 66 • 6 8 68 • 38 61 • 5 8 95 • 4 6		

Calculated Pattern (Integrated)					
d (Å)	I	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$		
5.07 3.09 2.916 2.536 2.429 2.191 1.823 1.790 1.716 1.629	2 10 100 1 5 11 21 6 1 1 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	17.47 28.65 30.63 35.37 36.97 41.17 49.99 50.97 53.36 56.44		
1.546	6	2 0 2	59.77		
1.480	1	1 1 6	62.72		
1.458	2	0 2 4	63.78		
1.401	1	2 0 5	66.69		
1.371	2	1 0 10	58.39		
1.277	1	0 2 7	74.18		
1.268	1	1 0 12	74.83		
1.179	3	1 2 2	81.59		
1.139	1	2 1 4	85.14		
1.053	1	3 0 0	94.08		
1.041	?	1 1 12	95.47		
1.028	1	0 1 14	97.12		
.804	1	1 2 14	146.93		

Hexagonal, $R\overline{3}m$ (166), Z=3 [Pringle and Noakes, 1968]

Lattice parameters

 $a=3.646\pm.002$, $c=15.214\pm.005Å$, (published value: $c=15.213\pm.005$) [ibid.]

Density

(calculated) 1.849 g/cm³

Thermal parameters

Isotropic [ibid.]

Scattering factors

 Na° [3.3.1A] $N^{-\circ\,\cdot\,8}$ and $N^{+\,\circ\,\cdot\,6}$ calculated from N^{-1} and N° [3.3.1A]

Scale factor

(integrated intensities) 0.4484 \times 10^4

Polymorphism

A monoclinic polymorph, $\alpha-NaN_3\,, \text{exists}$ at -90 to -100 $\,^\circ\text{C}\,.$

Reference

Pringle, G.E. and D.E. Noakes (1968). The crystal structures of lithium, sodium, and strontium azides, Acta Cryst. B24, 262-269.

Calculated Pattern (Peak heights)					
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \Lambda}$		
5.05	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	17.56		
3.11	7		28.70		
2.99	6		29.85		
2.95	35		30.32		
2.87	100		31.16		
2.53	2	0 0 2	35.52		
2.47	12	1 1 1	36.36		
2.31	11	-2 0 2	32.92		
2.25	8	2 0 1	39.98		
2.14	8	-1 1 2	42.14		
1.829	10	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	49.82		
1.817	7		50.16		
1.798	18		50.74		
1.731	2		52.85		
1.713	3		53.44		
1.683 1.674 1.595 1.554 1.495	1 1 5 4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	54.46 54.80 57.72 59.44 62.04		
1.434 1.420 1.385 1.262 1.250	2 2 1 1	-2 2 2 2 2 1 + 1 1 3 6 0 4 -2 2 3	64.96 65.70 67.50 75.20 76.06		
1.179	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	81.58		
1.157	2		83.46		
1.098	1		85.06		
1.067	1		92.40		
1.050	1		54.40		
1.039	1	0 2 4	95.70		
1.011		-1 1 5	99.22		

C	alculated	l Pattern (Integro	uted)
d (Å)	Ι	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \stackrel{\circ}{A}$
5.05	1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	17.55
3.11	6		28.70
2.99	5		29.87
2.95	34		30.31
2.87	100		31.15
2.52	1	0 0 2 1 1 1 -2 0 2 2 0 1 -1 1 2	35.52
2.47	12		36.35
2.31	11		38.92
2.25	8		39.97
2.14	8		42.15
1 • 82 3	12	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	49.81
1 • 817	7		50.16
1 • 798	20		50.74
1 • 730	2		52.86
1 • 713	3		53.43
1.683 1.674 1.596 1.554 1.513	1 1 6 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	54.46 54.81 57.72 59.43 61.21
1,495	5	-4 0 2	62.05
1.481	1	0 2 2	62.67
1.434	3	-2 2 2	64.96
1.420	1	-3 1 3	65.68
1.420	2	2 2 1	65.69
1.387	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	67.50
1.263	2		75.20
1.250	1		76.05
1.235	1		77.20
1.190	1		80.69
1.179	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	81.58
1.172	1		82.16
1.157	3		83.45
1.127	1		86.25
1.122	1		86.74
1.098 1.067 1.050 1.039 1.011	2 2 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	89.06 92.41 94.39 95.70 99.21
1.002 .959 .914 .909 .899	1 1 1 1	-3 1 5 4 2 2 0 4 0 2 2 4 -6 2 2	100.45 106.82 114.77 115.95 117.95

Structure		1 1 1		
Monoclinic,P21/c (14),Z=4 [Cocco et al.,	Ca	lculated	Pattern <i>(Peak he</i>	ights)
1967]	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 A}$
Lattice parameters				
a= 5.583±0.004, b=5.508±0.005, c=16.127±	8.01	2.6	0 0 2	11.04
0.006Å, B=96°26′±3′ [ibid.]	5.55	1	1 0 0	15.96
	5.21	2	0 1 1	17.02
Develter	4.54	1	0 1 2	19.54
Density	4.34	4	1 0 2	20.46
(calculated) 2.974 g/cm ³ [ibid.]				
	4.0.05	43	0 0 4	22.18
Thermal parameters	3.907	10.0	1 1 0	22.74
Isotropic [ibid.]	5.867	16		22.98
TROPIO [mord.]	3.834	5		23.18
	3.021	1	-1 1 /	74+32
Polymorphism	3 4 75		-1 0 //	25 92
Thomsenolite is dimorphous with pachno-	3.4.09	20	1 1 2	26.12
lite which is also monoclinic [Gerhard,	3.2.81	15	-1 1 3	27 15
1966]	3.241			27 50
	3 -0.87		1 0 4	28.90
Seattoning factors	3 66 67		1 0 4	7 0 0 00
Scattering factors $N_{-0}^{0} \rightarrow 1^{0} = N_{-0}^{0} \rightarrow 1^{0} = N_{-0}^{0} = N_{-0}^$	3.042	1 1 1	1 1 3	29.34
Na', Al', F', O', and Ca' [Hanson et al.,	2.915	4.8	-1 1 4	30.64
1964]	2.774	25	200+	32.24
	2.754	8	0 2 0	32.48
Scale factor	2.714	1.6	0 2 1	32.98
(integrated intensities) 1.498 $ imes$ 10^4				
	2 .6 93	14	1 1 4	33.24
	2.580	2	-1 1 5	34.74
Additional patterns	2.535	3	202	35.38
1. PDF 5-343 [Ferguson,1946]	2.485	7	-2 1 1 2 1 0	36+10 36+22
	2 11 55		1 2 0	36 40
Reterences	2.400	6		16+40 70 ED
Cocco, G., P.C. Castiglione, and G. Vagli-	2 .4 60	4		76 96
asindi (1967). The crystal structure of	2 .4 20	5	1 2 1	37.12
thomsenolite, Acta Cryst. 23, 162-166.	2.412	â	2 1 1 +	37.24
Ferguson, R.B. (1946). Trans.Roy. Soc. Can.				3,0,,
40, Sec.IV, 11-25.	2.391	2	-1 2 2	37.58
Gerhard, F.B.Jr. (1966). The crystal struc-	2.339	2	-2 1 3	38.46
ture of the mineral pachnolite. Acta	2.308	5	1 0 6	39.00
Cryst 21 Moscow abstracts A 54	2.283	11	-1 2 3	39.44
Handon U.D. F. Horman J.D. Lea and S	2.270	8	024	39.68
Chillman (1964) UES stomic cost toring				
Skillman (1964). HFS alonget Scattering	2.2.08	2	-2 1 4	40.84
factors, Acta Cryst. 17, 1040-1044.	2.198	2	1 2 3	41.02
	2.169	18	2 11 4 +	41.60
	2.148	4		42.(12
	2.120	. ⁵	1 1 6	47.44
	2.114	1	0 1 7	42.74
	2.0.89	17	0 2 5	43.28
	2.062	2	-2 1 5	4 4.86
	2.055	8	1 2 4	44.02
	2.042	3	-2 0 6	44.52
	2.019	4	2 1 4	44.86
	2.004	₹8	N N 8 +	45.22
	1.958	4 0	-2 2 1	46.32
	1.955	56	2 2 0 +	46.42
	1.934	4	-1 1. 2	46.94

Ca	lculated	Pattern (Peak he	ights)	C	alculated	Pattern (Integr	ated)
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$	d (Å)	I	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$
1.922 1.917 1.915 1.910 1.883	10 9 8 5 11	2 2 1 0 2 6 -2 1 6 1 2 5 0 1 8	47.26 47.38 47.44 47.58 48.30	8 •0 1 5 •5 5 5 •2 1 4 •5 4 4 •3 4	2 1 1 2 1 4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 1.03 1 5.96 1 7.01 1 9.54 2 0.45
1 .8 72 1 .8 65 1 .8 48 1 .P 43 1 .8 25	4 3 3 7 6	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	48.60 48.78 49.28 49.42 49.42 49.94	4 •0 06 3 •9 09 3 •8 68 3 •8 35 3 •6 28	4 3 10 0 1 3 3 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	22.17 22.73 22.97 23.18 24.52
1.820 1.814 1.791 1.760 1.756	6 3 5 9 7	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	50.08 50.24 50.96 51.90 52.04	3 •4 36 3 •4 09 3 •2 80 3 •2 40 3 •0 88	7 20 15 12 5	$ \begin{array}{cccccc} -1 & 0 & 4 \\ 1 & 1 & 2 \\ -1 & 1 & 3 \\ 0 & 1 & 4 \\ 1 & 0 & 4 \end{array} $	25.91 26.12 27.16 27.51 28.89
1 .7 52 1 .7 43 1 .7 39 1 .7 31 1 .7 21	6 4 10 2 6	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	52.16 52.46 52.58 52.86 53.18	3 • 0 42 2 • 9 15 2 • 7 74 2 • 7 70 2 • 7 5 4	11 52 27 2 7	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	29.33 30.64 32.24 32.29 32.48
1.718 1.704 1.694 1.691 1.675	8 1 1 2 11	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	53.28 53.74 54.08 54.20 54.74	2 • 7 1 4 2 • 6 9 4 2 • 5 8 0 2 • 5 3 5 2 • 4 8 6	17 15 2 3 8	$\begin{array}{ccccccc} 0 & 2 & 1 \\ 1 & 1 & 4 \\ -1 & 1 & 5 \\ 2 & 0 & 2 \\ -2 & 1 & 1 \end{array}$	32.97 33.23 34.74 35.38 36.10
1.672 1.640 1.638 1.615 1.612	8 14 10 2 3	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	54.86 56.02 56.10 56.96 57.10	2 • 4 77 2 • 4 67 2 • 4 57 2 • 4 37 2 • 4 20	2 7 2 5 8	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	36.23 36.39 36.55 36.86 37.12
1 .6 07 1 .6 03 1 .5 93 1 .5 54 1 .5 47	2 3 1 1 2	-3 0 6 0 0 10 + 0 3 5 -1 3 5 3 1 4 +	57.28 57.44 57.82 59.42 59.72	2.412 2.411 2.391 2.339 2.308	5 4 2 5	2 1 1 -2 0 4 -1 2 2 -2 1 3 1 0 6	37.24 37.27 37.58 38.46 39.00
1 • 5 42 1 • 5 39 1 • 5 19 1 • 5 15 1 • 4 96	3 3 4 3 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	59.92 60.08 60.96 61.12 62.00	2.291 2.283 2.270 2.208 2.198	1 12 9 2 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	39.29 39.43 39.68 40.83 41.02
1 •4 83 1 •4 79 1 •4 58 1 •4 48 1 •4 40	2 2 3 1 2	3 2 2 -1 2 9 -2 2 8 2 3 3 3 2 3	62.60 62.76 63.80 64.25 64.66	2 •1 70 2 •1 66 2 •1 49 2 •1 28 2 •1 14	20 9 4 6 1	2 0 4 2 1 3 -1 2 4 1 1 6 0 1 7	41.59 41.66 42.01 42.44 42.74
1 .4 32 1 .4 16 1 .4 08 1 .3 93 1 .3 87	1 1 2 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	65.10 65.92 66.32 67.14 67.48	2.089 2.063 2.055 2.042 2.019	2 0 2 9 3 5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	43.28 43.86 44.02 44.33 44.86

Calculated Pattern (Integrated)			uted)	Calculated Pattern (Integrated)			
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$
2.004 2.003 1.959 1.955 1.954	19 29 40 27 28	-1 2 5 0 0 8 -2 2 1 -1 0 8 2 2 0	4 5 • 22 4 5 • 23 4 6 • 32 4 6 • 40 4 6 • 4 2	1.543 1.542 1.539 1.521 1.518	2 2 1 1 5	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	59.91 59.94 6 n. 08 6 n. 25 6 n. 97
1 •9 34 1 •9 22 1 •9 17 1 •9 14 1 •9 09	4 1 2 3 7 1	-2 2 2 2 2 1 1 2 6 -2 1 6 1 2 5	4 6. 94 4 7. 26 4 7. 38 4 7. 45 4 7. 58	1 •5 15 1 •4 96 1 •4 95 1 •4 83 1 •4 79	1 1 1 2 2	3 2 1 1 0 10 0 2 9 3 2 2 -1 2 9	61.12 62.00 62.01 62.61 62.77
1.883 1.872 1.865 1.848 1.843	13 5 3 4 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	48.31 48.61 48.79 49.27 49.42	1.458 1.448 1.440 1.432 1.416	4 2 1 1	-2 2 8 2 3 3 3 2 3 2 7 -2 3 5	63.80 54.26 64.66 65.10 65.91
1 •825 1 •824 1 •820 1 •814 1 •790	Б 1 3 2 6	2 0 6 7 3 1 1 0 8 -2 2 4 2 2 3	49.94 49.96 5	1 •4 08 1 •3 93 1 •3 87 1 •3 77 1 •3 72	1 3 2 1 6	0 1 11 -4 0 2 4 0 0 0 4 1 0 4 1	6 6 . 31 6 7 . 13 6 7 . 47 6 8 . 03 6 8 . 31
1.763 1.760 1.759 1.756 1.753	2 9 2 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	51.81 51.89 51.93 52.05 52.13	1 • 3 71 1 • 364 1 • 3 47 1 • 3 42 1 • 3 36	2 1 2 1 2	-2 2 9 1 3 7 2 2 8 4 0 2 1 4 0	68.35 68.77 69.77 70.08 70.39
1 •752 1 •743 1 •739 1 •730 1 •721	4 3 1 1 1 6	$\begin{array}{cccccc} -3 & 1 & 2 \\ 1 & 3 & 0 \\ -1 & 3 & 1 \\ -2 & 2 & 5 \\ -3 & 1 & 3 \end{array}$	52.17 52.45 52.57 52.86 53.19	1 • 3 34 1 • 3 33 1 • 3 33 1 • 3 21 1 • 3 14	1 1 3 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	7 N. 55 7 Q. 57 7 N. 61 7 I. 31 7 I. 76
1 •718 1 •704 1 •694 1 •691 1 •676	8 1 2 11	-2 0 8 2 2 4 0 1 9 1 3 2 3 1 2	53.28 53.74 54.08 54.20 54.73	1 • 3 07 1 • 3 03 1 • 2 98 1 • 2 95 1 • 2 90	1 2 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	72.22 72.45 72.81 72.97 73.30
1 •6 75 1 •6 73 1 •6 40 1 •6 40 1 •6 38	6 5 12 6 7	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	54.77 54.84 56.02 56.03 56.11	1 •2 88 1 •2 77 1 •2 67 1 •2 58 1 •2 46	3 2 2 1 1	2 1 10 -3 2 8 2 2 9 1 4 4 -1 4 5	73.45 74.18 74.86 75.54 76.41
1.616 1.613 1.612 1.607 1.603	2 1 3 1 2	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	56.95 57.05 57.10 57.28 57.43	1 • 2 4 5 1 • 2 4 2 1 • 2 3 8 1 • 2 3 5 1 • 2 3 4	2 1 1 1 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	76.47 76.68 76.97 77.16 77.21
1 •603 1 •593 1 •554 1 •548 1 •547	2 1 2 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	57.46 57.83 59.41 59.68 59.73	1 •2 33 1 •2 28 1 •2 24 1 •2 22 1 •2 20	1 3 2 1 1	2 4 0 1 2 11 3 2 7 1 4 5 - 3 2 9	77.29 77.71 78.03 78.16 78.29

Sodium Calcium Beryllium Aluminum Fluorosilicate, meliphanite, (Na_{0.63}Ca_{1.37})Be(Al_{0.13}Si_{0.87}) (O_{6.25}F_{0.75}) (tetragonal)

Structure

Tetragonal, $I\overline{4}$ (82), Z=8 [Dal Negro et al., 1967]

Lattice parameters

a=10.516±0.002, c=9.887±0.002Å [ibid.]

Density

(calculated) 3.024 g/cm³ [ibid.]

Thermal parameters

Isotropic [ibid.]

Scattering factors

 Na^{+1} , F^{-1} , Be^{+1} , Si^{+2} , O^{-1} [3.3.1A] Ca^{+2} [3.3.1B]

Scale factor

(integrated intensities) 8.679×10^4

Additional patterns

 PDF 17-204 [Neumann and Bergstol,Geol.-Min. Museum, Oslo, Norway]

Reference

Dal Negro, A., G. Rossi, and L. Ungaretti (1967). The crystal structure of meliphanite, Acta Cryst. 23, 260-264.

Calculated Pattern (Peak heights)							
d (Å)	Ι	hkl			$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$		
7 •202 5 •254 4 •940 4 •247 4 •115	5 2 3 1 3 3	n 0 2 1	1 2 0 1 1	1 0 2 1 + 2	12.28 16.86 17.94 20.90 21.58		
3.601 3.326 3.144 2.970 2.798	37 2 39 4	n 3 2 2	2 1 1 2 3	2 0 + 3 2 1 +	24.70 26.78 28.36 30.06 31.96		
2.759 2.699 2.629 2.471 2.401	100 4 7 3 1	1 2 0 0	3 1 4 0 3	2 + 3 + 0 4 + 3	32.42 33.16 34.08 36.32 37.42		
2.352 2.346 2.721 2.237 2.216	18 20 20 5 15	4 1 0 3	2 1 4 2 3	0 + 4 2 4 2	38.24 38.34 38.76 40.28 40.68		
2 .1 84 2 .1 23 2 .1 57 2 .1 17 1 .984	1 3 1 1 21	2 2 1 3	3 4 5 4 1	3 2 + 1 + 3 + 4 +	41.30 42.54 43.98 44.90 45.70		
1.9156 1.9035 1.8589 1.8226 1.8031	1 2 8 1 7	5 1 4 2 3	2 5 4 1 5	1 2 + 0 5 + 0 +	47.42 47.74 48.96 50.00 50.58		
1 • 8 01 1 1 • 7 7 3 0 1 • 7 5 2 8 1 • 7 3 9 7 1 • 7 0 3 7	6 1 8 2 2 4'	0 0 4 4	45642	4 3 0 2 4 +	50.64 51.50 52.14 52.56 53.76		
1.6944 1.6800 1.6626 1.6521 1.6478	7 1 7 6 5	3 5 7 1 1	5 2 6 0	2 + 3 + 0 + 2 6	54.08 54.58 55.20 55.58 55.74		
1 •6 36 4 1 •5 8 3 4 1 •5 75 9 1 •5 72 5 1 •5 06 5	1 2 1 2 1	2 5 6 0 2	3 1 2 2 2	5 + 4 + 2 + 6 6	56.16 58.22 58.52 58.66 61.50		
1.4763 1.4700 1.4568 1.4297 1.3986	6 1 1 1 2	1 4 3 0 6	3 5 5 6 4	6 + 3 + 4 + 2 +	62.90 53.20 63.84 65.20 66.84		

Sodium Calcium Beryllium Aluminum Fluorosilicate, meliphanite, $(Na_{0.63}Ca_{1.37})Be(AI_{0.13}Si_{0.87})$ $(O_{6.25}F_{0.75})$ (tetragonal) – continued

Calculated Pattern (Peak heights)			Calculated Pattern (Integrated)				
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 A}$	đ (Å)	I	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$
1 • 3 96 3 1 • 3 7 9 6 1 • 3 7 2 2 1 • 3 4 9 3 1 • 3 30 0	4 2 1 2 7	Π 4 6 6 2 4 + 3 3 6 2 4 6 + 7 3 2 +	66.96 67.88 68.30 69.62 70.78	7 • 2 0 3 5 • 2 5 8 4 • 9 4 3 4 • 2 4 7	8 4 5 19	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	12.28 16.85 17.93 20.90
1 • 3 14 6 1 • 2 87 4 1 • 2 74 3 1 • 2 70 5 1 • 2 55 9	4; 1 1 1 1	Л 8 0 1 5 6 + 8 2 0 + П 8 2 4 6 4 +	71.74 73.50 74.38 74.64 75.66	4 • 1 17 3 • 6 02 3 • 325 3 • 325 3 • 304	5 66 2 1 1	1 1 2 0 2 2 3 1 0 1 3 0 0 3 1	21.57 24.70 26.79 26.79 26.96
1 •2 393 1 •2 36 0 1 •2 33 0 1 •2 16 4 1 •2 05 4	3 2 1 . 4 2	660 008 446 356+ 374+	76.86 77.10 77.32 78.58 79.44	3 •1 45 2 •9 71 2 •7 97 2 •7 97 2 •7 97 2 •7 59	4 79 3 4 96	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	28.36 30.05 31.97 31.97 32.42
1.2006 1.1868 1.1606 1.1584 1.1439	2 1 1 1 2	D 6 6 5 7 2 + D 8 4 1 3 8 8 4 2 +	79.82 80.94 83.16 83.36 84.66	2.759 2.699 2.699 2.629 2.472	10 0 5 4 1 4 4	1 3 2 2 1 3 1 2 3 0 4 0 0 0 4	32.42 33.17 33.17 34.07 36.32
1 •1 33 3 1 •1 30 5 1 •1 18 4 1 •1 07 9 1 •1 05 9	1 2 1 2 1	8 2 4 + 1 9 2 + 0 4 8 6 6 4 3 3 8	85.64 85.90 87.06 88.10 88.30	2.470 2.401 2.351 2.351 2.346	2 2 18 16 21	1 4 1 0 3 3 4 2 0 2 4 0 1 1 4	36.35 37.42 38.24 38.24 38.34
1 •1 04 1 1 •0 95 7 1 •0 93 9 1 •0 92 0 1 •0 58 4	1 2 2 1	7 1 6 + 7 5 4 + 2 4 8 + 6 4 6 + 3 7 6 +	88.48 89.34 89.52 89.72 93.40	2.321 2.237 2.215 2.184 2.123	4 1 1 1 3 3 2 3	17 4 2 17 2 4 3 3 2 2 3 3 4 2 2	38.76 40.28 40.69 41.30 42.54
1.0512 1.0094 .9764	1 1 2	1 9 4 + 2 10 2 + 4 10 0 +	94.24 99.48 104.16	2.123 2.058 2.057 2.017 2.017	4 1 1 1 1	2 4 2 2 2 4 0 5 1 4 1 3 1 4 3	4 2 • 5 4 4 3 • 95 4 3 • 98 4 4 • 90 4 4 • 90
				1.984 1.984 1.9158 1.9034 1.9034	23 25 3 2 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	45.70 45.70 47.42 47.74 47.74
				1.8590 1.8228 1.8228 1.8035 1.8035	19 1 1 7 8	4 4 0 1 2 5 2 1 5 5 3 0 3 5 0	48.95 49.99 49.99 50.57 50.57
				1 • 8 00 8 1 • 7 7 2 9 1 • 7 5 2 7 1 • 7 40 0 1 • 7 0 3 7	7 1 18 5 30	0 4 4 0 5 3 0 6 0 4 4 2 4 2 4	5 N . 6 5 5 1 . 5 N 5 2 . 1 4 5 2 . 5 5 5 3 . 7 6
Sodium Calcium Beryllium Aluminum Fluorosilicate, meliphanite, $(Na_{0.63}Ca_{1.37})Be(Al_{0.13}Si_{0.87})$ $(O_{6.25}F_{0.75})$ (tetragonal) – continued

