C13.44:25/sec.8

A UNITED STATES DEPARTMENT OF COMMERCE PUBLICATION

NBS MONOGRAPH 25—SECTION 8

Standard X-ray Diffraction Powder Patterns

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Standard X-ray Diffraction Powder Patterns

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

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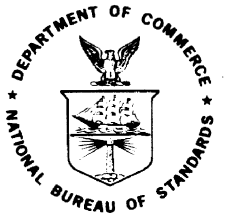

National Bureau of Standards Monograph 25—Section 8

Nat. Bur. Stand. (U.S.), Monogr. 25—Section 8, 171 pages (Sept. 1970)
CODEN: NBSMA

Issued September 1970

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402
(Order by SD Catalog No. C13.44:25/Sec. 8), Price $1.50.

Library of Congress Catalog Card Number: 53–61386

Contents

Errata

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_{6h}^{2} -$P6_3/m$ (No. 176)

Section 6, pg. 32; the formula in the page heading should be $K_2Co_2(SO_4)_3$

Section 7, { pg. iii / pg. 177 } 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:

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NBS Circular 539, Volume 8, Standard X-ray Diffraction Powder Patterns (Data for 61 substances).
NBS Circular 539, Volume 9, Standard X-ray Diffraction Powder Patterns (Data for 43 substances).
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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. Evans[2]

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."[4]

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.

Optical data, color. 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 $b:a:c$ [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 variance-covariance 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

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

[3] Joint 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.

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

[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 α_1 peaks because the internal standard corrections for all regions were established in terms of the $K\alpha_1$ 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 °C. The following angles for high-purity tungsten, silver, and cadmium oxide were computed using cell dimensions without index of refraction corrections.

Calculated 2θ Angles

$CuK\alpha_1$ = 1.54056 Å

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

All of our patterns were made at 25 °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 $K\alpha_1$ was assumed to be 1.54056 A [Bearden, 1964).

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm, 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.

Scattering factors. 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:

$$B = [\beta_{11}\beta_{22}\beta_{33}]^{1/3}$$

Integrated intensities. Intensity calculations were based on the copper K_{α_1} wavelength, 1.54056 A, determined by Bearden [1964]. The integrated intensities were computed from the formula:

$$I = F^2 \text{ (Lp) (FAC)}$$

where F is the standard structure factor

FAC is the powder multiplicity

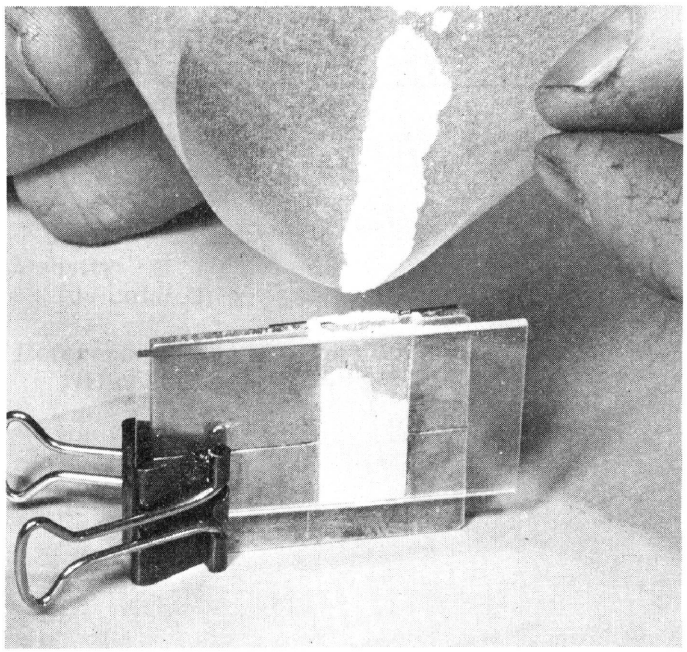
and $\text{Lp} = \dfrac{1 + 2\cos^2 2\theta}{\sin^2\theta \cos\theta}$.