C	alculated	l Pattern (Integra	ated)	Ca	alculated	l Pattern <i>(Integr</i>	ated)
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 ^{\circ}}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$
1 •7 037 1 •7 030 1 •6 94 3 1 •6 94 3	27 2 7 7	2 4 4 1 6 1 5 3 2 3 5 2	53.76 53.78 54.08 54.08	1 •2359 1 •2331 1 •2165 1 •2165	3 3 5 6	П П 8 4 4 6 5 3 6 3 5 6	77.11 77.31 78.57 78.57
1.6800	2	5 2 3	54.58	1.2055	3	734	79.43
1.6627 1.6627 1.6519 1.6478	8 8 15 4	6 2 0 2 6 0 0 6 2 0 0 6	55.20 55.20 55.59 55.74	1 •2006 1 •1857 1 •1867 1 •1867 1 •1606	4 5 2 2 2	0 6 6 7 5 2 5 7 2 0 8 4	79.82 80.95 80.95 80.95 83.17
1.6367 1.6367 1.6201 1.6088 1.5835	1 1 2 2	325 235 451 116 514	56.15 56.15 56.78 57.21 58.21	1 •1 58 5 1 •1 4 3 8 1 •1 4 3 8 1 •1 3 3 3 1 •1 3 3 3	1 3 2 2	1 3 8 8 4 2 4 8 2 8 2 4 2 8 4	83.35 84.66 84.66 85.64 85.64
1 • 5 8 3 5 1 • 5 76 0 1 • 5 76 0 1 • 5 72 4 1 • 5 31 0	2 1 1 4 1	1 5 4 6 2 2 2 6 2 0 2 6 1 6 3	58.21 58.52 58.52 58.66 60.42	1 •1 30 5 1 •1 30 5 1 •1 18 5 1 •1 07 9 1 •1 06 0	2 2 2 5 2	9 1 2 1 9 2 0 4 8 6 6 4 3 3 8	85.90 85.90 87.05 88.10 88.23
1 • 5 06 5 1 • 4 76 5 1 • 4 76 5 1 • 4 69 9 1 • 4 56 9	4 8 1 1	2 2 6 3 1 6 1 3 6 4 5 3 5 3 4	61.50 62.89 62.89 63.21 63.84	1 •1 04 0 1 •1 04 0 1 •0 95 8 1 •0 95 8 1 •0 94 0	1 2 1 1 4	176 716 754 574 248	8 8.48 8 8.48 8 9.33 8 9.33 8 9.33 8 9.52
1 •4 56 9 1 •4 29 7 1 •3 98 7 1 •3 98 7 1 •3 98 7	2 3 3 9	354 064 642 462 046	63.84 65.20 66.83 66.83 66.97	1 • 0 94 0 1 • 0 92 1 1 • 0 92 1 1 • 0 58 4 1 • 0 58 4	3 3 3 2 2	428 6466 736 376	89.52 89.71 89.71 93.41 93.41
1 • 3894 1 • 3808 1 • 3796 1 • 3796 1 • 3723	1 1 2 2 3	5 2 5 7 3 0 2 6 4 6 2 4 3 3 6	67.34 67.81 67.88 67.88 67.88 68.23	1.0511 1.0511 1.0195 1.0195 1.0195 1.0100	1 1 1 , 1	9 1 4 1 9 4 3 5 8 5 3 8 7 6 8	94.25 94.25 98.15 98.15 98.39
1.3495 1.3495 1.3299 1.3299 1.3299	3 3 11 10 10	2 4 6 4 2 6 7 3 2 3 7 2 0 8 0	69.61 69.61 70.79 70.79 71.75	1.0095 1.0095 1.0003 1.0003 .9919	1 1 1 1 1	1 0 2 2 2 1 0 2 9 5 2 5 9 2 2 6 8	99.47 99.47 100.72 100.72 101.90
1 •2 874 1 •2 874 1 •2 75 3 1 •2 75 3 1 •2 75 3	1 2 1 1 1	5 1 6 1 5 6 8 2 0 2 8 0 7 1 4	73.50 73.50 74.32 74.32 74.38	.9919 .9764 .9764 .9717 .9677	1 3 4 2 1	6 2 8 10 4 0 4 10 0 0 2 10 0 10 4	101-90 104-17 104-17 104-88 105-50
1 •2 74 3 1 •2 70 4 1 •2 56 0 1 •2 56 0 1 •2 39 3	1 3 1 1	174 082 644 464 660	74.38 74.65 75.65 75.65 75.65	LL	1]

Structure Orthorhombic, P2 ₁ 2 ₁ 2 ₁ (19),Z=4 [Cannillo	Ca	lculated	ilated Pattern (Peak heights)		
et al., 1967]	$d(\overset{\circ}{A})$	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$	
Lattice parameters					
a=7.401±0.008, b= 7.420±0.008, c= 9.939±	5.94	20	0 1 1 +	14.90	
0.005Å [ibid.]	4.97	14	0 0 2	17.84	
	4.63	5	1 1 1	19.14	
	4 - 1 3	2	1 0 2 +	21.52	
Density	3.604	40	1 1 2	24.68	
(calculated) 2.961 g/cm ³ [ibid.]					
	3.469	13	2 0 1 +	25.66	
Thormal narometers	3.312	3	1 2 0 +	26.90	
	3.144	5	1 2 1 +	28.36	
Isotropic [ibid.]	3.023	11	0 1 3 +	29.52	
	2.972	30	0 2 2	30.04	
Scattering factors				70.00	
1 1	2.968	33	2 0 7	50.08	
Be ⁺¹ . F ⁻² . Na ⁺² . Si ⁺² . O ⁻¹ [3.3.1A]	2.756	100		32.46	
Ca^{+1} [3,3,1B]	2.620	9		14.20	
ou [310112]	2.534	1		75.40	
	2.485		0 0 4	30.17	
Scale factor			0 2 2	75 72	
(integrated intensities) 2.059 $ imes$ 10^4	2.471	1	0 2 1	37 111	
	2.400		1 0 4 +	79 18	
Additional matterns	2.355	10	1 3 0 4	30.10	
Additional patterns	2.346	14	3 1 0 +	30.37	
1. PDF 18-711 [Neumann and Bergstal, Min.	2.541	17		30.47	
Geol. Museum, Oslo, Norway]	2 710	20	2 2 2 2	38.82	
	2.318	78	1 3 1	30.02	
	2.270	5	3 1 1	39.52	
	2.218	4	1 1 4	40.14	
	2 2 2 1 //	12	0 3 2	40.72	
Reference	C . / 14	14			
Cannillo, E., G. Giuseppetti, and V.Tazzoli	2 210	16	3 0 2	40.80	
(1967). The crystal structure of leuco-	2.118	3	3 1 2	42.66	
r_{1}	2.055	2	2 2 3	44.02	
phanice, Acta cryst. 25, 255-255.	1.988	19	2 1 4 +	45.60	
	1.899	2	3 2 2 +	47.86	
	1.855	5	n 4 n	49.08	
	1.850	7	4 n n	49.20	
	1.803	4	2 2 4	50.58	
	1.799	4	1 4 0	50.70	
	1.795	4	4 1 0	50.82	
	1.770	2	1 4 1	.51.58	
	1.767	2	4 1 1	51.70	
	1.751	4	7 7 0 1	52.18	
	1.747	11	5 5 0 +	57.54	
	1.734	1	4 0 2	52.1h	
	1 700	1	3 3 1	53,20	
	1.705	1	1 3 4	53,70	
	1 - 7 85	10	3 1 4	53.74	
	1.502	1 / L	1 4 2	54.16	
	1.699	LL LL	4 1 2	54.30	
	1.000				
	1.656	7	4 2 0 +	55.44	
	1.648	5		55.74	
	1.616	1	3 2 11 4	58 22	
	1.583	3		58 78	
	1.579	5	1 1 0 *	10.10	

Ca	lculated	Pattern (Peak he	ights)	C	alculated	l Pattern (Integra	ated)
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$	d (Å)	Ι	hkl	$\begin{array}{c} 2\theta(^{\circ}) \\ \lambda \approx 1.54056 \stackrel{\circ}{A} \end{array}$
1.575	3	2 4 2	58.56	5.95	21	$\begin{array}{cccccc} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 0 & 0 & 2 \\ 1 & 1 & 1 \\ 0 & 1 & 2 \end{array}$	1 4. 89
1.571	1	4 2 2	58.72	5.94	7		1 4. 91
1.545	1	3 3 3	59.80	4.97	19		1 7. 83
1.515	2	3 1 5 +	61.10	4.64	8		1 9. 13
1.512	2	0 2 6 +	61.24	4.13	1		2 1. 50
1.482	5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	62.64	4 •1 3	2	1 0 2	21.52
1.466	1		63.38	3 •6 06	62	1 1 2	24.67
1.440	1		64.70	3 •4 76	10	0 2 1	25.61
1.400	4		66.76	3 •4 68	13	2 0 1	25.57
1.397	3		66.94	3 •3 17	3	1 2 0	26.86
1.393 1.377 1.375 1.352 1.332	2 2 3 1	5 1 2 4 2 4 + 0 3 6 + 3 1 6 + 1 5 3	67.12 68.00 68.14 69.44 70.64	3 • 3 12 3 • 1 46 3 • 1 42 3 • 0 25 3 • 0 24	3 6 3 1 0 8	2 1 0 1 2 1 2 1 1 . 0 1 3 1 0 3	2 6. 90 2 8. 34 2 8. 38 2 9. 50 2 9. 52
1.327	4	2 5 2	70.94	2 .9 73	36	n 2 2	30.03
1.325	5	5 2 2	71.10	2 .968	31	2 n 2	30.08
1.310	3	4 4 0	72.04	2 .7 59	94	1 2 2	32.43
1.306	2	1 2 7	72.26	2 .7 56	100	2 1 2	32.46
1.299	1	4 4 1	72.76	2 .6 20	15	2 2 n	34.20
1.290	1	326+	73.35	2 •5 33	2	2 2 1	35.40
1.272	1	350+	74.56	2 •4 85	3	n 0 4	36.12
1.267	2	442	74.90	2 •4 71	1	0 2 3	36.32
1.260	1	531	75.38	2 •4 00	3	n 3 1	37.44
J.253	1	514	75.84	2 •3 56	7	0 1 4	38.15
1 •2 42	1	П О 8	76.64	2 • 3 56	8	1 0 4	3 P. 17
1 •2 37	2	О 6 О +	77.06	2 • 3 46	1 K	1 3 0	3 R. 34
1 •2 34	3	6 О П +	77.28	2 • 3 44	4	1 2 3	3 R. 37
1 •2 19	2	1 4 6	78.40	2 • 3 42	4	2 1 3	3 R. 40
1 •2 17	2	4 1 6	78.50	2 • 3 41	1 4	3 1 0	3 R. 42
1.205	1	2 5 4	79.50	2 • 3 18	47	2 2 2	3 8. 82
1.202	2	3 3 6 +	79.72	2 • 2 83	4	1 3 1	3 9. 44
1.182	1	6 1 2	81.34	2 • 2 79	5	3 1 1	3 9. 52
1.174	1	1 5 5	82.00	2 • 2 45	8,	1 1 4	4 0. 13
1.172	1	2 4 6	82.20	2 • 2 14	18	1 3 2	4 0. 71
1.168	1	2 3 7	82.50	2 •2 10	18	3 0 2	4 0.80
1.141	1	2 6 2	84.88	2 •1 21	2	1 3 2	4 2.58
1.139	1	6 2 2	85.08	2 •1 18	4	3 1 2	4 2.66
1.132	1	3 5 4	85.76	2 •0 55	4	2 3	4 4.03
1.127	1	5 4 2 +	86.24	2 •0 14	1	2 3 1	4 4.98
1.123 1.110 1.107 1.105 1.097	1 1 2 3	2 2 8 1 3 8 + 0 6 4 3 4 6 + 3 1 8 +	86.66 87.88 88.18 88.42 89.16	1 •9 89 1 •9 87 1 •9 00 1 •8 98 1 •P 59	18 20 2 2 2	1 2 4 2 1 4 2 3 2 3 2 2 1 1 5	45.58 45.61 47.83 47.87 48.97
1.095 1.093 1.092 1.010	2 2 2 1	1 6 4 1 5 6 + 5 1 6 2 6 5	89.42 89.62 89.74 99.38	1 • 8 55 1 • 8 50 1 • 8 24 1 • 8 03 1 • 7 99	7 10 1 7 4	0 4 0 4 0 0 0 4 1 2 2 4 1 4 0	4 9.07 4 9.20 4 9.97 5 0.59 5 0.69

C	alculated	d Pattern (Integra	ated)	Ca	alculated	l Pattern (Integra	ited)
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \stackrel{\circ}{A}}$
1 •7 95 1 •7 71 1 •7 67 1 •7 52 1 •7 51	4 3 3 3 3 3	4 1 0 1 4 1 4 1 1 0 2 5 2 0 5	50.82 51.58 51.70 52.16 52.19	1 •3 75 1 •3 64 1 •3 62 1 •3 54 1 •3 53	2 1 1 1 1	5 2 0 2 5 1 5 2 1 0 5 3 3 4 3	6 8. 15 6 8. 75 6 8. 89 6 9. 33 6 9. 39
1 • 7 47 1 • 7 47 1 • 7 46 1 • 7 38 1 • 7 34	2 16 2 1 2	2 3 3 3 3 0 3 2 3 0 4 2 4 0 2	5 2. 32 5 2. 34 5 2. 36 5 2. 62 5 2. 75	1 • 3 53 1 • 3 52 1 • 3 52 1 • 3 51 1 • 3 32	3 1 3 1 2	1 3 6 4 3 3 3 1 6 5 0 3 1 5 3	69.40 69.43 69.45 69.50 70.65
1 •7 20 1 •7 06 1 •7 04 1 •6 92 1 •6 88	2 2 7 2 2 7 4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5 3.20 5 3.69 5 3.75 5 4.17 5 4.28	1 • 3 27 1 • 3 25 1 • 3 12 1 • 3 10 1 • 3 05	9 9 1 8 1	2 5 2 5 2 2 3 3 5 4 4 0 1 2 7	7 0. 95 7 1. 09 7 1. 90 7 2. 03 7 2. 33
1 •6 58 1 •6 56 1 •6 56 1 •6 48 1 •6 36	7 4 9 8 1	2 4 0 0 0 6 4 2 0 3 3 2 2 4 1	55.36 55.42 55.45 55.74 56.19	1 • 2 99 1 • 2 90 1 • 2 89 1 • 2 73 1 • 2 72	2 1 1 1 1	4 4 1 2 3 6 3 2 6 4 3 4 4 2 5	7 2. 75 7 3. 33 7 3. 36 7 4. 50 7 4. 52
1 .6 33 1 .5 17 1 .5 84 1 .5 84 1 .5 83	1 1 2 3	4 2 1 0 1 6 2 3 4 2 2 5 3 2 4	5 6 28 5 6 91 5 8 19 5 8 21 5 8 22	1 •2 72 1 •2 67 1 •2 60 1 •2 53 1 •2 42	1 7 2 1 3	3 5 0 4 4 2 5 3 1 5 1 4 0 0 8	7 4.56 7 4.90 7 5.38 7 5.84 7 6.63
1 • 5 81 1 • 5 79 1 • 5 78 1 • 5 73 1 • 5 71	2 5 4 1 1	1 4 3 1 1 6 4 1 3 2 4 2 4 2 2	58,31 58,38 58,42 58,64 58,73	1 •2 37 1 •2 36 1 •2 34 1 •2 34 1 •2 34 1 •2 24	4 1 1 3 1	0 6 0 0 4 6 4 0 6 6 0 0 6 0 1	77.05 77.13 77.24 77.29 77.99
1 •5 45 1 •5 17 1 •5 15 1 •5 13 1 •5 12	1 2 3 1 1	3 3 3 1 3 5 3 1 5 0 2 6 2 0 6	5 9.81 6 1.05 6 1.11 6 1.23 6 1.26	1 •2 19 1 •2 17 1 •2 05 1 •2 03 1 •2 02	5 4 2 3	1 4 6 4 1 6 2 5 4 5 2 4 3 3 6	78.40 78.50 79.50 79.63 79.71
1 •4 82 1 •4 81 1 •4 66 1 •4 55 1 •4 40	5 6 2 1 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	6 2 • 6 3 6 2 • 6 6 6 3 • 37 6 3 • 92 6 4 • 6 9	1 •1 85 1 •1 82 1 •1 74 1 •1 72 1 •1 68	1 2 7 1	1 6 2 6 1 2 1 5 5 2 4 6 2 3 7	8 1. 12 3 1. 35 3 2. 00 8 2. 18 8 2. 49
1 •4 29 1 •4 00 1 •3 96 1 •3 95 1 •3 93	1 9 2 1 2	3 3 4 2 2 6 1 5 2 0 1 7 5 1 2	6 5. 24 6 6. 75 6 6. 96 6 7. NA 6 7. 12	1 •1 65 1 •1 59 1 •1 42 1 •1 39 1 •1 32	1 1 2 2 2	2 6 1 4 4 4 2 6 2 6 2 2 3 5 4	8 2 80 8 3 32 8 4 87 9 5 08 8 5 76
1 • 3 79 1 • 3 78 1 • 3 77 1 • 3 76 1 • 3 75	7 3 1 7 7	2 4 4 4 2 4 2 5 0 0 3 6 3 0 6	67.90 67.98 68.01 68.05 68.13	1 •1 31 1 •1-27 1 •1 27 1 •1 23 1 •1 14	1 2 2 1	5 3 4 4 5 2 5 4 2 2 2 8 4 1 7	85.86 86.19 96.25 86.56 87.52

Structure

Orthorhombic, Pcnb (60), Z=4 [Pant and Cruickshank, 1968]

Lattice parameters

a=6.409±.002,b=15.423±.004,c=4.896±.002Å (published value, b=15.422Å) [ibid.]

Thermal parameters

Isotropic: Na 1.212,Si 0.634;0(1) 1.548; 0(2) 0.988; 0(3) 1.190 Density (calculated). 2.50 g/cm³ [ibid.]

Polymorphism

At 1 bar pressure, sodium disilicate glass can be crystallized to yield six crystalline polymorphs designated as α_{III} , α_{II} , α_{I} , β , γ , and δ phases. Only the α_{I} and β polymorphs have any true range of thermodynamic stability [Williamson and Glasser, 1966]

Scattering factors

 0° , Na $^{\circ}$, Si $^{\circ}$ [3.3.1A]

Scale factor

(integrated intensities) 1.969 X 104

Additional patterns

- PDF card 18-1241[Range and Willigallis, Mineralogisches Institut. Freie Universität, Berlin, Germany, 1964]
- 2. PDF card 19-1237 [Williamson and Glasser, 1966]

Reference

- Pant, A.K. and D.W.J. Cruickshank [1968]. The crystal structure of α-Na₂Si₂O₅,Acta Cryst. B24, 13-19.
- Williamson, J. and F.P. Glasser (1966). The crystallization of Na₂O·2SiO₂-SiO₂ glasses, Phys. Chem. Glasses 7, 127-128.

Ca	lculated	Pattern (Pe	eak he	rights)
d (Å)	Ι	hkl		$\frac{2\theta(°)}{\lambda = 1.54056 A}$
4.929	62	1 2	0	17.98
3.890	10	1 0	1	22.84
3.857	44	0 4	0	23.04
3.773	100	1 1	1	23.56
3.474	4	1 2	1	25.62
3.304	100	1 4	0	26.96
3.204	20	2 0	0	27.82
3.102	5	1 3	1	28.76
2.959	1	2 2	0	30.18
2.738	5	1 4	1	32.68
2.642	29	2 1	1	33.90
2.532	16	2 2	1	35.42
2.448	55	0 0	2	36.68
2.417	13	1 5	1	37.16
2.385	13	1 6	0	37.68
2.378	9	2 3	1	37.80
2.333	2	0 2	2	38.56
2.262	1	1 1	2	39.82
2.202	3	2 4	1	40.96
2.145	5	1 6	1	42.10
2.067	2	0 4	2	43.76
2.005	7	2 6	0	45.18
1.967	14	1 4	2	46.12
1.945	12	2 0	2 +	46.66
1.928	4	0 8	0 +	47.10
1.917 1.869 1.846 1.829 1.773	2 20 8 1 1	1 7 3 4 1 8 3 3 0 6	1 0 1 2	47.38 48.68 49.32 49.80 51.50
1.746	1	3 4	1	52.36
1.708	3	1 6	2	53.60
1.653	4	3 5	1 +	55.54
1.645	3	2 5	2	55.84
1.643	4	3 6	0	55.92
1.602 1.581 1.573 1.565 1.558	3 1 4 2 1	4 0 1 0 1 1 2 8 3 6	0 3 1 1	57.48 58.30 58.62 58.96 59.28
1.551	2	2 6	2	59.56
1.549	2	1 2	3	59.62
1.542	7	0 10	0	59.92
1.536	3	3 3	2	60.18
1.515	3	0 8	2 +	61.12
1.485	13	3 4	2	62.48
1.481	7	4 4	0	62.66
1.474	2	1 8	2	63.00
1.463	2	1 4	3	63.52
1.460	3	4 3	1	63.68

Ca	lculated	Pattern (Peak he	ights)	C	alculated	l Pattern <i>(Integro</i>	ated)
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$	d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$
1.448 1.444 1.431 1.429 1.407	5 9 3 5 2	2 1 3 2 9 1 3 8 0 2 2 3 1 5 3	64.28 64.48 65.14 65.24 66.36	4 • 929 3 • 891 3 • 856 3 • 772 3 • 474	55 7 43 95 4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	17.98 22.84 23.05 23.56 25.62
1 • 3 9 9 1 • 3 6 4 1 • 3 6 0 1 • 3 4 7 1 • 3 4 1	2 3 3 2	2 3 3 3 6 2 4 6 0 + 1 6 3 4 0 2	66.80 68.76 68.98 69.76 70.14	3.304 3.204 3.102 2.959 2.739	100 19 5 1 5	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	26.96 27.82 28.75 30.18 32.67
1.336 1.319 1.305 1.300 1.297	1 1 3 1 1	4 1 2 1 11 1 0 10 2 3 7 2 3 0 3	70.44 71.46 72.36 72.68 72.88	2.642 2.533 2.464 2.448 2.417	32 18 1 60 14	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	33.91 35.41 36.43 36.68 37.17
1.285 1.266 1.264 1.253 1.236	2 1 1 2	0 12 0 4 4 2 5 2 0 4 7 1 3 8 2 +	73.64 74.94 75.06 75.88 77.12	2.386 2.377 2.333 2.262 2.201	14 4 2 1 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	37.67 37.81 38.55 39.82 40.96
1.232 1.224 1.220 1.209 1.196	2 1 1 2	4 8 0 0 0 4 0 1 4 2 10 2 3 5 3	77.38 78.00 78.28 79.18 80.22	2.145 2.067 2.005 1.967 1.958	5 2 9 1 8 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	42.10 43.77 45.18 46.11 46.33
1.188 1.171 1.161 1.150 1.143	1 1 2 6 1	4 6 2 1 3 4 2 8 3 5 5 1 2 0 4	80.80 82.30 83.14 84.06 84.70	1.945 1.942 1.930 1.928 1.917	13 4 2 3 2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	46.65 46.73 47.04 47.10 47.38
1 • 1 38 1 • 1 35 1 • 1 1 1 1 • 1 0 9 1 • 1 06	3 3 1 3 1	4 9 1 + 1 13 1 4 10 0 2 9 3 0 6 4	85 • 20 85 • 48 87 • 78 88 • 00 88 • 30	1.869 1.846 1.830 1.773 1.746	24 10 1 2 2	3 4 0 1 8 0 3 3 1 0 6 2 3 4 1	48.69 49.32 49.79 51.51 52.36
1.001 1.086 1.041 1.040 1.024	1 1 1 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	88.76 90.40 95.42 95.56 97.58	1.709 1.653 1.652 1.645 1.643	3 5 1 2 4	1 6 2 3 5 1 2 8 0 2 5 2 3 6 0	53.59 55.54 55.59 55.83 55.92
1.023 1.012 1.009 1.005 .9941	1 1 1 1	$\begin{array}{cccccc} 6 & 3 & 1 \\ 4 & 10 & 2 \\ 2 & 11 & 3 \\ 5 & 9 & 1 \\ 1 & 15 & 1 \end{array}$	97.72 95.16 99.48 100.12 101.58	1.602 1.582 1.573 1.565 1.558	3 1 5 3 1	4 0 C 1 0 3 1 1 3 2 8 1 3 6 1	57.47 58.29 58.63 58.96 59.28
•9926 •9791 •9767 •9582 •9566	1 1 1 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	101.80 103.76 104.12 107.00 107.26	1.551 1.549 1.542 1.536 1.515	2 1 9 3 2	2 6 2 1 2 3 0 10 0 3 3 2 4 1 1	59.55 59.63 59.93 60.19 61.10

_	Ca	lculated	Pattern (Integra	ated)
	d (Å)	Ι	hkl	$\begin{array}{c} 2\theta(^{\circ})\\ \lambda = 1.54056 \stackrel{\circ}{A} \end{array}$
	1.515	3	0 8 2	61.14
	1.485	18	3 4 2	62.47
	1.480	2	4 4 0	62.75
	1.474	2	1 8 2	63.01
	1.463	2	1 4 3	63.53
	1.460	2	4 3 1	63.68
	1.448	6	2 1 3	64.28
	1.444	10	2 9 1	64.48
	1.431	3	3 8 0	65.12
	1.429	7	2 2 3	65.23
	1.407	3	1 5 3	66.37
	1.399	2	2 3 3	66.80
	1.364	4	3 6 2	68.75
	1.361	1	2 4 3	68.96
	1.360	2	4 6 0	69.01
	1.347	4	1 6 3	69.76
	1.341	2	4 0 2	70.14
	1.336	1	4 1 2	70.44
	1.319	2	1 11 1	71.46
	1.305	4	0 10 2	72.36
	1.300	1	3 7 2	72.69
	1.297	1	3 0 3	72.88
	1.285	2	0 12 0	73.64
	1.266	1	4 4 2	74.93
	1.264	1	5 2 0	75.06
	1.253 1.242 1.236 1.236 1.236 1.232	1 1 3 1	4 7 1 2 11 1 5 1 1 3 8 2 4 8 0	75.89 76.63 77.10 77.13 77.38
	1.224 1.220 1.209 1.196 1.189	1 1 4 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	78.00 78.29 79.19 80.23 80.78
	1 • 1 7 1	1	1 3 4	82.29
	1 • 1 6 1	2	2 8 3	83.13
	1 • 1 5 1	11	5 5 1	84.06
	1 • 1 4 3	1	2 0 4	84.70
	1 • 1 3 8	2	4 9 1	85.17
	1.138	1	0 12 2	85.20
	1.138	1	0 5 4	85.23
	1.135	2	1 13 1	85.50
	1.111	2	4 10 0	87.77
	1.109	4	2 9 3	88.00
	1.105 1.102 1.101 1.086 1.085	1 1 1 1	0 6 4 0 14 0 4 8 2 1 14 0 2 13 1	88.38 88.73 88.83 90.38 90.47

Calculated Pattern (Integrated)							
d (Å)	Ι	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \stackrel{\circ}{A}$				
1.072 1.055 1.049	1 1 1	2 12 2 1 7 4 1 11 3	91.83 93.75 94.48				
1.041 1.040	2 2	6 1 1 3 3 4	95.42 95.57				
1.024 1.023 1.012 1.009	3 1 2 1	3 4 4 6 3 1 4 10 2 2 11 3 5 9 1	97.58 97.73 99.16 99.48 100.13				
.9941 .9925 .9816 .9791	2 1 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	101.59 101.81 103.40 103.76 103.77				
.9771 .9707 .9631 .9582 .9567	1 1 1 2 1	6 1 2 4 1 4 2 12 3 5 5 3 3 7 4	104.07 105.03 106.23 107.01 107.25				
•9490 •9385 •9296 •9221 •9193	1 1 1 1	1 13 3 5 6 3 2 2 5 0 11 4 2 13 3	108.51 110.33 111.91 113.31 113.84				
•9091 •9059	2 1	3 14 2 1 6 5	115.84 116.49				

,

Structure

Hexagonal, R3 (148), Z=3, [Burns et al., 1968]

Lattice parameters

a=13.808, c=9.429Å (published value: a=13.807Å) [ibid.]

Density

(calculated) 4.304 g/cm³ [ibid.]

Thermal parameters

Anisotropic [ibid.]

Scattering factors

Na⁺, F⁻ [3.3.1A] Zr⁴⁺ values from 3.3.1B, corrected for dispersion using $\Delta f'=-0.6$ and $\Delta f''=2.4$ [Burns et al., 1968]

Scale factor

(integrated intensities) 74.02 \times 10⁴

Additional patterns

1. PDF card 10-177 [Insley et al., 1956]

Reference

Burns, J.H., R.D.Ellison, and H.A.Levy (1968). The crystal structure of Na₇Zr₆F₃₁, Acta Cryst. B24, 230-237.

Insley, H., T.N. McVay, R.E. Thoma, and G. D. White (1956). Optical properties and x-ray diffraction data for some inorganic fluoride and chloride compounds,ORNL-2192, page 58, (Oak Ridge National Laboratory, Tennessee).

Calculated Pattern (Peak heights)								
d ($\overset{\circ}{A}$)	Ι	hkl	$2\theta(\circ)$ $\lambda = 1.54056 \stackrel{\circ}{A}$					
7.41	76	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	11.34					
5.30	12		12.82					
5.65	21		17.56					
4.38	35		20.24					
4.67	41		21.80					
3.387	20	3 0 0	22 • 28					
3.702	6	2 0 2	24 • 02					
3.453	10	2 2 0	25 • 7 8					
3.262	10	2 1 -2 +	27 • 3 2					
3.142	38	0 0 3	28 • 38					
3.123	100	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	20.50					
2.850	6		31.36					
2.712	22		33.00					
2.635	3		34.00					
2.803	1		34.34					
2.458	3	3 0 3 +	36.38					

Ca	Calculated Pattern (Peak heights)							
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$					
2.371	2	3 2 -2	37.92					
2.324	2	2 2 -3	38.72					
2.318	3	0 5 1	38.82					
2.313	2	1 0 4	38.90					
2.197	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	41.04					
2.133	1		42.34					
2.090	5		43.26					
2.038	8		44.42					
2.008	9		45.12					
1.9545	12	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	46.42					
1.9209	46		47.28					
1.9148	59		47.44					
1.8625	9		48.86					
1.8575	6		49.00					
1.8511	2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	49.18					
1.8145	7		50.24					
1.7905	6		50.96					
1.7404	2		52.54					
1.7008	2		53.86					
1.6812	3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	54.54					
1.6391	17		56.06					
1.6348	39		56.22					
1.6311	22		56.36					
1.6060	2		57.32					
1.5873	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	58.06					
1.5838	2		58.20					
1.5715	2		58.70					
1.5643	5		59.00					
1.5114	2		61.28					
1.4753	1	0 8 1	62 • 3 0					
1.4622	2	0 3 6	53 • 5 8					
1.4564	1	5 4 -2	63 • 8 6					
1.4479	3	4 2 5	64 • 2 8					
1.4439	2	7 2 -1	64 • 4 8					
1.4427	2	1 6 4	64.54					
1.4301	2	2 2 6	65.18					
1.4250	1	8 0 2	65.44					
1.4170	3	5 1 -5	65.86					
1.3843	2	8 1 1 +	67.62					
1.3807	2	5 5 0	67.82					
1.3610	2	4 3 -5	68.94					
1.3565	9	2 6 -4 +	69.20					
1.3463	1	4 1 6 +	69.80					
1.2907	1	1 2 -7	73.28					
1.2481	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	76.22					
1.2453	5		76.42					
1.2425	8		75.52					
1.2341	1		77.24					
1.2148	3		78.70					
1.2115	3	6 5 - 2 +	78.96					

20(°)

 $\lambda = 1.54056 \stackrel{\circ}{A}$

54.55

54.55

56.05

56.05 56.20

56.20

56.20

56.20

56.28

56.35 57.32

58.05

58.20 58.70 59.00

59.00 61.23

51.35

62.90

53.59

63.87 64.23

64.49

64.56

65.17

65.45 65.65

67.E1

67.58

67.dl

58.94

69.15

69.21

69.80

69.80 71.37

73.08

73.27 74.95 76.23

76.42

75.62

76.52

77.25 77.59

70.71 70.71

78.71

78.96

78.96

C	Calculated	l Pattern <i>(Integr</i>	rated)	C	Calculated Pattern (Integrated,			
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$	d (Å)	Ι	hkl	λ =	
7.40 6.90 5.05 4.39 4.08	64 10 19 34 9	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	11.94 12.81 17.55 20.23 21.73	1.6809 1.6809 1.6393 1.6393 1.6353	1 3 18 1 17	$\begin{array}{cccc} 7 & 0 & 1 \\ 3 & 5 & 1 \\ 1 & 3 & -5 \\ 3 & 1 & 5 \\ 5 & 2 & 3 \end{array}$		
4.08 3.986 3.702 3.452 3.263	33 19 5 10 5	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	21.79 22.28 24.02 25.79 27.31	1.6353 1.6353 1.6353 1.6332 1.6313	2 4 17 17 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		
3.263 3.143 3.129 3.129 2.850	6 33 100 1 7	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	27.51 28.37 28.51 28.51 31.36	1.5061 1.5876 1.5839 1.5715 1.5643	2 2 1 2 6	5 3 2 1 5 -4 1 7 G 0 G 6 2 6 2		
2.713 2.713 2.634 2.609 2.468	1 23 3 1 2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32.99 32.99 34.31 34.34 36.37	1.5643 1.5113 1.5098 1.4763 1.4620	1 3 1 2 4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		
2.468 2.371 2.324 2.318 2.313	1 1 2 2 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	36 • 37 37 • 91 30 • 71 38 • 81 38 • 91	1.4562 1.4479 1.4437 1.4424 1.4303	2 4 1 2 2	5 4 -2 4 2 5 7 2 -1 1 6 4 2 2 6 $-2 -2 $		
2.198 2.133 2.094 2.090 2.038	4 1 6 6	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	41.04 42.34 43.16 43.25 44.42	1.4249 1.4171 1.3844 1.3832 1.3808	1 3 1 1	8 0 2 5 1 -5 8 1 1 3 5 4 5 5 0		
2.038 2.008 2.008 2.008 2.008	4 1 2 5 4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	44.42 45.12 45.12 45.12 45.12 45.12	1 • 3609 1 • 3574 1 • 3563 1 • 3462 1 • 3462	1 3 12 1, 1	4 3 -5 6 4 -1 2 6 -4 4 1 6 4 1 -6		
1.9545 1.9545 1.9245 1.9245 1.9245	11 4 1 4 55	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	46.42 46.42 47.15 47.19 47.27	1.3109 1.2937 1.2909 1.2661 1.2480	1 1 1 1 4	6 1 5 7 3 -2 1 2 -7 5 3 5 1 3 7		
1.9148 1.9148 1.8528 1.8563 1.8510	57 3 12 1 1	5 2 D 2 5 D 0 1 5 3 3 3 4 0 4	47.44 47.44 48.25 49.32 49.13	1.2453 1.2426 1.2426 1.2343 1.2281	5 4 5 1 1	2 6 5 6 5 1 9 1 -1 0 6 6 4 0 7		
1.8145 1.8145 1.7904 1.7404 1.7008	5 4 7 2 2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	50.24 50.24 50.96 52.54 53.86	1.2148 1.2148 1.2148 1.2146 1.2114 1.2114	2 1 1 1 2	2 5 -6 5 2 6 5 2 -6 9 1 2 6 5 -2		

Structure

Orthorhombic, Fddd (70),Z=8 [Pringle and Noakes, 1968]

Lattice parameters

a=11.82, b=11.47, c=6.08 Å [ibid.]

Density

(calculated) 2.766 g/cm³

Thermal parameters

Anisotropic [ibid.]

Scattering factors

 Sr^{2+} , $N^{-\circ-8}$, $N^{+\circ-6}$, calculated from Sr° and K° averaged, from N^{-1} and N° [3.3.1A]

Scale factor

(integrated intensities) 15.021 \times 10⁴

Reference

Pringle, G.E. and D.E. Noakes (1968). The crystal structures of lithium, sodium, and strontium azides, Acta Cryst. B24, 262-269.

Calculated Pattern (Peak heights)						
d (Å)	Ι	,	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 ^{\circ}$		
4.89	51	1	1 1	18.12		
4.11	100	2	2 0	21.58		
3.177	85	3	1 1	28.06		
3.121	5	1	3 1	28.58		
2.868	27	0	4 0	31.16		
2.703	27	2	0 2	33 • 1 2		
2.685	39	0	2 2	33 • 34		
2.501	60	3	3 1	35 • 8 8		
2.445	8	2	2 2	36 • 7 2		
2.164	21	5	1 1	41 • 7 0		
2.112 2.058 1.988 1.967 1.909	18 6 13 28 19	1 4 2 5	5 1 4 0 2 2 4 2 + 3 1	42.78 43.96 45.60 46.10 47.60		
1.885	5	3	5 1	48.24		
1.863	7	6	2 0	48.84		
1.819	7	2	6 0	50.12		
1.780	6	3	1 3	51.28		
1.770	7	1	3 3	51.58		
1.653	5	6	0 2	55 • 5 4		
1.630	4	3	3 3	56 • 4 0		
1.618	8	0	6 2	56 • 8 4		
1.611	3	7	1 1	57 • 1 2		
1.589	4	5	5 1 +	58 • 00		
1.568	4	1	7 1	58.84		
1.561	1	2	6 2	59.14		
1.525	3	5	1 3	60.68		
1.520	2	0	0 4	60.88		
1.507	1	1	5 3	61.50		
1.497 1.478 1.468 1.432 1.426	1 4 5 6	7 8 3 6 2	3 1 0 0 7 1 4 2 + 2 4 +	61.94 62.84 63.28 65.08 65.40		
1.419	3	4	62	65.74		
1.417	6	3	53	65.84		
1.372	2	6	60	68.32		
1.352	3	4	44	69.48		
1.343	3	0	44	70.00		
1.327	3	7	5 1	70.96		
1.315	2	5	7 1	71.74		
1.313	3	8	4 0	71.82		
1.295	4	8	2 2	73.02		
1.290	4	4	8 0 +	73.34		
1.278	3	5	5 3	74 •1 4		
1.275	2	9	1 1	74 •36		
1.267	3	2	8 2 +	74 •30		
1.240	1	1	3 1	76 •78		
1.228	1	7	3 3	77 •6 6		

Ca	lculated	Pattern (Peak he	ights)
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 ^{\circ}}$
1.223	1	4 4 4	78.10
1.212	2	3 7 3	78.90
1.189	1	3 9 1	80.74
1.178	2	6 2 4	81.70
1.166	2	2 5 4	82.66
1.158 1.156 1.155 1.153 1.126	1 2 2 1	10 2 0 3 1 5 7 7 1 1 3 5 2 10 0	83.42 83.58 83.70 83.82 86.32
1.122	2	5 7 3	86 • 7 4
1.120	2	9 5 1	86 • 8 8
1.103	1	5 9 1	88 • 5 8
1.102	1	10 0 2	88 • 7 2
1.097	1	9 1 3	89 • 2 0
1.091	3	8 6 2	89.82
1.083	2	6 8 2	90.66
1.077	1	5 1 5	91.36
1.073	1	0 10 2	91.74
1.059	1	9 3 3 +	93.32
1.054 1.043 1.040 1.037 1.028	1 2 2 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	93.94 95.22 95.52 96.00 97.00
1.024	1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	97.58
1.020	1		98.10
1.018	2		98.28
1.011	1		99.32
1.009	1		99.58
.9978 .9938 .9913 .9815 .9782	1 2 1 1	0 2 6 + P 4 4 + 6 10 0 5 9 3 5 5 5	101.06 101.62 101.98 103.40 103.90
.9555	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	107.44
.9460	1		109.02
.9455	1		109.12
.9431	1		109.52
.9247	1		112.82
. 3211	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	113.50
. 9048	1		116.72
. 9025	2		117.18
. 9011	2		117.48
. 8965	1		118.46

C	Calculated Pattern (Integrated)					
d (Å)	Ι	hkl	$2\theta(°)$ $\lambda = 1.54056 \stackrel{\circ}{A}$			
4.89	59	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	18.12			
4.12	100		21.57			
3.177	92		26.06			
3.122	5		28.57			
2.868	30		31.16			
2.703	31	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	33 • 1 1			
2.686	45		33 • 3 3			
2.501	70		35 • 8 8			
2.445	9		36 • 7 2			
2.164	27		41 • 7 1			
2.112	22	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	42.78			
2.058	8		43.96			
1.988	15		45.60			
1.968	14		46.09			
1.967	23		46.11			
1.909	26	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	47.59			
1.885	6		48.24			
1.863	10		48.84			
1.819	9		50.11			
1.780	8		51.27			
1.770	9	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	51.58			
1.653	7		55.54			
1.630	6		56.39			
1.618	11		56.85			
1.611	3		57.13			
1.589	4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	57.99			
1.589	1		58.01			
1.568	5		58.84			
1.561	1		59.14			
1.525	4		60.63			
1.520	2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	60.90			
1.505	2		61.50			
1.497	1		61.93			
1.478	6,		62.84			
1.468	5		53.29			
1.434	1	0 8 0	64.99			
1.432	8	6 4 2	65.07			
1.427	3	5 3 3	65.32			
1.426	7	2 2 4	65.40			
1.419	3	4 5 2	65.73			
1 • 417	8	3 5 3	65.85			
1 • 372	3	6 6 0	58.31			
1 • 352	4	4 0 4	69.48			
1 • 343	5	0 4 4	70.00			
1 • 327	4	7 5 1	70.96			
1.315	3	5 7 1	71.72			
1.313	4	8 4 0	71.81			
1.295	7	8 2 2	73.03			
1.290	4	4 3 0	73.33			
1.289	3	7 1 3	73.39			

С	alculated	l Pattern <i>(Integ</i>	rated)
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$
1.278	5	5 5 3	74 •1 4
1.276	1	9 1 1	74 •2 8
1.267	1	1 7 3	74 •8 9
1.267	5	2 8 2	74 •9 1
1.240	2	1 9 1	76 •7 7
1.228	2	7 3 3	77.66
1.223	2	4 4 4	78.10
1.212	4	3 7 3	78.89
1.203	1	1 1 5	79.63
1.189	3	3 9 1	80.74
1.178 1.166 1.158 1.156 1.155	4 2 3 1	6 2 4 2 6 4 10 2 0 3 1 5 7 7 1	81 • 6 9 82 • 6 6 83 • 4 2 83 • 5 7 83 • 7 0
1.153 1.126 1.122 1.120 1.120	2 2 3 2 1	1 3 5 2 10 0 5 7 3 9 5 1 3 3 5	83 • 8 1 86 • 3 3 86 • 7 5 86 • 8 8 87 • 7 2
1.103	2	5 9 1	88.57
1.102	1	10 0 2	88.73
1.097	2	9 1 3	89.19
1.091	5	8 6 2	89.81
1.083	3	6 8 2	90.66
1.077	2	5 1 5	91.37
1.074	1	1 9 3	91.61
1.073	2	0 10 2	91.74
1.059	1	8 0 4	93.28
1.059	2	9 3 3	93.33
1.054 1.043 1.041 1.041 1.041	2 3 1 3	11 1 1 0 8 4 3 3 3 5 3 5 3 5 5	93.95 95.21 95.51 95.51 96.00
1.029 1.028 1.024 1.029 1.029 1.018	1 2 3 3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	96.94 97.01 97.59 98.11 98.29
1.011	2	9 7 1 4 10 2 10 6 0 7 9 1 2 0 6	99.33
1.009	2		39.57
1.005	1		100.02
1.003	1		100.31
.9988	1		100.93
.9979	3	0 2 6	101.05
.9945	1	3 11 1	101.53
.9938	4	8 4 4	101.63
.9912	2	6 10 0	101.99
.9815	2	5 9 3	103.41

Calculated Pattern (Integrated)					
d (Å)	Ι	hkl	$2\theta(°)$ $\lambda = 1.54056 \stackrel{\circ}{A}$		
• 9781	2	5 5 5	103.91		
• 9732	1	1 7 5	104.65		
• 9609	1	11 5 1	106.58		
• 9558	1	0 12 0	107.39		
• 9554	2	7 3 5	107.45		
. 94 78 . 94 61 . 94 54 . 94 32 . 94 32	1 1 2 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	108.72 109.01 109.12 109.51 109.62		
.9316	1	12 4 0	111.56		
.9248	2	12 2 2	112.80		
.9214	1	11 3 3	113.44		
.9210	2	10 2 4	113.52		
.9046	3	2 10 4	116.72		
.9044	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	116.79		
.9026	2		117.18		
.9025	1		117.18		
.9012	3		117.47		
.9011	1		117.48		
.8965	2	13 1 1	118.46		
.8953	1	0 6 6	118.71		
.8896	1	9 1 5	119.97		

Structure

Orthorhombic, Pnnm (58), Z=12 [Owens et al., 1967]

Lattice parameters

a=11.35, b=14.06, c=3.32Å [ibid.]