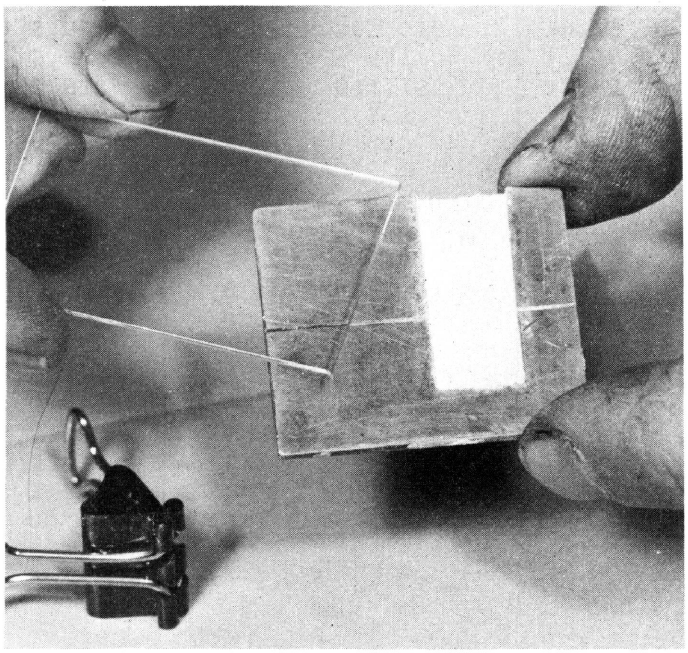
The intensities were scaled to the strongest line as 100. Reflections which had intensities of 0.7 or less were not reported.

Scale factors. 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° (2θ). 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.





REFERENCES

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, I (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 Centroid 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.

Ammonium Cadmium Sulfate Hydrate, $(NH_4)_2Cd(SO_4)_2 \cdot 6H_2O$ (monoclinic)

Sample

The sample was made by slow evaporation at room temperature of a 1 : 1 aqueous solution of $(NH_4)_2SO_4$ 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, $P2_1/a$ (14), Z=2, structure determined by Montgomery and Lingafelter [1966]. Isostructural with other "Tutton" salts [Tutton, 1916].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Hofmann [1931]	9.35*	12.705*	6.27*	106°41′*
Montgomery et al. [1966]	9.43	12.82	6.29	106°52′
NBS, sample 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

$I/I_{corundum}$ = 1.8

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	$\bar{1}11$	16.66
5.21	17	120	17.00
4.500	40	200	19.71
4.388	40	021	20.22
4.316	30	$\bar{1}21$	20.56
4.239	100	210,$\bar{2}$01	20.94
4.205	75	111	21.11
4.022	8	$\bar{2}11$	22.08
3.849	100	130	23.09
3.678	30	220	24.18
3.655	10	121	24.33
3.531	18	$\bar{2}21$	25.20
3.478	12	031	25.59
3.442	35	$\bar{1}31$	25.86
3.193	6	040,201	27.92
3.099	19	211	28.78
3.077	8	131	28.99
3.057	60	$\bar{1}12$	28.19
3.014	4	002	29.61
3.006	4	$\bar{2}31$	29.70
2.934	10	012	30.44
2.921	20	$\bar{2}02$,310	30.58
2.855	35	221	31.30
2.823	20	041,122	31.67
2.759	7	$\bar{3}21$	32.42
2.729	5	022	32.79
2.659	11	$\bar{2}22$	33.68
2.603	15	240	34.43
2.584	9	112	34.68
2.552	8	231,$\bar{2}$41	35.13
2.529	4	$\bar{1}32$	35.46
2.485	40	$\bar{3}31$	36.11
2.471	7	$\bar{3}12$	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 Å $CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
2.339	8	$\bar{1}51,\bar{4}01$	38.46
2.264	20	321	39.78
2.258	12	241	39.89
2.243	6	$132,\bar{1}42$	40.17
2.227	3	202	40.48
2.215	9	151,410	40.70
2.193	18	$\bar{2}12,042$	41.13
2.187	15	$\bar{2}51,340$	41.24
2.169	6	$\bar{3}32$	41.61
2.156	15	$\bar{2}42$	41.87
2.122	20	420	42.56
2.103	3	222	42.98
2.072	5	$160,\bar{2}03$	43.64
2.068	5	$\bar{1}13$	43.74
2.044	2	$\bar{2}13$	44.28
2.009	15	061	45.10
1.992	3	$\bar{1}23$	45.50
1.960	9	$\bar{3}51$	46.29
1.945	7	350	46.66
1.926	14	$260,\bar{2}52$	47.16
1.919	7	023	47.33
1.902	7	$\bar{2}61$	47.77
1.888	3	$\bar{4}41$	48.17
1.879	6	$\bar{1}33$	48.40
1.859	8	$\bar{5}11$	48.95
1.850	7	421	49.21
1.833	8	113	49.70
1.827	7	242	49.86
1.795	6	$\bar{3}52$	50.83
1.782	9	510	51.22
1.773	6	$\bar{4}03,\bar{3}33$	51.49
1.770	4	$261,\bar{5}12$	51.59
1.757	7	$351,\bar{4}13$	52.00
1.746	1	$\bar{3}61,071$	52.35
1.737	9	$\bar{2}43,360$	52.66
1.719	6	$\bar{5}31$	53.25