Density

(calculated) 4.809 g/cm³

Thermal parameters

Isotropic [ibid.]

Scattering factors

S°, Ti[°] [Hanson et al., 1964]

Scale factor

(integrated intensities) 5.806 \times 10⁴

Reference

Hanson,	H.P.	, F. H	Herman,	J.D.	Lea,	and	s.
Skill	.man (1964)	. HFS a	atomic	sca	atter	ing
facto	rs, A	cta Ci	ryst. 1	7, 104	40-104	14.	
Owens,	J.P.,	B.R.	Conard	, and	H.F.	Fran	zen

(1967). The crystal structure of Ti₂S, Acta Cryst. 23, 77-82.

Ca	Calculated Pattern (Peak heights)					
d (Å)	Ι		hk	1	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$	
5.97	3	1	2	0	14.82	
4.41	3	2	2	0	20.10	
3.654	2	3	1	0	24.34	
3 - 331	1	3	2	0	26.74	
3.232	2	n	1	1	27.58	
3-108	9	,	1	1	28.70	
2.838	Ĝ	4	'n	ñ	31.50	
2.730	3	1	5	n	32.78	
2.709	7		3	1	33.04	
2.654	12	2	2	1	33.74	
	•••					
2.632	3	4	2	0+	34.04	
2.574	1	3	4	Ω	34.82	
2.520	3	2	5	0	35.60	
2.495	45	3	0	1	35.96	
2.457	22	3	1	1	36.54	
3 4 3 9			7	~	77.00	
2 361	11	1	5	1	70 00	
2 3 7 5 4	50	7	2	1	79 20	
2 7 4 7	37		ć	0	70 70	
2 256	20	7	ç	0	70 07	
	22	,	,	0	, , , , , , , , , , , , , , , , , , , ,	
2.241	29	5	1	O	40.20	
2.771	100	2	4	1	40.58	
2.203	95	3	3	1	40.94	
2.166	9	2	Б	0	41.56	
2.160	23	5	2	0	41.78	

Ca	Calculated Pattern (Peak heights)					
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$			
2 •146	46	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42.08			
2 •132	15		42.36			
2 •108	5		42.86			
2 •062	23		43.86			
2 •043	7		44.30			
2.035 2.007 1.997 1.992 1.978	6 3 10 16	3 4 1 2 5 1 4 5 0 3 6 0 1 7 0	44.48 45.14 45.38 45.50 45.84			
1.907	14	540	47.66			
1.892	1	600	48.06			
1.875	3	610	48.52			
1.857	19	511	49.00			
1.857	1	620	49.88			
1 •774	1	3 7 0	51.45			
1 •754	2	5 3 0	52.10			
1 •737	1 1	1 8 0	52.66			
1 •719	1	0 7 1	53.25			
1 •711	1	4 5 1	53.50			
1.708	3	3 6 1	53.60			
1.679	1	2 8 0	54.62			
1.660	40	0 0 2	55.30			
1.655	23	5 4 1	55.46			
1.640	1	4 7 0	56.04			
1.631	1	5 6 0	56.38			
1.611	2	7 1 0	57.14			
1.600	4	6 2 1	57.54			
1.587	3	4 6 1	58.08			
1.551	3	6 3 1	59.56			
1.548	3	1 9 0	59.70			
1.506	.9	2 9 0	61.52			
1.504	8	5 7 0	61.60			
1.472	1 0	6 6 0 +	63.12			
1.463	1	5 6 1	63.52			
1.457	1	$\begin{array}{ccccccc} 7 & 0 & 1 \\ 7 & 1 & 1 \\ 4 & 0 & 2 \\ 7 & 2 & 1 \\ 6 & 5 & 1 \end{array}$	63.84			
1.449	1		64.22			
1.433	2		65.04			
1.427	8		65.36			
1.419	4		65.76			
1.412 1.406 1.403 1.391 1.387	2 2 7 1	8 1 0 0 10 0 1 9 1 + 7 3 1 + 2 5 2	66.14 66.44 65.62 67.24 67.46			
1 • 370	10	5 7 1 +	Б8.42			
1 • 362	3	4 8 1	Б8.86			
1 • 354	6	7 6 7	Б9.32			
1 • 346	7	6 6 1	Б9.84			
1 • 337	14	3 5 2	70.34			

 $\frac{2\theta(^{\circ})}{\lambda = 1.54056 \stackrel{\circ}{A}}$

14.81 20.09 24.34 26.74 27.58 28.70 31.50 32.78 33.04 33.75 33.99 34.04 34.81 35.60 35.96 36.54 37.00 38.09 38.24 38.38 39.91 40.21 40.58 40.84 4 0. 94 41.65 41.78 42.07 42.3F 42.85 43.87 44.30 44.49 45.14 45.37 45.49 45.84 47.65 48.06 48.52 4 9.00 49.88 51.47 52.09 52.66 53.26 53.50 5.3.61 54.62 55.29

Calcula	ated Pattern (Peak he	ights)	Ca	lculated	Pattern (Integra	ated)
d (Å) 1	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{ Å}}$	d (Å)	Ι	hkl	λ =
1.334 1 1.327 1.324 1 1.316 1.299	5 1 2 4 4 4 2 1 3 9 1 8 5 2 2 3 8 1 1	70.54 70.98 71.14 71.64 72.74	5.98 4.42 3.653 3.332 3.231	2 2 1 1 2	1 2 0 2 2 0 3 1 0 3 2 0 0 1 1	
1.288 1.286 1.282 1.277 1.275	3 5 3 2 4 1 10 1 + 6 5 8 1 4 4 5 2 4 3 6 2	73.44 73.56 73.86 74.22 74.30	3 .1 08 2 .8 38 2 .7 29 2 .7 09 2 .6 54	7 9 1 6 1 2	1 1 1 4 n 0 1 5 n n 3 1 2 2 1	
1.272 1.265 1.262 1.259 1.256	8 1 7 2 2 4 9 1 3 2 10 1 2 4 10 0 3 9 1 0	74.55 75.00 75.22 75.42 75.64	2 .6 35 2 .6 31 2 .5 75 2 .5 20 2 .4 95	1 2 1 2 4 3	1 3 1 4 2 0 3 4 0 2 5 0 3 0 1	
1.252 1.247 1.243 1.228 1.225	7 5 4 2 2 2 11 0 2 6 1 2 1 6 2 2 6 3 10 1	75.94 76.30 76.60 77.66 77.92	2 .4 57 2 .4 27 2 .3 61 2 .3 52 2 .3 43	20 11 50 4 17	3 1 1 4 3 0 1 4 1 3 2 1 0 6 0	
1.214 1.212 1.211 1.206 1.200	1 8 6 0 1 3 7 2 1 3 11 0 1 6 3 2 8 1 8 2	78.80 78.92 79.02 79.42 79.86	2 • 2 57 2 • 2 41 2 • 2 21 2 • 2 08 2 • 2 03	39 28 100 9 88	3 5 0 5 1 0 2 4 1 4 4 <i>n</i> 3 3 1	
1.192 1.186 1.180 1.178 1.178 1.175	1 7 8 0 1 1 11 1 1 2 8 2 2 4 10 1 2 9 1 1	80.54 80.98 81.48 81.68 81.94	2 •1 66 2 •1 60 2 •1 46 2 •1 32 2 •1 08	7 1 8 4 6 1 3 5	2 6 0 5 2 0 0 5 1 4 1 1 1 5 1	
1.172 1.165 1.163 1.153 1.153 1.156	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	82.20 82.74 82.98 83.32 83.58	2 •0 62 2 •0 43 2 •0 35 2 •0 07 1 •9 97	24 7 5 3 8	4 2 1 5 3 0 3 4 1 2 5 1 4 5 0	
1 •1 43 1 •1 38 1 •1 32 1 •1 25 1 •1 22	6 9 3 1 3 3 11 1 2 1 9 2 4 5 10 1 3 7 8 1	84.72 85.24 85.75 86.46 86.74	1 .9 92 1 .9 78 1 .9 07 1 .8 92 1 .8 75	6 17 16 1 3	360 170 540 600 610	
1.121 1.113 1.115 1.110 1.103	2 10 2 0 2 9 4 1 8 2 9 2 3 9 6 0 3 10 3 0	86.84 87.12 87.36 87.84 88.58	1 .8 57 1 .8 27 1 .7 74 1 .7 54 1 .7 37	2 1 1 2 1 2	5 1 1 6 2 0 3 7 0 6 3 0 1 8 0	
1.101 1.094 1.084 1.083 1.077	8 6 6 2 8 8 7 1 1 2 12 1 2 4 12 0 3 1 13 0	88.76 89.50 90.52 90.68 91.36	1 • 7 19 1 • 7 11 1 • 7 08 1 • 6 79 1 • 6 60	1 1 3 1 4 7	n 7 1 4 5 1 3 6 1 2 8 0 n 0 2	

C	Calculated	d Pattern (Integr	rated)	С	alculated	l Pattern (Integr	ated)
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$	d (Å)	Ι	hkl	λ =
1 •6 54	1	5 4 1	55.53	1 •2 56	3	9 1 0	
1 •6 39	1	4 7 0	56.05	1 •2 52	9	5 4 2	
1 •6 30	1	5 6 0	56.39	1 •2 47	2	2 11 0	
1 •6 11	2	7 1 0	57.14	1 •2 43	2	6 1 2	
1 •6 00	4	6 2 1	57.54	1 •2 29	1	6 2 2	
1 •5 87	3	4 6 1	56.07	1 .2 25	8	3 10 1	
1 •5 51	4	6 3 1	59.56	1 .2 14	1	9 6 0	
1 •5 48	1	1 9 0	59.70	1 .2 12	1	3 7 2	
1 •5 06	1 ()	2 9 0	61.52	1 .2 11	1	3 11 0	
1 •5 04	7	5 7 0	61.60	1 .2 06	1	6 3 2	
1 .4 72	1 3	6 6 0	6 3 • 11	1 •2 00	8	1 8 2	
1 .4 70	1	4 7 1	6 3 • 20	1 •2 00	3	5 9 1	
1 .4 63	1	5 6 1	6 3 • 52	1 •1 92	2	7 8 0	
1 .4 57	1	7 0 1	6 3 • 83	1 •1 86	1	1 11 1	
1 .4 49	1	7 1 1	6 4 • 22	1 •1 80	1	2 8 2	
1 .4 33	3	4 0 2	55.04	1 .1 78	2	4 10 1	
1 .4 27	10	7 2 1	65.36	1 .1 75	2	9 1 1	
1 .4 19	4	6 5 1	65.75	1 .1 72	1	0 12 0	
1 .4 12	2	8 1 0	66.14	1 .1 66	1	4 7 2	
1 .4 06	2	0 10 0	66.44	1 .1 65	2	4 11 0	
1 .4 04	1	4 2 2	6 6. 55	1 •1 63	1	9 2 1	
1 .4 03	7	1 9 1	5 6. 62	1 •1 59	6	8 7 0	
1 .3 91	17	7 3 1	6 7. 24	1 •1 56	2	7 1 2	
1 .3 91	6	8 2 0	6 7. 27	1 •1 43	9	9 3 1	
1 .3 86	1	2 5 2	6 7. 51	1 •1 38	5	3 11 1	
1 •3 72 1 •3 70 1 •3 70 1 •3 69 1 •3 62	5 4 8 1 4	2 9 1 4 3 2 5 7 1 4 9 0 4 8 1	58.33 58.41 58.41 58.41 58.51 55.85	1 .1 32 1 .1 32 1 .1 31 1 .1 26 1 .1 25	1 2 1 1 5	6 9 1 1 9 2 1 0 1 0 7 3 2 5 10 1	
1 • 3 55	7	0 6 2	59.31	1 .1 22	2	7 8 1	
1 • 3 46	8	6 6 1	59.84	1 .1 20	2	10 2 0	
1 • 3 37	17	3 5 2	70.34	1 .1 18	1	9 4 1	
1 • 3 34	12	5 1 2	70.54	1 .1 15	9	2 9 2	
1 • 3 27	4	4 4 2	70.98	1 .1 15	7	5 7 2	
1 .3 24	13	3 9 1	7 1. 14	1 •1 11	4	9 6 0	
1 .3 18	4	2 6 2	7 1. 55	1 •1 03	3	10 3 0	
1 .3 16	8	5 2 2	7 1. 64	1 •1 01	12	6 6 2	
1 .3 16	1	8 4 0	7 1. 67	1 •1 00	1	1 12 1	
1 .2 99	4	8 1 1	7 2. 73	1 •1 00	1	4 11 1	
1 •2 88	3	5 3 2	73.44	1 • 1 94	13	A 7 1	
1 •2 87	1	5 9 0	73.53	1 • 1 85	2	2 12 1	
1 •2 85	3	1 10 1	73.57	1 • 1 83	2	4 12 0	
1 •2 82	7	5 8 1	73.87	1 • 1 77	4	1 13 0	
1 •2 77	4	4 5 2	74.22	1 • 1 75	2	8 1 2	
1 •2 75	3	3 6 2	7 4 • 31	1 .073	2	2 2 3	
1 •2 72	9	1 7 2	7 4 • 57	1 .073	2	1 10 2	
1 •2 65	2	4 9 1	7 5 • 01	1 .066	6	2 2 2	
1 •2 62	3	2 10 1	7 5 • 21	1 .065	1	7 9 1	
1 •2 60	1	4 10 0	7 5 • 38	1 .062	3	2 13 0	

20(°) $\lambda \approx 1.54056 \text{ Å}$

75.65

75.93

76.30

76.60

77.66

77.93

78.79

78.91

7 9.00

79.41

79.85

79.87

80.53

80.98

81.47

81.68 81.94

8 2. 21

82.55 82.75

82.98

83.32

83.57

84.71

85.23

85.73

85.76

85.82

86.33

85.46

86.74

85.85

87.13

87.35

87.42

87.84

88.58

8 8. 76

88.93

88.93

89.50 90.51

90.68

91.36

91.50

91.71

91.77 92.53

92.59

92.94

20(°)

 $\lambda = 1.54056 \text{ Å}$

20.58

21.72

23.90

24.18

25.50

26.44

26.58

28.36

28.46

29.12 29.26

29.46

30.32

30.70

31.00 31.24

31.92

32.32

33.20

33.94

34.56

35.56

36.08

36.24 37.40

37.68

37.88

38.38 38.48

38.80

38.92

39.42 40.54

41.04

41.86

42.36 42.44

43.94 45.76

46.04

46.48

46.60

47.76

47.96

48.10

48.92

49.66

Structure			1 10	Ca	lculated	Patteri	1 (P	eak h	eights)
cioli et	al. 19	68]	=4 [Gramac-	d (Å)	Ι		hki	!	$\begin{array}{c} 2\\ \lambda = 1 \end{array}$
Lattice para	ameters			4.312	10		2		
a = 23	7858 ±.0	0008Å, b = 7.3	580 ±.0007Å.	4.512	10	4	U	1	20
c = 6.264	5 + 0.004	LÅ (published a	a -23 70/0+	7 7 20	5	5	1	1	21
0000 %		$\pm 0007 = 0007$	$3 \alpha - 23.70402$	3.720	100	4	1	1	22
a,8000.	=/.35//	±.0007,C=6.26	$42 \pm .0004 \text{A},)$	3.678	13	0	2	0	24
[ibid.]				3.490	13	6	1	0	25
Thermal na	rameter			3.368	5	5	1	1	26
Anigotr				3.351	5	6	0	1	26
Anisotro	obic [1]	bid.j		3-144	6	1	2	1	28
				3.134	5	0	0	2	28
Density				3.064	5	2	2	1	29
(calculat	ed) 1.55	7 g/cm ³ [ibid	.1						
•	,	5, 2	-	3.050	6	6	1	1	29
				3.029	4	2	۵	2	29
Scattering f	actors			2.945	7	3	2	1	30
H° [McWe	eeny, 19	951]		2.910	7	5	2	Ô	30
C° , N° ,	0°, [C1	omer and Wabe	r, 1965]	2.882	2	0	1	2	31
				2,861	7	1		2	
Scale factor	•			2.801	17		1	2	2.
lintograd	tod into	maiting) 6 200	2×10^{4}	2.768	1	2	1	2 4	2
(Integrat	Lea Inte	ensities) 6.280	3 × 10	2.696	9		1	1 *	20
				2 6 7 9		6	2	u 1	
Reference				2:035	0	5	2	1	د <u>ا</u>
Cromer, D.	T. and	J.T. Waber (19	965). Scat-	2.597				~	
tering f	actors	computed from	n relativis-	2 5 2 7	1	4	1	2	1 34
tia Dima		eompaeca 110	tiona Nata	2	2	8	1	1	5:
tic Dira	ac-State	r wave funct	LIONS, ACLA	2.401	2	9	1	0	36
Cryst. 1	104-	109.		2.411	10	6	2	1	56
Gramacciol	li, C.M.	, R.Destro, an	nd M. Simon-	2.403	1	2	3	٥	. 3
etta (19	968). Th	e structure of	f 2,4,6-fri-	2.385	1	0	2	2	2
nitrophe	enetole,	Acta Cryst. 1	B24,129-136.	2.373	1	1	2	2	7
McWeeny,R.	. (1951)	. X-ray scatte	ering by ag-	2.343	2	7	7	0	7
gregates	s of bor	ded atoms. I	. Analvtical	2.338	2	2	ר ה	2	7
approvin	ations	in single_ator	n scattering	2 3 3 9	2	2	2	2	20
Acta Cry	/st 4, 5	13 - 519	" beaccering	2.0313			2	1	
-	•			2.312	3	8	2	0 +	38
				2.284	1	3	2	2	39
	-			2.223	2	10	a	1	40
·				2.197	2	7	1	2 +	4
Ca	lculated	Pattern (Peak he	eights)	2.156	1	8	Ō	2	4
0	· · · · ·	1	28(°)	2,132		<u>د</u>	2	2.4	
d (A)	I	hkl	2017	2.128	7	10	د ۱	2 1	
			$\lambda = 1.54056 \ A$	2,059	2	10	7	1 .	-
				1,9812	2	5	1	7	4
11.87	29	200	7.44	1,9699	5	2	1	3	4
7.357	39	0 1 0	12.02	1.3030	1	4	U	2	46
7.031	37	1 1 0	12.58	1.000		_			
6.258	18	2 1 0	14.14	1.9521	1	1	2	2	41
5.941	5	4 0 0	14.90	1.9474	2	3	1	3	41
		\$		1.9028	1	10	2	1	4
5.542	20	2 0 1	15.98	1.8953	2	7	3	1	4
5 70/	22	3 1 0	16.42	1.8901	2	12	0	1	4:

4.677

4.624

4.427

1.8603

1.8343

18.96

19.18

20.04

Cá	Calculated Pattern (Integrated)				
d (Å)	Ι	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \stackrel{\circ}{A}$		
11.89	23	2 0 0	7.43		
7.358	32	0 1 0	12.02		
7.029	31	1 1 0	12.58		
6.257	15	2 1 0	14.14		
5.946	5	4 0 0	14.89		
5.543	17	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	15.98		
5.393	20		16.42		
4.677	23		18.96		
4.625	4		13.17		
4.427	9		20.04		
4.313	9	4 0 1	20.58		
4.087	3	3 1 1	21.73		
3.721	100	4 1 1	23.90		
3.679	11	0 2 0	24.17		
3.490	13	6 1 0	25.50		
3.368 3.350 3.145 3.132 3.065	5 5 3 5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	26.44 26.59 28.36 28.47 29.11		
3.049 3.029 2.945 2.910 2.882	6 4 3 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	29.27 29.46 30.32 36.70 31.00		
2.861	3	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	31.24		
2.801	17		31.93		
2.799	3		31.95		
2.771	5		32.28		
2.768	7		32.32		
2.697	1	6 2 0	33.19		
2.639	7	5 2 1	33.94		
2.593	2	4 1 2	34.56		
2.523	3	8 1 1	35.55		
2.487	1	9 1 0	36.08		
2 • 4 7 7	12	6 2 1	36.24		
2 • 4 6 5	1	5 1 2	36.42		
2 • 4 0 2	2	2 3 0	37.41		
2 • 3 8 5	1	0 2 2	37.69		
2 • 3 7 3	1	1 2 2	37.88		
2.343 2.338 2.319 2.312 2.312 2.312	2 1 1 2 1	3 3 0 2 2 2 7 2 1 8 2 0 9 1 1	38.38 38.47 38.80 38.91 38.93		
2.284 2.224 2.198 2.195 2.156	1 2 1 1	3 2 2 10 0 1 7 1 2 3 3 1 8 0 2	39.42 40.53 41.03 41.10 41.86		

	1 > 1	20101
	hkl	$\lambda = 1.54056 \stackrel{\circ}{A}$
5 4 10 5 2 2 4 7 3 10 7 12 8 10	2 2 3 1 1 1 3 1 0 3 1 3 0 3 2 2 1 3 2 1 3 1 0 1 2 2 1 2 2 1 1 2 2 1 2 1 2 2 2 1 3 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1	42.36 42.36 42.43 43.94 43.99 45.77 46.03 46.48 46.60 47.75 47.95 48.11 48.92 49.66
	5 4 10 5 2 2 4 7 3 10 7 12 8 10	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

Structure

Monoclinic, P21 /a (14), Z=4[Ringertz, 1966]

Lattice parameters

a=14.465±.003,b=7.403±.002,c=6.208±.001Å β =65.10°±.05°,(published value:a=14.464Å) [ibid.]

Density

(calculated) 1.851 g/cm³ [ibid.]

Thermal parameters

Isotropic:									
С		н		N		0			
(1)	2.18	(1)	2.28	(1)	2.28	(1)	3.10		
(2)	1.83	(2)	2.06	(2)	2.06	(2)	2.46		
(3)	2.02	(3)	1.92	(3)	1.92	(3)	2.42		
(4)	1.98	(4)	1.86	(4)	1.86				
(5)	1.78								

Scattering factors

 C° , N° , O° , H° [3.3.1A]

Scale factor

(integrated intensities) 1.914 \times 10⁴

Additional patterns

1. PDF card 19-1995 [Shirley, 1966].

Reference

- Ringertz,H.(1966). The molecular and crystal structure of uric acid, Acta Cryst. 20, 397-403.
- Shirley, R. (1966). Uric acid dihydrate: crystallography and identification, Science 152, 1512-1513.

Calculated Pattern (Peak heights)								
d (Å)	Ι	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \hat{A}}$					
6.55	43	2 0 0	13.50					
6.45	2	1 1 0	13.72					
5.63	20	0 0 1	15.72					
4.91	51	2 1 0	18.06					
4.76	7	1 1 1	18.64					
4.48	1	0 1 1	19.80					
3.264	42	1 1 -1	23.00					
3.837	20	3 1 1	23.16					
3.702	6	0 2 0	24.02					
3.590	3	2 0 -1	24.78					

Calculated Pattern (Peak heights)								
d (Å)	Ι	hkl	$\frac{2\theta(°)}{\lambda = 1.54056 \text{ Å}}$					
3.281 3.222 3.209 3.180 3.093	14 3 55 100	4 0 0 2 2 0 4 1 1 1 2 1 0 2 1	27 .16 27 .66 27 .78 28 .04 28 .84					
3.087	69	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	28.90					
3.000	3		29.76					
2.866	25		31.18					
2.826	1		31.64					
2.815	2		31.76					
2.796 2.632 2.615 2.566 2.454	9 2 15 3	4 0 2 1 2 4 1 2 4 2 1 4 2 0	31 • 9 8 34 • 0 4 34 • 2 6 34 • 9 4 36 • 5 8					
2.425	3	4 0 -1	37.04					
2.404	2	1 1 -2	37.38					
2.310	4	2 3 0	38.96					
2.277	3	5 2 1	39.54					
2.265	2	2 0 -2	39.76					
2.245 2.240 2.186 2.166 2.148	7 5 2 1	6 0 2 0 2 2 6 0 0 1 3 -1 + 6 1 2	40.14 40.22 41.26 41.66 42.02					
2.096	1	1 2 -2	43.12					
2.028	2	4 2 -1	44.64					
1.910	1	3 3 2	47.58					
1.877	2	0 0 3	48.46					
1.8071	2	6 1 3 +	50.46					
1.7978	3	7 2 1	50.74					
1.7912	2	2 2 3 +	50.94					
1.7685	1	3 2 -2	51.64					
1.7584	1	0 4 1	51.96					
1.7478	1	6 1 -1	52.30					
1.7447	1	1 2 3	52.40					
1.6648	2	6 2 3	55.12					
1.5402	1	8 0 0	56.02					
1.6180	2	5 2 -1	55.86					
1.5117	2	4 4 0 +	57.10					
1.6045	1	8 2 2	57.38					
1.5898	3	2 4 2	57.36					
1.5789	1	1 4 2	58.40					
1.5745	1	5 1 -2	58.58					
1.5466	4	3 4 2	58.74					
1.5132	.1	204+	61.20					

C	alculated	Pattern (Integra	uted)	Ca	alculated	l Pattern (Integra	ited)
d (Å)	I	hkl	$\frac{2\theta(^{\circ})}{\lambda = 1.54056 \text{\AA}}$	d (Å)	Ι	hkl	λ =
6.56 6.45 5.63 4.91 4.76	37 1 18 46 E	2 G G 1 1 O 0 O 1 2 1 O 1 1 1	13.49 13.72 15.72 18.05 18.64	2.167 2.166 2.148 2.095 2.028	2 1 1 1 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
4.48 3.864 3.838 3.701 3.590	1 39 18 6 2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	19.79 23.00 23.15 24.02 24.78	1.909 1.277 1.8076 1.8062 1.7978	1 2 1 3	3 3 2 0 0 3 6 1 3 3 2 3 7 2 1	
3.280 3.224 3.209 3.179 3.093	14 2 4 55 100	4 0 0 2 2 0 4 1 1 1 2 1 0 2 1	27.10 27.65 27.78 28.04 28.64	1.7912 1.7899 1.7633 1.7582 1.7430	2 1 1 1 1	2 2 3 8 0 1 3 2 -2 0 4 1 6 1 -1	
3.087 2.999 2.866 2.862 2.825	7 3 24 5 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	28.90 29.77 31.18 31.22 31.64	1.7443 1.6741 1.6648 1.6401 1.6179	1 1 2 1 2	1 2 3 10 2 3 16 2 3 18 0 0 16 2 -1	
2.815 2.796 2.632 2.616 2.577	1 10 2 1 1	0 0 2 4 0 2 3 1 2 4 1 2 2 2 -1	31.76 31.98 34.04 34.25 34.78	1.6119 1.6114 1.6043 1.5896 1.5789	1 1 3 1	4 4 0 8 2 1 8 2 2 2 4 2 1 4 2	4
2.566 2.455 2.425 2.404 2.310	16 3 2 5	4 2 1 4 2 0 4 0 -1 1 1 -2 2 3 0	34.94 36.57 37.04 37.37 38.96	1 • 5741 1 • 5465 1 • 5133 1 • 5124	1 6 1 1	5 1 -2 3 4 2 2 0 4 5 4 0	
2.278 2.265 2.244 2.241 2.187	3 2 7 4	5 2 1 2 0 -2 6 3 2 6 2 2 6 8 0	39.53 39.77 40.14 40.21 41.25				

2θ(°)

 $\lambda = 1.54056 \text{ Å}$

41.64

41.87

42.03 43.14

44.64

47.58

48.46

50.45 50.49

50.74

50.94

50.98 51.65 51.97

52.29

52.39

54.79

55.12

56.03

56.86

57.09

57.11

57.39

57.97

58.40

58.60

59.74

51.20

51.23

CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONOGRAPH 25, SECTIONS 1, 2, 3, 4, 5, 6, 7, and 85

	Vol. or	
	sec.	Page
4-Acetyl-2 '-fluorobiphenyl, C ₁₄ H ₁₁ OF	8m	91
L-Alanine, C ₃ H ₂ O ₃ N	8m	93
Aluminum, Al	1	11
Aluminum antimony, AlSb	4	72
Aluminum calcium sulfate hydrate (ettring-		
ite), Al.O. 6CaO 3SO 31H.O.	8	3
Aluminum chloride hexahydrate (chlor-	-	-
aluminite), AlCl. 6H.O.	7	3
Aluminum fluosilicate, topaz, Al.SiO.(F.OH).	1 m	4
Aluminum metaphosphate Al(PO.)	2m	3
Aluminum nickel AlNi	6m	82
Aluminum orthophosphate (berlinite) AIPO	om	02
(trigonal)	10	3
Aluminum orthophosphate AIPO (ortho-	10	0
rhombia)	10	4
Aluminum avida (aarundum) alpha Al O	10	4 9
Aluminum oxide monohydroto (höhmito), alpha	9	0
Alo Ho	0	20
$AI_2 \cup_3 \cdot \Pi_2 \cup \dots $	3	38
Aluminum oxide mononydrate, diaspore, beta	0	
$AI_2 \cup H_2 \cup H_2$	3	41
Aluminum silicate (mullite) $3AI_2O_3 \cdot 2SIO_2 \dots$	3m	3
Ammonium acetate, NH ₄ ·CH ₃ CO ₂	8m	95
Ammonium aluminum sulfate dodecahydrate		
(teschermigite), $NH_4Al(SO_4)_2 \cdot 12H_2O \dots$	6	3
Ammonium azide, NH ₄ N ₃	9	4
Ammonium bicarbonate (teschemacherite),		
(NH ₄)HCO ₃	9	5
Ammonium bromide, NH ₄ Br	2	49
Ammonium bromoosmate, $(NH_4)_2OsBr_6$	3	71
Ammonium bromoplatinate, $(NH_4)_2 PtBr_6 \dots$	9	6
Ammonium bromoselenate, $(NH_4)_2SeBr_6$	8	4
Ammonium bromotellurate, $(NH_4)_2 TeBr_6 \dots$	8	5
Ammonium cadmium sulfate, (NH ₄), Cd, (SO ₄),	7m	5
Ammonium cadmium sulfate hydrate,		
$(\mathrm{NH}_4)_2\mathrm{Cd}(\mathrm{SO}_4)_2\cdot 6\mathrm{H}_2\mathrm{O}$	8m	5
Ammonium cadmium trichloride, NH ₄ CdCl ₃	5m	6
Ammonium calcium sulfate, $(NH_4)_2 Ca_2(SO_4)_3$	8m	7
Ammonium chloride (sal-ammoniac), NH ₄ Cl	1	59
Ammonium chloroiridate, (NH ₄), IrCl ₆	8	6
Ammonium chloroosmate, (NH ₄) ₂ OsCl ₆	1m	6
Ammonium chloropalladate, (NH ₄) ₂ PdCl ₆	8	7
Ammonium chloropalladite, (NH ₄) ₂ PdCl ₄	6	6
Ammonium chloroplatinate, (NH ₄) ₂ PtCl ₆	5	3
Ammonium chlorostannate (NH ₄) ₂ SnCl ₆	5	4
Ammonium chlorotellurate, (NH ₄), TeCl ₆	8	8
Ammonium chromium sulfate dodecahydrate,		
$NH_{4}Cr(SO_{4})_{2} \cdot 12H_{2}O$	6	7
Ammonium cobalt fluoride, NH4CoF,	8m	9
Ammonium cobalt (II) trichloride, NH, CoCl,	6m	5
Ammonium copper chloride, NH, CuC1,	7m	7
Ammonium dihydrogen phosphate, NH,H,PO,	4	64
Ammonium fluoberyllate, (NH ₄), BeF ₄	3m	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.

	Vol. or	
	sec.	Page
Ammonium fluoborate, NH ₄ BF ₄	. 3m	6
Ammonium fluogermanate, $(NH_4)_2 GeF_6 \dots$. 6	8
Ammonium fluosilicate (cryptohalite),		
$(\mathrm{NH}_4)_2 \mathrm{SiF}_6 \ldots \ldots$. 5	5
Ammonium gallium sulfate dodecahydrate,		
$NH_4Ga(SO_4)_2 \cdot 12H_2O$. 6	9
Ammonium iodide, NH ₄ I	. 4	56
Ammonium iron sulfate dodecahydrate,		
$NH_{4}Fe(SO_{4})_{2}\cdot 12H_{2}O$. 6	10
Ammonium magnesium chromium oxide hydrat	e,	
$(NH_4)_2Mg(CrO_4)_2 \cdot 6H_2O$. 8m	10
Ammonium manganese sulfate, (NH ₄) ₂ Mn ₂ (SO ₄), 7m	8
Ammonium manganese sulfate hydrate,		
$(NH_4)_{2}Mn(SO_4)_{2}\cdot 6H_{2}O_{1}$	8m	12
Ammonium manganese(II) trifluoride, NH_MnF	, 5m	8
Ammonium mercury chloride, NH ₄ HgCl ₃	-	
(revised)	. 8m	14
Ammonium metavanadate, NH, VO,	. 8	9
Ammonium nickel chromium oxide hydrate.		
$(NH_{4})_{a}Ni(CtO_{4})_{a}\cdot 6H_{a}O_{4}$. 8m	16
Ammonium nickel (II) trichloride. NH.NiCl.	. 6m	6
Ammonium nitrate (ammonia-niter), NH, NO,	. 7	4
Ammonium oxalate monohydrate (oxammite)	•	-
(NH) CO.HO	. 7	5
Ammonium perchlorate NH ClO (ortho-	• •	Ŭ
rhombic)	. 7	6
Ammonium nerrhenate NH ReO	 q	7
Ammonium phosphomolybdate tetrahydrate	. 0	•
(NH) PO (M_0O_1) , 4H O	8	10
$\begin{array}{c} (\mathrm{NH}_4)_{31} O_4(\mathrm{MOO}_3)_{12}, \mathrm{HI}_2 O_{111}, \mathrm{HI}_2 O_{111}$. 0	10
(revised) $(\operatorname{Inascagnite}), (\operatorname{Ini}_4)_2 \otimes \mathcal{O}_4$	Q	8
(10VISCU) $(11VISCU)$		0
Animonium yttiium oxalate nyulate, $NH_{41}(C_2($) ₄) Qm	07
$_2 \cdot \Pi_2 \cup \dots $. 0111 9m	10
Ammonium zine nuonde, N_{H_4} Zinr ₃	. om	10
Antimony Sh	. 0	14
Antimony, SD	. J 	14
Antimony(III) indonde, SbI	. 200 C	16
Antimony(III) rounde, Sol ₃	. 0	10
(aubia) (11) oxide (senamonite), 50_20_3	2	21
(CUDIC)	. ა	51
Antimony(III) Oxide, valentinite, SD_2O_3	10	C
(orthornonibic)	. 10	0
Antimony(IV) oxide (cervanite), SD_2O_4	. 10	8
Antimony (v) oxide, Sb_2O_5	. 10 4m	10
Antimony scalaride Sh So	. <u>4</u> 111	44
Antimony Scienide, So ₂ Se ₃	. 300	(
Antimony (III) suffice (subnite), So_2S_3	. 0	6
Antimony telluride, Sb ₂ 1e ₃	. 3m	8
Antimony terbium, Solo	. 5m	61
Antimony thorium, Spin	. 4m	44
Antimony thullum, Solm	. 4m	45
Antimony ytterblum, Sbyb	. 4m	45
Anumony yturium, SbY	. 4m	46
Arsenic acid, H, AS ₃ O ₁₀	7m	84
Arsenic, As	. 3	6
Arsenic(III) iodide, AsI ₃	. 6	17
Arsenic trioxide (arsenolite), As_2O_3 (cubic).	. 1	51
Arsenic trioxide, claudetite, As_2O_3 (mono-	0	
Clinic)	. 3m	Q

** *

v	01. OF	_		Vol. or	
	sec.	Page		sec.	Page
ℓ -Ascorbic acid, C ₆ H ₈ O ₆	8m	99	Cadmium, Cd	3	10
Azobenzene, $C_{12}H_{10}N_2$	7m	86	Cadmium bromide, CdBr ₂	9	17
Barium aluminum oxide, $BaAI_2O_4$	2m	11	Cadmium carbonate (otavite), CdCO ₃	- 7	11
Barium arsenate, $Ba_3(ASO_4)_2$	2111	0 7		5m	63
Barlum, Ba	4	10	Cadmium chioride, CdCl ₂	9	18
Barium borate, BaB ₈ O ₁₃	7 m 4 m	10	Cadmium chromite, $CdCr_2O_4$	Om	10
Barium boron oxide, Ingi Ionii, BaB ₂ O ₄	4m	4	Cadmium cyanue, $Cu(CN)_2$	Zm	8
Barium boroli oxide, BaB_4O_7	94111 9 m	10	Cadmium Imidazole mirate,	0	
Barium bromido monohydrato, $BaRr H O$	0111 2m	19	$Cu(C_{3}H_{4}N_{2})_{6}(NO_{3})_{2}$	8m Em	23
Barium carbonato (witherite) BaCO (ortho-	JIII	10	Cadmium malubdate. CdMaQ	Jill E	03
rhombic)	2	54	Cadmium nitrato tetrahydrato	0	21
Barium carbonate $BaCO(cubic)$ at 1075 °C	10	11	$Cd(NO) \cdot dHO$	7m	0.2
Barium chlorate hydrate Ba(ClO ₁) H O	8m	21	Cadmium oxide CdO	2	93
Barium fluoride. BaF	1	70	Cadmium oxide, CdO (ref. standard)	8m	2
Barium fluosilicate. BaSiF	4m	7	Cadmium perchlorate hexahydrate.	0	-
Barium molybdate. BaMoO	7	7	Cd(ClO.)6H.O	3m	19
Barium nitrate (nitrobarite), Ba(NO,),	1	81	Cadmium praseodymium, CdPr	5m	64
Barium perchlorate trihydrate, Ba(ClO ₄), 3H ₂ O	2m	7	Cadmium selenide, CdSe (hexagonal)	7	12
Barium peroxide, BaO,	6	18	Cadmium sulfate, CdSO,	3m	20
Barium selenide, BaSe	5m	61	Cadmium sulfate hydrate, 3CdSO, .8H,O	6m	8
Barium stannate, BaSnO ₃	3m	11	Cadmium sulfate monohydrate, CdSO ₄ ·H ₂ O	6m	10
Barium sulfate (barite), BaSO ₄	3	65	Cadmium sulfide (greenockite), CdS	4	15
Barium sulfide, BaS	7	8	Cadmium telluride, CdTe	3m	21
Barium titanate, BaTiO ₃	3	45	Cadmium tungstate, CdWO ₄	2m	8
Barium tungstate, BaWO ₄	7	9	tri-Calcium aluminate, 3CaO·Al ₂ O ₃	5	10
Barium zirconate, BaZrO ₃	5	8	Calcium aluminate, 12CaO.7A1 ₂ O ₃	9	20
Beryllium aluminum oxide (chrysoberyl),			Calcium aluminum germanate, $Ca_3Al_2(GeO_4)_3$	10	15
BeAl ₂ O ₄	9	10	Calcium bromide hexahydrate, CaBr ₂ .6H ₂ O	8	15
Beryllium aluminum silicate, beryl,			Calcium carbonate (aragonite), CaCO ₃ (or-		
$\operatorname{Be}_{3}\operatorname{Al}_{2}(\operatorname{SiO}_{3})_{6}$	9	13	thorhombic)	3	53
Beryllium calcium oxide, Be,,Ca,,O,,	7m	89	Calcium carbonate (calcite) CaCO, (hexagonal)) 2	51
Beryllium chromium oxide, $BeCr_2O_4$	10	12	Calcium chromate, CaCrO,	7	13
Beryllium cobalt, BeCo	5m	62	Calcium chromium germanate, $Ca_3Cr_2(GeO_4)_3$	10	16
Beryllium germanate, Be ₂ GeO ₄	10	13	Calcium chromium silicate (uvarovite),	10	1.7
Beryllium nioblum, Be,Nb	7m	92	$Ca_3 Cr_2(SIO_4)_3$ $Ca_5 Ca_5$	10	17
Beryllium orthostiticate, phenacite, $BeSi_2O_4$	8	26	Calcium fluoride (fluorite), CaF ₂	1	09
Beryllium palladium BeDd	5m	.00	Ca E(PO)	3m	22
Bis (o-dodecacarborane) C B H	6m	7	Calcium formate $Ca(HCO)$	8	16
Bismuth Bi	3	20	Calcium gallium germanate Ca.Ga.(GeO.)	10	18
Bismuth cerium BiCe	4m	20 46	Calcium hydroxide (portlandite), Ca(OH),	10	58
Bismuth dysprosium, BiDy	4m	47	Calcium iron germanate. Ca. Fe. (GeO.).	10	19
Bismuth erbium. BiEr	4m	47	Calcium iron silicate (andradite).		
Bismuth fluoride, BiF,	1m	7	Ca,Fe,Si,Q,	9	22
Bismuth holmium, BiHo	4m	48	Calcium magnesium silicate (diopside),		
Bismuth(III) iodide, Bil,	6	20	CaMg(SiO ₃) ₂	5m	17
Bismuth lanthanum, BiLa	4m	48	Calcium molybdate (powellite), CaMoO,	6	22
Bismuth neodymium, BiNd	4m	49	Calcium nitrate, Ca $(NO_3)_2$	7	14
Bismuth orthophosphate, BiPO ₄ (monoclinic)	3m	11	Calcium oxide, CaO	1	43
Bismuth orthophosphate, BiPO ₄ (trigonal)	3m	13	Calcium phosphate, beta-pyro-, Ca,P,O,	7m	95
Bismuth orthovanadate, low form, BiVO ₄			Calcium selenide, CaSe	5m	64
(tetragonal)	3m	14	Calcium sulfate (anhydrite), CaSO ₄	4	65
Bismuth orthovanadate, high form, BiVO ₄			Calcium sulfide (oldhamite), CaS	7	15
(monoclinic)	3m	14	Calcium telluride, CaTe	4m	50
Bismuth oxybromide, BiOBr	8	14	Calcium tungstate, scheelite, CaWO ₄	6	23
Bismuth oxychloride (bismoclite), BiOCl	4	54	Carbon, diamond, C	2	5
Bismuth oxylodide, BiOI	9	16	Cerium, antimony Cesp	4m	40
Bismuth praseodymium, BiPr	4m	49	Cerium arsenate, CeAsO ₄	4m	8
Distinuul sullide ($DISMULTINITE$), Bl_2S_3 (revised) Rismuth tolluride $BiTe$	om	13	Cerium arsenide, CeAs	4m	51
Dismuth telluride (tellurebienuthite). Di Te	4m	50	Cerium (III) chloride, CeCl ₃	111	8
Bismuth triovide (bismite), $alpha Bio$	200	10	Cerium (III) fluoride CeF	/m 8	99
Disingui utorige (Disinite), aiplia Bl ₂ U ₃	.9m	10	Cerium magnesium CeMg	5m	65
m-Monograph 25.			Cerium magnesium nitrate 24-hydrate	011	00
A mineral name in () indicates a synthetic sample			Ce_Mg_(NO_)24H_O	10	20
() interest a synancial sumpre			2 03 3/12 2		

A mineral name in () indicates a synthetic sample.