References

Hofmann, W. (1931). Die Struktur der Tuttonschen Salze, Z. Krist., **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.

Sample

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, $P2_13$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The structure of langbeinite, $K_2Mg_2(SO_4)_3$, 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

$I/I_{corundum} = 2.3$

Additional patterns

1. PDF card 11-241, [M. Hoshino, Dept. Applied Chem., Tohoku Univ.,Sendai, Japan].

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	622	58.04
1.5706	4	630	58.74
1.5535	4	631	59.45
1.5206	1	444	60.87
1.5052	2	632	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

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
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	2	810	72.24
1.2967	1	811	72.89
1.2871	1	733	73.52
1.2776	1	820	74.16
1.2682	1	821	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

References

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

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, $K_2Mg_2(SO_4)_3$, Acta Cryst. **10**, 409 - 413.

Ammonium Cobalt Fluoride, NH_4CoF_3 (cubic)

Sample

The material was formed by the reaction of methanol solutions of $CoBr_2$ and NH_4F, 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]----------	4.129
Crocket and Haendler[1960]------	4.129
NBS, sample at 25 °C----------	4.1320 ±.0001

Density

(calculated) 3.153 g/cm^3 at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.2

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

d (Å)	I	hkl	2θ(°)
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

References

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.

Sample

The sample was prepared at room temperature by slow evaporation of an aqueous equimolar solution of $(NH_4)_2CrO_4$ and $MgCrO_4$.

Color

Unground: vivid yellow
Ground: vivid greenish yellow

Optical data

Biaxial(+) N_α=1.637, N_β=1.638, N_γ=1.653, 2V is small.

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	9.508 ±.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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
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	$\bar{1}21$	20.71
4.249	70	$\bar{2}01$	20.89
4.213	30	111	21.07
4.026	8	$\bar{2}11$	22.06
3.832	80	130	23.19
3.649	19	121	24.37
3.453	20	031	25.78
3.414	12	$\bar{1}31$	26.08
3.222	18	201	27.66
3.167	30	040	28.15
3.123	16	211	28.56
3.071	5	$\bar{1}31$	29.05
3.029	30	$\bar{1}12$	29.46
2.996	20	$\bar{3}11, \bar{2}31, +$	29.80
2.957	3	$\bar{3}10$	30.20
2.907	13	$\bar{2}02$	30.73
2.873	13	221	31.10
2.832	2	$\bar{2}12$	31.57
2.798	25	$041, \bar{1}22$	31.96
2.774	15	$\bar{3}21$	32.24
2.742	5	320	32.63
2.710	1	022	33.02
2.586	7	$141, 112$	34.66
2.563	11	$\bar{2}31$	34.98
2.541	6	$\bar{2}41$	35.29
2.491	25	$\bar{3}31$	36.02
2.445	3	032	36.72
2.394	3	232	37.53