	Vol. or			Vol. or	
	sec.	Page		sec.	Page
Cerium niobium titanium oxide (eschynite),			Cesium nickel (II) trichloride, CsNiCl ₃	6m	12
CeNbTiO,	3m	24	Cesium nitrate, CsNO,	9	25
Cerium nitride. CeN	4m	51	Cesium perchlorate, CsClO., (orthorhombic)	1m	10
Cerium(IV) oxide (cerianite) CeO	1	56	Cosium strontium trichloride CeStCl	6m	13
Corium phosphido. CoP	.4m	50	Cesium substa Ca SO	7	17
Certuin phosphilde, Cer	1	52	Cestum suffate Cs_2SO_4	1	11
Cerium(III) vanadate, CevO ₄	Im	9	Cesium vanadium sullate dodecanydrate,		
Cerium zinc, CeZn	5m	65	$CsV(SO_4)_2 \cdot 12H_2O$	1m	11
Cesium aluminum sulfate dodecahydrate,			Cesium zinc sulfate hexahydrate,		
$CsAl(SO_4)_2 \cdot 12H_2O$	6	25	$Cs_2Zn(SO_4)_2 \cdot 6H_2O$	7m	25
Cesium bromate, CsBrO,	8	18	Chromium, Cr	5	20
Cesium bromide. CsBr	3	49	Chromium fluoride Cr.F.	$7 \mathrm{m}$	108
Cesium bromoosmate(IV) Cs.OsBr	2m	10	Chromium(III) fluoride trihydrate CrF. 3H O	5m	25
Cesium bromonlatinate Cs PtBr	8	19	Chromium iridium 2:1 Cr. Ir	6m	14
Cesium bromogalanata, Cs SoPr	0	20	Chromium arthaphaenhota alpha CrDO	0m	10
Cestum bromosetenate, Cs ₂ SeBr ₆	0	20	Chromitum orthophosphate, alpha, CIPO,	2111	12
Cesium bromotellurate, CS ₂ leBr ₆	9	24	Chromium orthophosphate, beta, CrPO ₄	9	26
Cesium cadmium trichloride, CSCdCl ₃			Chromium(III) oxide, Cr_2O_3	5	22
(hexagonal)	5m	19	Chromium rhodium 3:1, Cr ₃ Rh	6m	15
Cesium calcium fluoride, CsCaF ₃	8m	25	Chromium silicide, Cr ₃ Si	6	29
Cesium calcium sulfate, $Cs_2Ca_2(SO_4)_3$	7m	12	Cobalt, Co (cubic)	4m	10
Cesium calcium trichloride, CsCaCl,	5m	21	Cobalt aluminum oxide, CoAl ₂ O ₄	9	27
Cesium cerium chloride. Cs.CeC1.	7m	101	Cobalt antimony oxide. CoSb.O.	5m	26
Cesium chlorate CsClO	8	20	Cobalt arsenide (skutterudite), CoAs	10	21
Cosium chlorido. CsCl	2	44	Cobalt (II) corbonate (sphereachaltite)	10	
Gasium shlatar smats(NI). Ga OaGl	2	11	Cobart(II) carbonate (spherocobartite),	10	0.4
Cestum chloroosmate(IV), CS_2OSCI_6	210	11		10	24
Cesium chloroplatinate, CS ₂ PtCl ₆	5	14	Cobalt diarsenide, CoAs ₂ (revised)	4m	10
Cesium chlorostannate, Cs ₂ SnCl ₆	5	16	Cobalt fluosilicate hexahydrate,		
Cesium chromate, Cs ₂ CrO ₄	3m	25	$\operatorname{CoSiF}_{6} \cdot 6H_{2}O$	3m	27
Cesium chromium sulfate dodecahydrate,			Cobalt gallate, CoGa,O,	10	27
$CsCr(SO_{2}) \cdot 12H_{2}O_{2}$	8	21	Cobalt germanate, Co. GeO.	10	27
Cesium cobalt (II) trichloride, CSCoCl.	6m	11	Cobalt jodide. Col.	4m	52
Cesium conner sulfate heyahydrate			Cobalt iron arsenide (safflorite) CoFeAs	10	28
Cestulii copper suffate flexally diate,	17 m	1.4	Cobalt non arsenide (samorite), cor ens.	20	19
$C_{S,CU}(SO_{4}), \cdot bH_{2}O \dots O C_{U}C$	/111 5 m	14	Cobalt mercury throcyanate, Co[Hg(CNS) ₄]	2111	00 T9
Cesium copper(II) trichtoride, CSCuCi ₃	2111	22		9	28
Cesium dichloroiodide, $CSICI_2$	3	50	Cobalt(II, III) oxide, Co_3O_4	9	29
Cesium fluoantimonate, CsSbF ₆	4m	9	Cobalt perchlorate hexahydrate,		
Cesium fluoborate, CsBF ₄	8	22	$Co(ClO_4)_2 \cdot 6H_2O$	3m	28
Cesium fluogermanate, Cs ₂ GeF ₆	5	17	Cobalt silicate, Co,SiO ₄ (orthorhombic)	4m	11
Cesium fluoplatinate, Cs, PtF,	6	27	Cobalt sulfate, beta, CoSO,	2m	14
Cesium fluoride. CsF	3m	26	Cobalt titanate. CoTiO.	4m	13
Cesium fluosilicate Cs SiF	5	19	Cohalt tungstate CoWO	4m	13
Cesium gallium sulfate dodecabydrate	0		Copper Cu	1	15
CeCo(SO) = 124 O	0	7 2	Copper, eu	5m	27
$CSGa(SO_4)_2 \cdot 12H_2O \cdot \dots \cdot D$	- 0	20	Copper antimoly oxide, $Cusb_2O_6$	JIII	21
Cesium iodine bromide, CSI, Br	'7 m	103	Copper(1) bromide, CuBr	4	.30
Cesium iodide, CSI	4	47	Copper carbonate, basic, azurite,		
Cesium iron sulfate dodecahydrate,			$CU_3(OH)_2(CO_3)_2$	10	30
$CsFe(SO_4)_2 \cdot 12H_2O$	6	28	Copper carbonate, basic, (malachite),		
Cesium iron sulfate hexahydrate,			CU ₂ (OH) ₂ CO ₃	10	31
$Cs_{a}Fe(SO_{a}) \rightarrow 6H_{a}O_{a}$	7m	16	Copper (I) chloride (nantokite), CuC1	4	35
Cesium lead fluoride, CsPbF,	8m	26	Conner glutamate dihydrate	_	
Cesium lead(II) trichloride CsPbCl	0		CuC H NO 22H O	7m	1 10
(tetragonal)	5m	24	Conner(I) iodide (marchite) Cul		30
Creive lithing funcide Cel iT	- OIII	105	Copper(I) Iodide (marchite), Cu O	r O	00
Cesium Inthium Indonde, CSLIF,	(111	105	Copper (1) oxide (cupitte), Cu_2O	4	23
Cesium magnesium chromium oxide,			Copper(II) oxide (tenorite), CuO	1	49
$Cs_2Mg_2(CrO_4)_3$	8m	27	Copper phosphate, alpha-pyro-, Cu ₂ P ₂ O ₇	7m	113
Cesium magnesium chromium oxide hydrate,			Copper pyrazole chloride, $Cu(C_3H_4N_2)_4Cl_2$	8m	31
$Cs_2Mg(CrO_4)_2 \cdot 6H_2O$	8m	29	Copper sulfate (chalcocyanite), CuSO ₄	3m	29
Cesium magnesium sulfate hexahydrate,			Copper(II) sulfide (covellite), CuS	4	13
$Cs_Mg(SO_*)_{\circ} \cdot 6H_{\circ}O_{\circ}$	7m	18	Dibenzovlmethane, C. H. O.	7m	115
Cesium manganese sulfate hexahydrate	,		Dysprosium antimony, DySb	4m	41
Cs Mn(SO) +6H O	7 m	20	Dysprosium arsenate DyAsO	Rm	20
Cosium moreury chlorido CollaC1	7111	20	Dyenrosium arsonido DyAc	4m	50
Cesium nickel culfate benchritete	7111	22	Dysprosium collium ovide Dr. Co. (CoC.)	4111	23
Cesium nickel sulfate nexanydrate,			Dy sprostum gattium oxide, $Dy_3Ga_2(GaO_4)_3$	2m	15
$Cs_Ni(SO_4)_{2} \cdot 6H_{2}O$	7m	23	Dysprosium nitride, DyN	4m	53
			Dysprosium sesquioxide, Dy ₂ O ₃	9	30
m-Monograph 25.			Dysprosium telluride, DyTe	4m	54
A mineral name in () indicates a synthetic samp	le.		Dysprosium vanadate, DyVO ₄	4m	15

V	'ol. or			Vol. or	
	sec.	Page		sec.	Page
Erbium antimony, ErSb	4m	41	Holmium sesquioxide, Ho ₂ O ₃	9	32
Erbium arsenate, ErAsO ₄	.3m	31	Holmium vanadate, HoVO,	4m	18
Erbium arsenide, ErAs	4m	54	Hydrogen iodate, Hl ₃ O ₈	8m	104
Erbium gallium oxide, Er,Ga,(GaO ₄),	1m	12	Hydroquinone, gamma, $C_6H_6O_2$	8m	107
Erbium manganite, ErMnO ₃	2m	16	Imidazole nickel nitrate, $(C_3H_4N_2)_8Ni(NO_3)_2$	7m	27
Erbium nitride, ErN	4m	55	Imidazole zinc chloride, $(C_3H_4N_2)$, ZnC1,	7m	123
Erbium phosphate, ErPO,	9	31	Indium, In	3	12
Erbium sesquioxide, Er ₂ O ₃	8	25	Indium antimony, InSb	4	73
Erbium telluride, ErTe	4m	55	Indium arsenide, InAs	.3m	35
Erbium vanadate, ErVO ₄	5m	29	Indium oxide, In ₂ O ₃	5	26
Europium arsenate, EuAsO ₄	3m	32	Indium phosphate, InPO ₄	8	29
Europium(III) chloride, EuCl ₃	1m	13	Iodic acid, HIO,	5	28
Europium gallium oxide, Eu,Ga,(GaO ₄),	2m	17	Iodine, I_2	3	16
Europium nitride, EuN	4m	56	Iridium, Ir	4	9
Europium oxide, EuO	4m	56	Iridium dioxide, IrO ₂	4m	19
Europium oxychloride, EuOCl	1m	13	Iridium niobium 1:3, IrNb ₃	6m	19
Europium(III) vanadate, EuVO ₄	4m	16	Iridium titanium 1:3, IrTi ₃	6m	20
Gadolinium antimony, GdSb	4m	42	Iridium vanadium 1:3, IrV_3	6m	21
Gadolinium arsenate, GdAsO ₄	4m	17	Iron, alpha Fe	4	3
Gadolinium arsenide, GdAs	4m	57	Iron arsenide, FeAs	1m	19
Gadolinium chloride hexahydrate,	_		Iron arsenide (loellingite), FeAs ₂	10	34
$GdC1, \cdot 6H, O$	7m	118	Iron bromide, $FeBr_2$	4m	59
Gadolinium fluoride, GdF ₃	1m Dm	14	Iron lodide, Fel ₂	4m	60
Gadolinium gallium oxide, $Gd_3Ga_2(GaO_4)$,	∠m ⊑	18	Iron(II,III) oxide (magnetite), Fe_3O_4	Sm	31
Gadolinium indium, Gdin	5111 4 m	67	Iron sulfate hydrate (melanterite), $FeSO_4 \cdot 7H_2C$) 8m	38
Gadolinium nitride, GdN	4m	57	Iron sulfide (pyrite), FeS_2	5	29
Gadolinium oxide, Gd_2O_3	1m	10	bis-(N-Isopropyi-3-ethylsalicylaidiminato)	_	
Gadolinium oxychioride, GdOCI	1111	17	palladium, (C, H, NO), Pd.	-7m 4m	144
Gadolinium titanium oxide, $Gd_2 I IO_5 \dots \dots$	810 5m	32	Lanthanum antimony, Laso	4111 2m	44
Gallium Ga	0111 0	30	Lanthanum arsenate, LaAsO ₄	Jiii Am	30 60
Callium arconido. Co Ac	2 2m	9	Lanthanum arsenide, LaAs	4111 1m	20
Gallium antimonide GaSb	6	30	Lanthanum chloride, LaCl	1m	20
Gallium ovide alpha Ga O	4	25	Lanthanum fluorido LaE	7	20
Gallium phosphato hydrato $GaBO 2^{2}HO$	2 Rm	20	Lanthanum magnesium LaMg	5m	69
Gallium phosphate (\sim quartz type) GaPO	8	27	Lanthanum magnesium nitrate 24-hydrate	0	00
Germanium Ge	1	18	La Mg (NO) .24H O	1m	22
Germanium dioxide GeO (hexagonal)	1	10	Lanthanum niohium titanium oxide LaNhTiO	3m	37
(low form)	1	51	Lanthanum nitrate hydrate La(NO ₂).·6H ₂ O	8m	40
Germanium dioxide, GeO, (tetragonal)	-	01	Lanthanum nitride. LaN	4m	61
(high form)	8	28	Lanthanum oxide. La.O.	3	33
Germanium iodide. GeL	4m	58	Lanthanum oxychloride, LaOCl	7	22
Germanium(IV) jodide. Gel.	5	25	Lanthanum phosphide, LaP	5m	69
Glyoxime, H ₂ C ₂ (NOH),	8m	102	Lanthanum selenide. LaSe	4m	61
Gold. Au	1	33	Lanthanum zinc. LaZn	5m	70
Gold antimony 1:2 (aurostibite). AuSb	7	18	Lead. Pb	1	34
Gold(I) cyanide, AuCN	10	33	Lead boron oxide, PbB ₄ O ₇	4m	19
Gold dysprosium, AuDy	5m	66	Lead bromide, PbBr,	2	47
Gold holmium, AuHo	5m	68	Lead carbonate (cerrussite), PbCO ₃	2	56
Gold magnesium, AuMg	6m	83	Lead chloride (cotunnite), PbCl ₂	2	45
Gold niobium 1:3, AuNb,	6m	16	Lead formate, Pb(HCO ₂) ₂	8	30
Gold potassium cyanide, AuK(CN) ₂	8m	36	Lead fluochloride (matlockite), PbFCl	1	76
Gold tin, 1:1 AuSn	7	19	Lead fluoride, alpha PbF, (orthorhombic)	5	31
Gold titanium 1:3, AuTi ₃	6m	17	Lead fluoride, beta PbF ₂ (cubic)	5	33
Gold vanadium 1:3, AuV ₃	6m	18	Lead(II) iodide, PbI2	5	34
Hafnium, Hf	3	18	Lead molybdate (wulfenite), PbMoO ₄	7	23
Hexamethylenediammonium adipate,			Lead monoxide (litharge), PbO (red) tetrag-		
$C_{12}H_{26}N_{2}O_{4}$	7m	121	onal	2	30
Holmium arsenate, HoAsO ₄	3m	34	Lead monoxide (massicot), PbO (yellow)		
Holmium ethylsulfate nonahydrate,			(orthorhombic)	2	32
$Ho[(C_2H_5)SO_4]_3 \cdot 9H_2O \dots$	1m	18	Lead nitrate, Pb(NO ₃) ₂	5	36
Holmium nitride, HoN	4m	58	Lead(II, III) oxide (minium), Pb ₃ O ₄	8	32
Holmium selenide, HoSe	4m	59	Lead oxybromide, Pb ₃ O ₂ Br ₂	5m	32
			Lead phosphate hydrate, $Pb_s(PO_4)_3OH$	8	33
m-Monograph 25.			Lead selenide (clausthalite), PbSe	5	38
A mineral name in () indicates a synthetic sample	э.		Lead sulfate (anglesite), PbSO ₄	.3	67

V	ol. or			Vol. or	
	sec.	Page		sec.	Page
Lead sulfide (galena), PbS	2	18	Magnesium hydrogen phosphate trihydrate,		
Lead titanate, PbTiO ₃	5	39	newberyite, MgHPO.3H,O	7m	139
Lead tungstate (stolzite), PbWO ₄ (tetragonal)	_		Magnesium hydroxide (brucite), Mg(OH) ₂	6	30
(revised)	5m	34	Magnesium molybdate, MgMoO	7m	28
Lead uranium oxide, Pb_3UO_6	8m	109	Magnesium oxide (periclase), MgO	1	37
Lithium aluminum fluoride, alpha, Li_3AlF_6	8m	111	Magnesium perchlorate hexahydrate,		
Lithium arsenate, LI ₃ ASO ₄	Zm	19	$Mg(C 1O_A)$, GH_2O	7m	30
Lithium harium trifluorido, LiBoE	8m 5m	113	Magnesium selenite hydrate Mase	0m	116
Lithium boullium fluorido, Li BoF	5111 77m	190	Magnesium silicato enstatite $MgSeO_3 On_2O$	oni 6	110
Lithium beryllium huoride, Li ₂ Der ₄	9m	120	Magnesium silicate (forsterite) Mg SiO	1	22
Lithium bromide LiBr		30	Magnesium silicate (lorstenice), Mg_2OO_4	1	00
Lithium carbonate LiCO	2 Sm	42	Magnesian sineate nuonae (norbergite), Ma SiO .MaF	10	39
Lithium chloride. LiCl	1	62	Magnesium silicate fluoride (humite).	10	00
Lithium fluoride. Li F	î	61	3Mg.SiO.·MgF.	1 m	30
Lithium iodate, LiIO,	7	26	Magnesium sulfate heptahydrate (epsomite).		
Lithium molybdate, Li ₂ MoO ₄ (trigonal)	1m	23	MgSO ₄ ·7H ₂ O	7	30
Lithium niobate, LiNbO ₃	6m	22	Magnesium sulfide, MgS	7	31
Lithium nitrate, LiNO,	7	27	Magnesium tin, Mg ₂ Sn	5	41
Lithium oxide, Li ₂ O	1m	25	Magnesium titanate (geikielite), MgTiO ₃	5	43
Lithium perchlorate trihydrate, LiC10 ₄ ·3H ₂ O	8	.34	Magnesium tungstate, MgWO ₄	1	84
Lithium phosphate, low form (lithiophos-			Manganese, alpha, Mn	7m	142
phate), Li_3PO_4 (orthorhombic) revised	4m	21	Manganese aluminate (galaxite), MnAl ₂ O ₄	9	35
Lithium phosphate, high form, Li_3PO_4	3m	39	Manganese bromide, MnBr ₂	4m	63
Lithium rubidium fluoride, LiRbF,	$7 \mathrm{m}$	128	Manganese(II) carbonate (rhodochrosite),	_	
Lithium sodium sulfate, LiNaSO ₄	6m	24	MnCO ₃	7	32
Lithium sulfate, $L_{1_2}SO_4$	6m	26	Manganese ferrite (Jacobsite), $MnFe_2O_4$	9	36
Lithium suffate monohydrate, $Ll_2SO_4 \cdot H_2O \dots$	410	22	Manganese louide, MnI_2	410	63
Lipo 200	9m	20	Manganoso(III) oxide (manganosite), MnO	0	97
Lithium tungstate Li WO (trigonal)	2111 1m	20	Manganese selenide $MnSe$	9 10	41
Lithium tungstate hemihydrate Li WO $\frac{1}{4}$ H O	2m	20	Manganese sulfide (alabandite) alpha MnS	4	11
Lithium uranium fluoride, LiUF.	7m	131	Manganese(II) tungstate (huebnerite), MnWO,	2m	24
Lutetium arsenate, LuAsO,	5m	36	Mercury(I) bromide, Hg,Br,	7	33
Lutetium gallium oxide, Lu ₃ Ga ₂ (GaO ₄) ₃	2m	22	Mercury(I) chloride (calomel), Hg ₂ Cl ₂	1	72
Lutetium manganite, LuMnO ₃	2m	23	Mercury(II) chloride, HgCl ₂	1	73
Lutetium nitride, LuN	4m	62	Mercury(II) cyanide, Hg(CN) ₂	6	35
Lutetium oxide, Lu ₂ O ₃	1m	27	Mercury(II) fluoride, HgF ₂	2m	25
Lutetium vanadate, LuVO ₄	5m	37	Mercury(I) iodide, HgI	4	49
Magnesium, Mg	1	10	Mercury iodide, HgI ₂ (tetragonal) (revised)	7m	32
Magnesium aluminate (spinel), MgAl ₂ O ₄	2	35	Mercury magnesium, HgMg	6m	8.4
Magnesium aluminum silicate (pyrope),			Mercury(II) oxide (montroydite) HgO (revised)	9	39
$Mg_3AI_2(SIU_4)_3$	4m	24	Mercury(II) selenide (tiemannite), HgSe	4	35
arita) Ma Al Si O (arthorhombia)	1m	20	agonal)	4	17
Magnesium aluminum silicate (high cordi-	1	28	Mercury(II) sulfide (metacinnahar) HaS	4	17
erite) Mg Al Si O (hexagonal)	1m	20	(cubic)	4	21
Magnesium ammonium phosphate hexaby-	1	20	Mercury sulfide chloride alpha Hg.S.Cl	r 8m	118
drate (struvite). MgNH.PO6H.O	3m	41	Metaboric acid. HBO, (cubic)	4m	27
Magnesium boron oxide, Mg, B,O, (triclinic).	4m	25	N-methylphenazinium tetracyanoguinodi-		
Magnesium bromide, MgBr,	4m	62	methanide, C., H., N.	7 m	146
Magnesium carbonate (magnesite), MgCO ₃	7	28	Molybdenum, Mo	1	20
Manganese chloride (scacchite), MnCl ₂	8m	43	Molybdenum disulfide (molybdenite), MoS ₂	5	47
Magnesium chloride dodecahydrate,			Molybdenum osmium 3:1, Mo ₃ Os	6m	28
MgC1, 12H, O	$7 \mathrm{m}$	135	Molybdenum trioxide (molybdite), MoO ₃	3	30
Magnesium chromite (picrochromite),			2-Naphthylamine, n-phenyl-, C ₁₆ H ₁₃ N	6m	29
MgCr ₂ O ₄	9	34	Neodymium antimony, NdSb	4m	43
Magnesium nuoride (sellaite), MgF ₂	4	33	Neodynium arsenate, NdASO,	4m	28
Magnesium gallate, MgGa ₂ O ₄	10	36	Neodymium arsenide, NdAS	4m	64
Magnesium germanate, Mg_GeO ₄ (CuDiC)	10	37	Neodymium chloride NdC	1m	32
rhombic)	10	20	Neodymium ethylsulfate popabydrate	111	33
(inombic)	10	30	Nd[(C H)SO].9H O	0	41
			Neodymium fluoride. NdF.	9	36
m-Monograph 25.			Neodymium gallium oxide, Nd.Ga.(GaO.).	1m	34
A mineral name in () indicates a synthetic sample	÷.		Neodymium oxide, Nd ₂ O,	.4	26

V	ol. or			Vol. or	
	sec.	Page		sec.	Page
Neodymium oxychloride, NdOCl	8	37	Potassium chlororuthenate(IV), K ₂ RuCl ₆	10	46
Neodymium selenide, NdSe	5m	71	Potassium chlorostannate, K ₂ SnCl ₆	6	38
Neodymium vanadate, NdVO ₄	4m	30	Potassium chromium sulfate dodecahydrate,		
Neptunium nitride, NpN	4m	64	$\text{KCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6	39
Nickel, Ni	1	13	Potassium cobalt (II) sulfate, $K_2Co_2(SO_4)_3 \ldots$	6m	35
Nickel aluminate, NiAl ₂ O ₄	9	42	Potassium cobalt (II) trifluoride, KCoF ₃	6m	37
Nickel arsenic 1:2 (rammelsbergite), NiAs ₂	10	42	Potassium cobaltinitrite, $K_3Co(NO_2)_6$	9	45
Nickel arsenic sulfide (gersdorffite), NiAsS	1m	35	Potassium copper chloride, KCuCl	$7 \mathrm{m}$	41
Nickel(II) carbonate, NiCO ₃ (trigonal)	1m	.36	Potassium copper (II) trifluoride, KCuF ₃	6m	38
Nickel ferrite (trevorite), NiFe ₂ O ₄	10	44	Potassium cyanate, KCNO	7	39
Nickel fluosilicate hexahydrate, NiSiF ₆ ·6H ₂ O	8	38	Potassium cyanide, KCN	1	77
Nickel gallate, NiGa ₂ O ₄	10	45	Potassium dihydrogen arsenate, KH ₂ AsO ₄	1m	38
Nickel germanate, Ni ₂ GeO ₄	9	43	Potassium dihydrogen phosphate, KH ₂ PO ₄	3	69
Nickel(II) oxide (bunsenite), NiO	1	47	Potassium fluogermanate, K ₂ GeF ₆	6	41
Nickel pyrazole chloride, $Ni(C_{3}H_{4}N_{2})_{4}Cl_{2}$	8m	44	Potassium fluoplatinate, K ₂ PtF ₆	6	42
Nickel sulfate, NiSO,	2m	26	Potassium fluoride, KF	1	64
Nickel sulfate hexahydrate (retgersite),			Potassium fluosilicate (hieratite), K_2SiF_6	5	50
$NiSO_4 \cdot 6H_2O$	7	36	Potassium fluotitanate, $K_2 TiF_6 \dots$	7	40
Nickel sulfide, millerite, NiS	1m	37	Potassium heptafluozirconate, K ₃ ZrF ₇	9	46
Nickel tungstate, NiWO ₄	2m	27	Potassium hydroxide, KOH at 300 °C	4m	66
Niobium osmium 3:1, Nb ₃ Os	6m	30	Potassium hydroxy-chlororuthenate,		
Niobium oxychloride, NbOC1,	7m	148	$K_4 Ru_2 Cl_{10} O \cdot H_2 O \dots$	10	47
Niobium platinum 3:1, Nb ₃ Pt	6m	31	Potassium iodide, KI	1	68
Niobium silicide, NbSi ₂	8	39	Potassium iron (II) trifluoride, KFeF ₃	6m	39
Osmium, Os	4	8	Potassium lithium sulfate, KLiSO ₄	3m	43
Osmium titanium, OsTi	6m	85	Potassium magnesium chloride hydrate		
Palladium, Pd	1	21	(carnallite), KMgCl ₃ .6H ₂ O	8m	50
Palladium hydride, PdH _{0.706}	5m	72	Potassium magnesium chromium oxide,		
Palladium oxide, PdO	4	27	$K_2Mg_2(CrO_4)_3$	8m	52
Palladium vanadium 1:3, PdV ₃	6m	32	Potassium magnesium sulfate (langbeinite),		
Phosphorus bromide, PBr ₇	7m	150	$K_2Mg_2 (SO_4)_3 \dots$	6m	40
Pimelic acid, C ₇ H ₁₂ O ₄	$7 \mathrm{m}$	153	Potassium magnesium sulfate hydrate		
Platinum, Pt	1	31	(picromerite), $K_2Mg(SO_4)_2 \cdot 6H_2O$	8m	54
Platinum titanium 1:3, PtTi ₃	6m	33	Potassium magnesium trifluoride, KMgF ₃	6m	42
Platinum vanadium 1:3, PtV_3	6m	34	Potassium manganese (II) sulfate		
Plutonium arsenide, PuAs	4m	65	(manganolangbeinite), $K_2Mn_2(SO_4)_3$	6m	43
Plutonium phosphide, PuP	4m	65	Potassium manganese (II) trifluoride, KMnF,	6m	45
Plutonium telluride, PuTe	4m	66	Potassium nickel fluoride, KNiF,	7m	42
Potassium acid phthalate,			Potassium nickel (II) sulfate, $K_2Ni_2(SO_4)_3$	6m	46
$C_6H_4(COOH)(COOK)$	4m	30	Potassium niobium fluoride, K ₂ NbF ₇	8m	120
Potassium aluminum sulfate dodecahydrate,			Potassium nitrate (niter), KNO ₃	3	58
(alum), KAl(SO ₄) ₂ ·12H ₂ O	6	36	Potassium nitroso chlororuthenate,		
Potassium borohydride, KBH ₄	9	44	K,RuCl,NO	2m	29
Potassium bromate, KBrO ₃	7	38	Potassium perchlorate, KClO ₄	6	43
Potassium bromide, KBr	1	66	Potassium perchromate, K, CrO _a	3m	44
Potassium bromide chloride, KBro,s Clos	8m	46	Potassium periodate, KIO ₄	7	41
Potassium bromoplatinate, K ₂ PtBr ₆	8	40	Potassium permanganate, KMnO ₄	7	42
Potassium bromoselenate, K ₂ SeBr ₆	8	41	Potassium perrhenate, KReO ₄	8	41
Potassium cadmium fluoride, KCdF ₃	8m	47	Potassium phosphomolybdate tetrahydrate,		
Potassium cadmium sulfate, K ₂ Cd ₂ (SO ₄),	7m	34	$K_2 PO_4 (MOO_3)_{12} \cdot 4H_2 O$	8	43
Potassium cadmium trichloride, KCdCl ₃	5m	38	Potassium sodium sulfate, KNaSO ₄	6m	50
Potassium calcium carbonate (fairchildite),			Potassium sodium sulfate, K.67Na1.33SO4	6m	48
$K_2Ca(CO_3)_2$	8m	48	Potassium sodium sulfate (aphthitalite),		
Potassium calcium chloride (chlorocalcite),			$K_3 Na (SO_4)_2 \dots \dots$	6m	52
KCaC1,	7m	36	Potassium sulfate (arcanite), K_2SO_4	3	62
Potassium calcium fluoride, KCaF,	8m	49	Potassium thiocyanate, KCNS	8	44
Potassium calcium magnesium sulfate,			Potassium vanadium oxide, KV ₃ O ₈	8m	56
$K_2CaMg(SO_4)_3$	7m	37	Potassium zinc decavanadate 16 hydrate,		
Potassium calcium sulfate, K,Ca, (SO.)	7m	39	$K_{2}Zn_{2}V_{10}O_{28} \cdot 16H_{2}O$	3m	45
Potassium chlorate, KClO,	3m	42	Potassium zinc fluoride, KZnF,	5	51
Potassium chloride (sylvite), KCl	1	65	Potassium zinc sulfate hexahydrate,		
Potassium chloroplatinate, K, PtCl	5	49	$K_2Zn(SO_4)_2 \cdot 6H_2O$	7m	43
Potassium chlororhenate, K.ReCl.	2m	28	Potassium zinc sulfate, K ₂ Zn ₂ (SO ₄) ₃	6m	54
,2 6			Praseodymium antimony, PrSb	4m	43
m-Monograph 25.			Praseodymium arsenate, PrAsO,	4m	32
A mineral name in () indicates a synthetic sample	e.		Praseodymium arsenide, PrAs	4m	67

1	701. or			Vol. or	
	sec.	Page		sec.	Page
Praseodymium chloride, PrCl ₃	1m	39	Rubidium zinc sulfate hexahydrate,		
Praseodymium fluoride, PrF,	5	52	$Rb_{a}Zn(SO_{a})_{a}\cdot 6H_{a}O_{a}$	7 m	55
Praseodymium oxychloride, PrOCl	9	47	Ruthenium, Ru	4	5
Praseodymium sulfide, PrS	4m	67	Ruthenium titanium, RuTi	6m	86
Praseodymium vanadate, PrVO,	5m	40	Samarium arsenate, SmAsO,	4m	33
Praseodymium zinc. PrZn	5m	72	Samarium arsenide, SmAs	4m	68
Reservine C. H. N.O.	8m	123	Samarium chloride SmCl.	1m	40
Rhenium Re	2	13	Samarium fluoride SmF	1m	41
Rhodium Bh	3	9	Samarium gallium oxide Sm Ga (GaO)	1m	42
Rhodium vanadium 1:3 RhV	6m	56	Samarium oxide $Sm \cap (cubic)$	4m	34
Rubidium aluminum sulfate dodogahydrate	UII	00	Samarium oxychlorido $SmOCl$	1m	43
Rubidium alumnium surfate dodecanydrate,	c	44	Samarium tin oxido. Sm Sn O	2	70
$RDAI(SO_4)_2 \cdot 12\Pi_2O$	50	44	Samarium unodato $\operatorname{Sm}_2\operatorname{Sm}_2\operatorname{O}_7$	0111 5 m	11
Rubidium annue, RoNA ₂	200	13	Samarium vanadate, SinvO ₄	JIII 4m	41
Rubidium bromate, RbBrO ₃	8	45	Scandium arsenate, ScAsO ₄	4111	30
Rubidium bromide, RbBr	7	43	Scandium arsenide, ScAs	4m	68
Rubidium bromotellurate, $Rb_2 leBr_6$	8	46	Scandium oxide, Sc_2O_3	3	27
Rubidium cadmium sulfate, Rb,Cd,(SO ₄) ₃	7m	45	Scandium phosphate, ScPO ₄	8	50
Rubidium cadmium trichloride, high form,	_		Scandium silicate (thortveitite), $Sc_1Si_2O_7$	7m	58
RbCdCl ₃ (tetragonal)	5m	43	Selenium, Se	5	54
Rubidium cadmium trichloride, low form,			Selenium oxide (selenolite), SeO, (revised).	7m	60
RbCdCl ₃ (orthorhombic)	5m	41	Silicon, Si	2	6
Rubidium calcium chloride, RbCaC1,	7m	47	Silicon dioxide, alpha or low quartz, SiO_2		
Rubidium calcium fluoride, RbCaF ₃	8 m	57	(hexagonal)	3	24
Rubidium calcium sulfate, $Rb_2Ca_2(SO_4)_3$	7m	48	Silicon dioxide (alpha or low cristobalite),		
Rubidium chlorate, RbClO ₃	8	47	SiO ₂ (tetragonal) (revised)	10	48
Rubidium chloride, RbCl	4	41	Silicon dioxide (beta or high cristobalite),		
Rubidium chloroplatinate, Rb, PtCl,	5	53	SiO, (cubic)	1	42
Rubidium chlorostannate, Rb,SnCl,	6	46	Silver, Ag	1	23
Rubidium chlorotellurate, Rb, TeCl,	8	48	Silver, Ag (reference standard)	8m	2
Rubidium chromate, Rb, CrO,	.3m	46	Silver antimony sulfide, AgSbS, (cubic)	5m	48
Rubidium chromium sulfate dodecahydrate.			Silver antimony sulfide (miargyrite).		
$BbCr(SO_{1}) + 12H_{2}O_{1}$	6	47	AgShS (monoclinic)	5m	49
Rubidium cobalt fluoride RbCoF.	8m	58	Silver antimony sulfide (nyrargyrite) Ag.SbS.	0	10
Rubidium cobalt sulfate. Bb Co (SO)	8m	59	(trigonal)	5 m	51
Rubidium cobalt (II) trichloride $PbCoC1$	Gm	57	Silver antimony telluride AgShTe	3m	47
Rubidium copper sulfate hydrate	Om	01	Silver arconate Ag AsO	5	56
Rubhalum copper suitate hydrate, Ph $Cu(SO)$, $EU O$	9 m	61	Silver arsenia culfide venthegenite Ar Ass	0 m	196
$Rb_2 Cu(SO_4)_2 On_2 O \dots Db PtE$	oiii	40	Silver brometo A_{α} Pro	om	120
Rubidium fluorida. BhE	0 0m	40	Silver bromide (bromunite) AgDr	4	10
Rubidum fluoriliente. Dh SiE	0111	03	Silver bronide (bronyrite), AgBr	- 4 1 m	40
Rubidum indide Dh	0	49	Silver carbonate, Ag_2CO_3	1111	44
Rubialum loaide, Rbi	4	43	Silver chlorate, AgClO ₃	(44
Rubidium iron sulfate nydrate,			Silver chloride, (cerargyrite), AgCl	- 4	44
$Rb_2Fe(SO_4)_2 \cdot 6H_2O$	8m	64	Silver dysprosium, AgDy	5m	66
Rubidium magnesium chromium oxide,			Silver erbium, AgEr	5m	67
$Rb_2Mg_2(CrO_4)_3$	8m	66	Silver gadolinium, AgGd	6m	87
Rubidium magnesium chromium oxide hydrate,			Silver holmium, AgHo	5m	68
$Rb_2Mg(CrO_4)_2 \cdot 6H_2O$	8m	68	Silver iodide (iodyrite), AgI (hexagonal)	8	51
Rubidium magnesium sulfate, Rb,Mg,(SO ₄) ₃	7m	50	Silver iodide, gamma, AgI (cubic)	9	48
Rubidium magnesium sulfate hydrate,			Silver molybdate, Ag ₂ MoO ₄	7	45
$Rb_2Mg(SO_4)_2$ GH_2O	8m	70	Silver neodymium, AgNd	5m	71
Rubidium manganese sulfate, Rb ₂ Mn ₂ (SO ₄) ₃	7m	52	Silver nitrate, AgNO ₃	5	59
Rubidium manganese(II) trifluoride, RbMnF ₃	5m	44	Silver nitrite, AgNO ₂	5	60
Rubidium nickel sulfate, Rb ₂ Ni ₂ (SO ₄) ₃	8 m	72	Silver oxide, Ag ₂ O	1m	45
Rubidium nickel sulfate hydrate,			Silver(II) oxynitrate, Ag,O,NO,	4	61
$Rb_2Ni(SO_4)_2 \cdot 6H_2O$	8m	74	Silver periodate, AgIO,	9	49
Rubidium nickel (II) trichloride, RbNiCl,	6m	58	Silver permanganate, AgMnO,	7m	155
Rubidium nitrate, RbNO, (trigonal)	5m	45	Silver perrhenate. AgReO.	8	53
Rubidium perchlorate, RbClO	2m	30	Silver phosphate, Ag.PO.	5	62
Rubidium periodate, RbIO.	2m	31	Silver potassium cvanide. AgK(CN).	8m	78
Rubidium potassium chloride Rh. K. Cl	8m	76	Silver samarium. AgSm	5m	73
Rubidium strontium chloride RbSrC1	7m	54	Silver selenate Ag SeO	2m	20
Rubidium sulfate Rb.SO	8	48	Silver Sodium chloride Ag Na Cl	2m	70
Rubidium zine fluoride RhZnF	-7m	57	Silver subfluoride Ag F	5m	52
Rubidium zine mubilue, Ruzinra	(111	57	Silver sulfate Ag SO	7	10
m Monograph 25			Silver sulfide (argentite) $A \in S$	10	40
A minorel nome in () indicates a sufficient	-		Silver torbium AgTh	10	51
A mineral name in () indicates a synthetic sampl	е.		bilver terbium, Agib	DIII	14

Vol a

	VOI. 01	
	sec.	Page
Silver thulium AgTm	5m	74
Silver uttrium $\Delta \alpha V$	5m	75
Gadium anid fluorida NoVIE		10
Sodium acid fluoride, NaHF ₂	5	63
Sodium aluminum chloride silicate, sodalite,		
$Na_{si_{4}}A1_{O_{4}}C1_{2}$	$7 \mathrm{m}$	158
Sodium azide, alpha, NaN, at-90 to -100° C	8m	129
Sodium azida bata NaN	0	120
Soutum azide, beta, NaN_3		130
Sodium borate, $Na_{B}B_{B}O_{1}$,	$7 \mathrm{m}$	160
Sodium borohydride, NaBH ₄	9	51
Sodium bromate, NaBrO,	5	65
Sodium bromide NaBr	3	47
Sodium polaium oluminum fluorido hydroto	0	
Sourum carcium aruminum riuoriue nyurate,	~	
thomsenolite, NaCaAlF ₆ ·H ₂ O	8m	132
Sodium calcium beryllium aluminum fluorosili-		
cate, meliphanite, (Na, a, Ca, 17)Be(Al, 17)		
Si_{2} (O, F_{2} F, F_{3})	8m	135
Solo \$77 (06 25 1 0 757) IIIIII fluorogilianto	0111	100
Sourum carcium berymum muorosmicate,		
leucophanite, NaCaBeFS1 ₂ O ₆	8m	138
Sodium calcium sulfate (glauberite),		
$Na_{a}Ca(SO_{a})_{a}$	6m	59
Sodium carbonate monohydrate (thermonatrite)		
No. CO. IL O.	0	F 4
$Na_2 C U_3 \cdot H_2 U$	ð	54
Sodium chlorate, NaClO ₃	3	51
Sodium chloride (halite), NaCl	2	41
Sodium cobalt (II) sulfate tetrahydrate		
No $Co(SO)$.44 O	Gm	61
$\operatorname{Na}_2 \cup (\operatorname{SU}_4)_2 \cdot \operatorname{II}_2 \cup \cdots \cup $	0	01
Sodium cyanate, NaCNO	2m	33
Sodium cyanide, NaCN (cubic)	1	78
Sodium cyanide, NaCN (orthorhombic) at 6 ° C	1	79
Sodium dichromate dihydrate Na Cr O • 2H O	7 m	62
Sodium fluorido (villigumito) NaE	1 1	62
Sourum Huonue (vinnaumite), Nar	1	03
Sodium nexametaphosphate hexahydrate,		
$Na_{6}P_{6}O_{16} \cdot 6H_{2}O \dots \dots$	5m	54
Sodium hydrogen silicate tetrahydrate.		
No H SiO .4H O	7m	169
$Na_{3}\Pi_{3}SIO_{4}$ $\Pi_{3}O$	4	103
Sourum nyuroxide, NaOH at 300 °C	4111	69
Sodium iodate, NaIO ₃	7	47
Sodium iodide, NaI	4	31
Sodium lanthanum fluosilicate		
(No Lo) (SO) E	7 m	C 4
$(Na_{J}La_{R})$ $(BIO_{4})_{\kappa}\Gamma_{2}$	1111	04
Sodium magnesium aluminum boron hydroxy		
silicate, dravite, NaMg, Al, B, Si, O ₂₇ (OH),	3m	47
Sodium magnesium sulfate tetrahydrate.		
bloedite Na Mg(SO), 4H O	6m	63
Sodium monganaga (II) trifluarida NoMnE	Cm	00 65
Sourum manganese (II) trinuoride, Namir ₃	0111	60
Sodium mercury (II) trichloride dihydrate,		
$NaHgCl_{3} \cdot 2H_{2}O$	6m	66
Sodium molybdate. Na.MoO	1m	46
Sodium neodymium fluosilicate		
(N-Nd) (Co) E		
$(\operatorname{Na},\operatorname{Nd}_{a})$ $(\operatorname{SlO}_{a})_{\kappa}F_{2}$	γm	66
Sodium nickel (II) sulfate tetrahydrate,		
$Na_{2}Ni(SO_{4})_{2}\cdot 4H_{2}O$	6m	68
Sodium nitrate (soda-niter), NaNO,	6	50
Sodium nitrite NaNO	1	62
Codium anthetic, Narroy_2 , \ldots , Narroy_2 , \ldots	7	02
Sodium ortholungstate(IV) dinydrate,	_	
$Na_2WO_4 \cdot 2H_2O$	2m	33
Sodium oxalate, $Na_2C_2O_4$	6m	70
Sodium perchlorate, NaClO, (orthorhombic)	7	49
Sodium periodate NaIO		10
Sources period a_1, a_2, \dots, a_n	(40
sourum praseodymium fluosificate,		
$(\operatorname{Na}_{2}\operatorname{Pr}_{a})$ $(\operatorname{SiO}_{4})_{6}F'_{2}$	7m	68
Sodium silicate, alpha (III), Na,Si,O,	8m	141
Sodium sulfate (thenardite). Na.SO.	2	59
	2	00

Vol. or sec. Page Sodium sulfite, Na₂SO₃..... 3 60 Sodium tetrametaphosphate tetrahydrate, alpha, Na P.O., 4H,O (monoclinic)..... 10 52 Sodium tetrametaphosphate tetrahydrate, beta, $Na_4P_4O_{12} \cdot 4H_2O$ (triclinic) 2m 35 Sodium tin fluoride, NaSn₂F₅..... 7m 166 Sodium trimetaphosphate, Na₃P₃O₉ 3m 49 Sodium trimetaphosphate monohydrate, Na, P, O, H, O..... 3m 50 Sodium tungstate, Na₂WO₄ 1m 47 Sodium zinc sulfate tetrahydrate, $Na_2Zn(SO_4)_2 \cdot 4H_2O$ 6m 72 Sodium zinc trifluoride, NaZnF, 74 6m Sodium zirconium fluoride, Na₇Zr₆F₃₁ 8m 144 Strontium arsenate, $Sr_3(AsO_4)_2$ 2m36 Strontium azide, $Sr(N_3)_2$ 8m 146 Strontium boron oxide, SrB₂O₄..... 3m 53 Strontium boron oxide, SrB₄O₇..... 4m 36 Strontium bromide hexahydrate, SrBr, 6H,O... 4 60 Strontium carbonate (strontianite), SrCO₁ 3 56 Strontium chloride, SrCl, 4 40 Strontium chloride hexahydrate, SrCl₂.6H₂O ... 58 4 Strontium fluoride, SrF₂..... 5 67 Strontium formate, Sr (CHO₂), 8 55 Strontium formate dihydrate, Sr(CHO₂)₂·2H₂O (orthorhombic) 8 56 Strontium indium hydroxide, Sr, In₂(OH)₁₂ 6m 76 Strontium iodide hexahydrate, SrI₂.6H₂O 8 58 Strontium molybdate, SrMoO₄ 7 50 Strontium nitrate, Sr(NO₃)₂..... 80 1 Strontium oxide, SrO 68 5 Strontium peroxide, SrO₂..... 6 52 Strontium scandium oxide hexahydrate, Sr₃Sc₂O₆·6H₂O 78 6m Strontium sulfate (celestite), SrSO, 2 61 Strontium sulfide, SrS 7 52 Strontium telluride, SrTe 69 4m Strontium tin oxide, SrSnO₃ 80 8m Strontium titanate, SrTiO₃ 3 44 Strontium tungstate, SrWO, 7 53 Strontium zirconate, SrZrO₃..... 9 51 7 Sulfamic acid, NH₃SO₃ 54 Sulfur, S (orthorhombic) 9 54 Tantalum, Ta 1 29 d-Tartaric acid, $C_4H_6O_6$ 7m 168 Tantalum silicide, TaSi, 8 59 Tellurium, Te..... 1 26 Tellurium(IV) oxide (paratellurite), TeO₂ (tetragonal)..... 7 56 Tellurium(IV) oxide, paratellurite, TeO₂ (tetragonal)..... 10 55 Tellurium(IV) oxide, tellurite, TeO, (ortho-57 rhombic) 9 Terbium arsenate, TbAsO, 3m 54 Terbium arsenide, TbAs..... 5m 75 Terbium nitride, TbN 4m 70 Terbium phosphide, TbP 76 5m 76 Terbium selenide, TbSe 5m Terbium sulfide, TbS 5m 77 77 Terbium telluride, TbTe..... 5m Terbium vanadate, TbVO, 56 5m Thallium aluminum sulfate dodecahydrate, 6 $TlAl(SO_4)_2 \cdot 12H_2O \dots \dots \dots \dots \dots \dots \dots$ 53 Thallium(I) arsenate, Tl,AsO, 2m 37 Thallium azide, TlN3..... 82 8m Thallium(I) bromate, TlBrO₃

8

60

m-Monograph 25.

A mineral name in () indicates a synthetic sample.

	Vo1.	or		Vol. or	
	sec.	Page		sec.	Page
Thallium bromide, TlBr	7	57	Titanium oxide (anatase), TiO, (revised)	7m	82
Thallium cadmium sulfate, $Tl_2Cd_2(SO_4)_3$	8m	83	Titanium oxide (rutile), TiO, (revised)	7m	83
Thallium(I) chlorate, TlClO,	8	61	Titanium(III) oxide. TiO.	9	59
Thallium(I) chloride. TlCl	4	51	Titanium silicide, Ti, Si,	8	64
Thallium chloroplatinate, Tl.PtCl.	5	70	Titanium sulfide TiS.	4m	72
Thallium chlorostannate Tl SnCl	6	54	Titanium sulfide Ti S	8m	140
Thallium chromate Tl CrO	3m	54	24.6 Tripitrophonotolo C II OC II (NO)	0m	150
Thallium chromium sulfate dedeaphydrate	0111	01	$2,4,0$ = 1111110phenetole, $C_{2}\Pi_{5}OC_{6}\Pi_{2}(1)O_{2}/_{3}$	1	102
TICKSO 1240	c	55	Tungsten, W (reference standard)	0	20 0
$\operatorname{Ticl}(\operatorname{SO}_4)_2 \cdot \operatorname{I2In}_2 \cup \ldots \dots \dots$	0	55	Tungsten, w (reference standard)	811	4
Inallium cobait sullate, $\Pi_2 CO_2(SO_4)_3$	вm	85	Tungsten sullide (tungstenite), WS_2	8	65
Thallium cobalt sulfate hexahydrate,			Uranium dioxide (uraninite), UO_2	_ 2	.33
$T_{1},C_{0}(S_{0}), 6H_{2}O$	7m	70	Uranium oxide, UO	5m	78
Thallium copper sulfate hexahydrate,			Uranium selenide, USe	5m	78
$T_{1}, Cu(SO_{4}), 6H, O$	$7 \mathrm{m}$	72	Uranium telluride, UTe	4m	73
Thallium fluosilicate, Tl ₂ SiF ₆	6	56	Urea, $CO(NH_2)_2$	7	61
Thallium gallium sulfate dodecahydrate,			Uric acid, $C_{5}H_{4}N_{4}O_{3}$	8m	154
$TlGa(SO_4)_2 \cdot 12H_2O$	6	57	Vanadium(V) oxide, V ₂ O ₅	8	66
Thallium(I) iodate, TlIO,	8	62	Ytterbium arsenate, YbAsO,	4m	38
Thallium(I) iodide, TlI (orthorhombic)	4	53	Ytterbium arsenide, YbAs	4m	73
Thallium iron sulfate hydrate.			Ytterbium gallium oxide, Yb, Ga, (GaO.),	1m	49
Tl-Fe(SO.).:6H-O	8m	87	Ytterbium nitride YbN	4m	74
Thallium magnesium chromium oxide	0		Vtterbium oxide Vb O	6m	80
TI Mg (Cro.)	8m	80	Vtterbium selenide VhSe	5m	79
Thallium magnosium sulfato hovehydrato	om	00	Vtterbium telluride, VbTe	5m	70
Thanfulli magnesium suffate nexaliyurate,	-7 m		Vttorbium (III) unnadato VbVO	5m	50
Π_{n} Mg(SO ₄), \bullet 6H, O \ldots The set of	7111	74	Itterbrum(III) vanadate, IDVO4	0m	20
Thallium manganese sulfate, 11, Mn, (SO ₄),	'7m	76	Yttrium arsenate, YASO,	2111	39
Thallium nickel sulfate nexalydrate,	_		Yttrium arsenide, YAS	4m	74
$T1_2N1(SO_4)_2 \cdot 6H_2O$	7m	78	Yttrium gallium oxide, Y,Ga,(GaO ₄),	Im	50
Thallium(I) nitrate, TINO ₃	6	58	Yttrium oxide, Y_2O_3	3	28
Thallium(III) oxide, Tl_2O_3	2	28	Yttrium oxychloride, YOCl	1m	51
Thallium(I) perchlorate, TlClO ₄	2m	38	Yttrium phosphate (xenotime), YPO ₄	8	67
Thallium(I) phosphate, Tl ₃ PO ₄	7	58	Yttrium sulfide, YS	5m	80
Thallium(III) phosphate, TlPO ₄	7	59	Yttrium telluride, YTe	4m	75
Thallium(I) sulfate, Tl ₂ SO ₄	6	59	Yttrium vanadate, YVO ₄	5m	59
Thallium(I) thiocyanate, TlCNS	8	63	Zinc, Zn	1	16
Thallium(I) tungstate, Tl,WO,	1m	48	Zinc aluminate (gahnite), ZnAl,O,	2	38
Thallium zinc sulfate hexahydrate.			Zinc antimony oxide. ZnSb.O.	4m	39
T_{1} , $Z_{n}(S_{0})$, 6H, 0	7m	80	Zinc borate. ZnB.O.	1	83
Thorium arsenide. ThAs	4m	70	Zinc carbonate, smith sonite, ZnCO,	8	69
Thorium oxide (thorianite) ThO	1	57	Zinc evanide $Zn(CN)$	5	73
Thulium arsenate TmAsO	3m	56	Zinc fluoride ZnF	ĥ	60
Thulium arsenide TmAs	4m	71	Zine fluosilicate hevelydrate ZnSiF .6H O	8	70
Thulium nitrido TmN	4m	71	Zine nuosineate nexangulate, Zhon ₆ .01 ₂ 0	10	56
Thulium accquievide Tm O		11 E0	Zine germanate, $\Sigma n_2 \text{deo}_4 \dots \dots \dots$	10	170
Thulium telluside $TmTe$	9 4m	00	Zinc glutamate dinyurate, ZnC, H, NO, 2H, O	-7m	170
Thulium terruride, Imie	410	14	\sum inc fourde, \sum in 2	- 9	60
Inulium vanadate, ImVO ₄	5m	57	Zinc molybdate, Zn,Mo,O,	7m	173
Tin, alpha, Sn (cubic)	2	12	Zinc orthosilicate (willemite), Zn_2SiO_4	7	62
Tin, beta, Sn (tetragonal)	1	24	Zinc oxide (zincite), ZnO	2	25
Tin arsenide, SnAs	4m	37	Zinc pyrosilicate hydrate, hemimorphite,		
Tin(II) fluoride, SnF_2	3m	51	$Zn_4(OH)_2Si_2O_7 \cdot H_2O \dots \dots \dots \dots \dots$	2	62
$Tin(IV)$ iodide, SnI_4	5	71	Zinc selenide, ZnSe	3	23
Tin(II) oxide, SnO	4	28	Zinc sulfate (zinkosite), ZnSO ₄	7	64
Tin(IV) oxide (cassiterite), SnO,	1	54	Zinc sulfate heptahydrate (goslarite),		
Tin(II) telluride, SnTe	7	61	ZnSO ₄ ·7H ₂ O	8	71
Titanium, Ti	3	1	Zinc sulfide (wurtzite), alpha ZnS (hexag-		
Titanium dioxide, brookite, TiO, (ortho-			onal)	2	14
rhombic)	3m	57	.,	-	- 1
		0.			

m_Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE MINERAL INDEX

	Vol. or			Vol. or	
	sec	Page		sec.	Page
Alabandite, MnS	4	11	Eschynite, CeNbTiO ₆	3m	24
Alum, $KAl(SO_4)_2 \cdot 12H_2O \dots$	6	36	Eskolaite, Cr ₂ O ₃	5	22
Ammonia-niter, NH,NO,	7	4	Ettringite, Al.O. 6CaO 3SO. 31H.O	8	3
Anatase, TiO. (revised)	7m	82	Fairchildite, K Ca(CO)	8m	48
Andradite Ca. Fe.Si.O.	9	22	Fluoranatite Ca. F(PO.).	3m	22
Anglesite PhSO	ž	67	Fluorite CaF	1	60
Anhydrite $C_0 S_0$	4	65	Findine, Car ₂	1	00
Aninyunte, $CaSO_4$	4	00	$\mathbf{Forsterrite}, \mathbf{Mg}_2 \mathbf{SIO}_4 \dots \mathbf{SIO}_4$	1	03
Apric April	611	54	Galaxite, MnAl ₂ O ₄	9	35
Aragonite, CaCO ₃	3	53	Galena, PbS	2	18
Argentite, Ag ₂ S	10	51	Gahnite, $ZnAl_2O_4$	2	38
Arcanite, K_2SO_4	3	62	Geikielite, MgTiO,	5	43
Arsenolite, As ₂ O ₃	1	51	Gersdorffite, NiAsS	1m	35
Aurostibite, AuSb ₂	7	18	Glauberite, $Na_2Ca(SO_4)_2$	6m	59
* Azurite, Cu ₂ (OH) ₂ (CO ₂),	10	.30	Goslarite, ZnSO, 7H, O	8	71
Barite, BaSO,	3	65	Greenockite. CdS	4	15
Berlinite AlPO	10	3	Halite NaCl	2	41
*Porvl Po Al (SiO)	10	12	*Homimorphite Zn (OH) Si O H O	2	62
$\operatorname{Picmite}_{(a)nba} \operatorname{Pi}_{O}$	3m	17	Hierotito K SiF	5	50
$\mathbf{Bismille}, (alpha) \mathbf{Bi}_2 \mathbf{O}_3 \dots \mathbf{Di}_2 \mathbf{O}_3$	1	E 4	Hughporite $MnWO$		24
Dismocrite, DiOCI	- 4 	54	Huebherite, MilwO ₄	2111	24
Bismutninite, Bi_2S_3 (revised)	5m	13	Humite, $3Mg_2SIO_4 \cdot MgF_2 \dots \dots \dots$	Im	30
*Bloedite, $Na_2Mg(SO_4)_2 \cdot 4H_2O \dots$	6m	63	Iodyrite, Agl	8	51
Böhmite, $Al_2O_3 \cdot H_2O \dots \dots$	3	38	Jacobsite, $MnFe_2O_4$	9	36
Bromellite, BeO	1	36	Langbeinite, $K_2Mg_2(SO_4)_3$	6m	40
Bromyrite, AgBr	4	46	*Leucophanite, NaCaBeFSi ₂ O ₆	8m	138
*Brookite, TiO ₂	3m	57	Litharge, PbO (red)	. 2	30
Brucite, Mg(OH),	6	30	Lithiphosphate, Li ₃ PO ₄	4m	21
Bunsenite, NiO	1	47	Loellingite, FeAs,	10	34
Calcite. CaCO,	2	51	Magnesite, MgCO,	7	28
Calomel. Hg.Cl.	1	72	Magnetite, Fe.O.	5m	31
Carnallite KMgCl. 6H-O	- 8m	50	Malachite, Cu.(OH), CO.	10	31
Cassiterite SnO	1	54	Manganolangheinite K Mn (SO)	6m	43
Calestite SrSO	2	61	Manganosite MnO	5	45
Corergyrite AgC	4	44	Marshite Cul	1	20
Cerianjita CoO	1	56	Macongrite (NH) SO (revised)	0	0
Certainte, CeO_2	2	50	Massignite, $(Nii_4)_2 SO_4$ (levised)	3	20
Cerussile, $FDCO_3$	10	00	Massicol, FDO (yellow)	1	34
Cervantite, SD_2O_4	10	8		1	10
Charcocyanite, CuSO,	311	29	Melanterite, $FeSO_4 \cdot 7H_2O$	8 m	38
Chloraluminite, $AlCl_3 \cdot 6H_2O$	4	3	*Meliphanite, Na.63Ca1 37BeA1.13S1.87O6.25 F 475	8m	135
Chlorocalcite, KCaC1,	$7 \mathrm{m}$	36	Metacinnabar, HgS	_ 4	21
Chrysoberyl, $BeAl_2O_4$	9	10	Miargyrite, AgSbS ₂	5m	49
Cinnabar, HgS	4	17	*Millerite, NiS	1m	37
*Claudetite, As ₂ O ₃	3m	9	Minium, Pb_3O_4	8	32
Clausthalite, PbSe	5	38	Molybdenite, MoS ₂	. 5	47
Cordierite, $Mg_A 1_4 Si_5 O_{18}$ (orthorhombic)	1m	28	Molybdite, MoO ₃	3	30
Cordierite, Mg ₂ A1 ₄ Si ₅ O ₁₆ (hexagonal)	1m	29	Montroydite, HgO (revised)	9	39
Corundum, Al ₂ O ₃	9	3	Mullite, $3Al_2O_3 \cdot 2SiO_2 \dots \dots \dots \dots$	3m-	3
Cotunnite, PbCl,	2	45	Nantokite, CuCl	4	35
Covellite, CuS	4	13	*Newbervite, MgHPO, 3H, O	7m	139
Cristobalite, (alpha or low) SiO, (revised)	10	48	Niter, KNO,	3	58
Cristobalite. (beta or high) SiO	1	42	Nitrobarite, Ba(NO.),	1	81
Cryptohalite. (NH.).SiF.	5	5	Norbergite Mg.SiQ.MgF.	10	39
Cuprite Cu O	2	23	Oldhamite CaS	7	15
*Diamond C	2	5	Otavite CdCO	7	11
*Diaspore Al O.H O	2	41	Oxammite $(NH) C O H O$. 7	5
Dionside CaM $\sigma(SiO)$.0 5m	17	*Paratallurita TaO	10	55
*Dravito NaMa Al $\mathbf{R} \in \mathcal{O}(\mathbf{OU})$	0m	47	\mathbf{P}_{a}	7	56
*Enctotite MaSiO	SIII	20	Portridgoito Mn O	0	27
Ensemite $Maso 740$	0	34	Participante, Mm_2O_3	5	27
Epsonate, $MgSO_4 \cdot In_2O$	1	30	*Dhenosite, Do SiO	1	11
			Phenacite, $Be_2 SIO_4 \dots$	ð	11
*Natural mineral.			Picrochromite, $MgCr_2O_4$	9	34
M-Monagraph 25.			Picromerite, $K_2Mg(SO_4)_2$ ·6H ₂ O	8m	54

CUMULATIVE MINERAL INDEX—Continued

	Vol. or		,	Vol. or	
	sec.	Page		sec.	Page
Portlandite, Ca(OH) ₂	1	58	Teschermigite, NH ₄ Al(SO ₄) ₂ ·12H ₂ O	6	3
Powellite, CaMoO,	6	22	Thenardite, Na ₂ SO ₄	2	59
Pyrargyrite, Ag ₃ SbS ₃	5m	51	Thermonatrite, $Na_2CO_3 \cdot H_2O$	8	54
Pyrite, FeS ₂	5	29	*Thomsenolite, NaCaAlF ₆ ·H ₂ O	8m	132
Pyrope, Mg ₃ Al ₂ (SiO ₄) ₃	4m	24	Thorianite, ThO ₂	1	57
*Quartz, SiO ₂ (alpha or low)	3	24	Thortveitite, Sc ₂ Si ₂ O ₇	$7 \mathrm{m}$	58
Rammelsbergite, NiAs ₂	10	42	Tiemannite, HgSe	7	35
Retgersite, NiSO ₄ .6H ₂ O	7	36	* Topaz, Al ₂ SiO ₄ (F,OH) ₂	1m	4
Rhodochrosite, MnCO ₃	7	32	Trevorite, NiFe ₂ O ₄	10	44
Rutile, TiO, (revised)	7m	83	Tungstenite, WS ₂	8	65
Safflorite, CoFeAs,	10	28	Uraninite, UO ₂	2	33
Sal-ammoniac, NH ₄ Cl	1	59	Uvarovite, $Ca_{2}Cr_{2}(SiO_{4})_{3}$	10	17
Sanmartinite, ZnWO ₄	2m	40	* Valentinite, Sb ₂ O ₃	10	6
Scacchite, MnCl ₂	8m	43	Villiaumite, NaF	1	63
*Scheelite, CaWO,	6	23	Willemite, Zn ₂ SiO ₄	7	62
Selenolite, SeO, (revised)	7m	60	Witherite, BaCO ₃	2	54
Sellaite, MgF ₂	4	33	Wulfenite, PbMoO,	7	23
Senarmontite, Sb ₂ O ₃	3	31	Wurtzite, ZnS	2	14
Skutterudite, CoAs,	10	21	*Xanthoconite, Ag ₃ AsS ₃	8m	126
*Smithsonite, ZnCO ₃	8	69	Xenotime, YPO,	8	67
*Sodalite, Na Si Al O, Cl,	7m	158	Zinc sulfide (sphalerite), beta ZnS (cubic)	2	16
Soda-niter, NaNO,	6	50	Zinc telluride, ZnTe	Зm	58
Sphalerite, ZnS	2	16	Zinc tungstate (sanmartinite), ZnWO ₄	2m	40
Spherocobaltite, CoCO,	10	24	Zincite, ZnO	2	25
Spinel, MgAl ₂ O ₄	2	35	Zinkosite, ZnSO,	7	64
Stibnite, Sb,S,	5	6	*Zircon, ZrSiO,	4	68
Stolzite, PbWO, (revised)	5m	34	Zirconium, alpha, Zr	2	11
Strontianite, SrCO,	3	56	Zirconium dihydride, ZrH,	5m	60
Struvite, MgNH ₄ PO ₄ ·6H ₂ O	3m	41	Zirconium iodate, Zr(IO ₃) ₄	1m	51
Sylvite, KCl	1	65	Zirconium nitride, ZrN	5m	80
*Tellurite, TeO,	9	57	Zirconium oxide, ZrO	5m	81
Tellurobismuthite, Bi ₂ Te ₃	3m	16	Zirconium phosphide, ZrP	4m	75
Tenorite, CuO	1	49	Zirconium silicate, zircon, ZrSiO,	4	68
Teschemacherite, NH ₄ HCO ₃	9	5	Zirconium sulfate tetrahydrate, Zr(SO ₄) ₂ ·4H ₂ O	7	66



.

Latest developments in the subject area of this publication, as well as in other areas where the National Bureau of Standards is active, are reported in the NBS Technical News Bulletin. See following page.

HOW TO KEEP ABREAST OF NBS ACTIVITIES

Your purchase of this publication indicates an interest in the research, development, technology, or service activities of the National Bureau of Standards.

The best source of current awareness in your specific area, as well as in other NBS programs of possible interest, is the TECHNICAL NEWS BULLETIN, a monthly magazine designed for engineers, chemists, physicists, research and product development managers, librarians, and company executives.

If you do not now receive the TECHNICAL NEWS BULLETIN and would like to subscribe, and/or to review some recent issues, please fill out and return the form below.

Mail to: Office of Technical Informatio National Bureau of Standards Washington, D. C. 20234	n and Publications			
Name				
Affiliation				
Address				
City	_ State Zip			
 Please send complimentary past issues of the Technical News Bulletin. Please enter my 1-yr subscription. Enclosed is my check or money order for \$3.00 (additional \$1.00 for foreign mailing). Check is made payable to: SUPERINTENDENT OF DOCUMENTS. 				

(cut here)
PERIODICALS

JOURNAL OF RESEARCH reports National Bureau of Standards research and development in physics, mathematics, chemistry, and engineering. Comprehensive scientific papers give complete details of the work, including laboratory data, experimental procedures, and theoretical and mathematical analyses. Illustrated with photographs, drawings, and charts.

Published in three sections, available separately:

• Physics and Chemistry

Papers of interest primarily to scientists working in these fields. This section covers a broad range of physical and chemical research, with major emphasis on standards of physical measurement, fundamental constants, and properties of matter. Issued six times a year. Annual subscription: Domestic, \$9.50; foreign, \$11.75*.

• Mathematical Sciences

Studies and compilations designed mainly for the mathematician and theoretical physicist. Topics in mathematical statistics, theory of experiment design, numerical analysis, theoretical physics and chemistry, logical design and programming of computers and computer systems. Short numerical tables. Issued quarterly. Annual subscription: Domestic, \$5.00; foreign, \$6.25*.

• Engineering and Instrumentation

Reporting results of interest chiefly to the engineer and the applied scientist. This section includes many of the new developments in instrumentation resulting from the Bureau's work in physical measurement, data processing, and development of test methods. It will also cover some of the work in acoustics, applied mechanics, building research, and cryogenic engineering. Issued quarterly. Annual subscription: Domestic, \$5.00; foreign, \$6.25*.

TECHNICAL NEWS BULLETIN

The best single source of information concerning the Bureau's research, developmental, cooperative and publication activities, this monthly publication is designed for the industry-oriented individual whose daily work involves intimate contact with science and technology—for engineers, chemists, physicists, research managers, product-development managers, and company executives. Annual subscription: Domestic, \$3.00; foreign, \$4.00*.

* Difference in price is due to extra cost of foreign mailing.

Order NBS publications from:

Superintendent of Documents Government Printing Office Washington, D.C. 20402

NONPERIODICALS

Applied Mathematics Series. Mathematical tables, manuals, and studies.

Building Science Series. Research results, test methods, and performance criteria of building materials, components, systems, and structures.

Handbooks. Recommended codes of engineering and industrial practice (including safety codes) developed in cooperation with interested industries, professional organizations, and regulatory bodies.

Special Publications. Proceedings of NBS conferences, bibliographies, annual reports, wall charts, pamphlets, etc.

Monographs. Major contributions to the technical literature on various subjects related to the Bureau's scientific and technical activities.

National Standard Reference Data Series. NSRDS provides quantitative data on the physical and chemical properties of materials, compiled from the world's literature and critically evaluated.

Product Standards. Provide requirements for sizes, types, quality and methods for testing various industrial products. These standards are developed cooperatively with interested Government and industry groups and provide the basis for common understanding of product characteristics for both buyers and sellers. Their use is voluntary.

Technical Notes. This series consists of communications and reports (covering both other agency and NBS-sponsored work) of limited or transitory interest.

Federal Information Processing Standards Publications. This series is the official publication within the Federal Government for information on standards adopted and promulgated under the Public Law 89–306, and Bureau of the Budget Circular A–86 entitled, Standardization of Data Elements and Codes in Data Systems..

U.S. DEPARTMENT OF COMMERCE WASHINGTON, D.C. 20230

OFFICIAL BUSINESS

-

PENALTY FOR PRIVATE USE, \$300



POSTAGE AND FEES PAID U.S. DEPARTMENT OF COMMERCE