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.282	6	400	39.46
2.260	15	241	39.86
2.246	5	410	40.12
2.216	7	250,$\bar{4}$21	40.68
2.195	9	340	41.09
2.178	14	042,$\bar{2}$51	41.43
2.147	12	420	42.05
2.121	4	331	42.60
2.028	4	$\bar{2}$13,142	44.64
2.000	2	003	45.31
1.994	6	251,061	45.46
1.959	6	401,$\bar{3}$51	46.32
1.939	4	341	46.81
1.917	10	260,$\bar{3}$13	47.39
1.911	8	$\bar{2}$52,161	47.53
1.852	8	$\bar{3}$23,440	49.15
1.847	7	$\bar{2}$33	49.30
1.828	3	113,152	49.83
1.822	2	$\bar{5}$21	50.03
1.807	12	510,033	50.46
1.775	2	123	51.45
1.750	3	$\bar{1}$62	52.23
1.730	4	$\bar{5}$22,$\bar{4}$51,+	52.88
1.725	5	$\bar{2}$43	53.05
1.696	3	450	54.03
1.678	6	171	54.65
1.667	3	441,271	55.06
1.652	2	213,$\bar{3}$43	55.56

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. 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.

Sample

The sample was prepared at room temperature by slowly evaporating a 1:1 aqueous solution of $(NH_4)_2SO_4$ and $MnSO_4$.

Color

Pale pink

Optical data

Biaxial (+) N_α=1.482, N_β=1.456, N_γ=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]	9.29	12.66	6.211	107.05°
Montgomery et al.[1966]	9.40	12.74	6.26	107°
NBS, 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 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	$\bar{1}11$	16.77
5.18	25	120	17.10
4.491	20	200	19.75
4.356	25	021	20.37
4.287	50	$\bar{1}21$	20.70
4.227	100	210,$\bar{2}$01	21.00
4.172	45	111	21.28
4.010	11	$\bar{2}11$	22.15
3.824	80	130	23.24
3.664	10	220	24.27
3.627	10	121	24.52
3.517	6	$\bar{2}21$	25.30
3.453	16	031	25.78
3.422	19	$\bar{1}31$	26.02
3.177	25	201	28.06
3.079	25	211,230	28.98
3.031	45	$\bar{1}12$	29.44
2.986	8	140,$\bar{2}$31	29.90
2.965	7	$\bar{3}11$	30.12
2.911	15	012,310	30.69
2.834	20	$\bar{2}12$	31.54
2.801	25	$\bar{1}22$,041	31.93
2.749	12	$\bar{3}21$	32.54
2.703	3	022,320	33.11
2.643	5	$\bar{2}22$	33.89
2.587	10	240	34.64
2.576	7	141	34.80
2.539	11	231	35.32
2.475	30	$\bar{3}31$	36.27
2.439	6	330,150	36.82
2.397	4	$\bar{2}32$	37.49
2.336	5	051,$\bar{4}$01	38.51
2.295	3	$\bar{4}11$	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 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.199	6	151,$\bar{3}$41	41.01
2.176	20	042,340	41.47
2.157	6	$\bar{3}$32	41.84
2.143	7	$\bar{2}$42	42.14
2.114	14	420,060	42.74
2.052	5	$\bar{1}$13	44.10
2.029	4	$\bar{2}$13	44.62
2.004	6	$\bar{4}$22	45.21
1.991	12	061	45.52
1.959	6	232	46.30
1.950	7	$\bar{3}$51	46.54
1.934	8	052,350	46.94
1.902	6	411,023	47.78
1.890	6	$\bar{2}$61,$\bar{4}$32	48.10
1.879	3	$\bar{4}$41	48.39
1.854	8	$\bar{5}$11,$\bar{3}$23	49.09
1.849	8	$\bar{2}$33	49.23
1.831	7	440	49.76
1.814	8	242	50.26
1.783	6	$\bar{3}$52	51.18
1.776	8	510,170	51.41
1.764	4	$\bar{4}$03,123	51.77
1.749	7	$\bar{1}$62,$\bar{4}$13	52.26
1.725	8	360,$\bar{2}$43,+	53.03

References

Cipriani, C. (1958). Manganese boussingaultite 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.

Ammonium Mercury Chloride, NH_4HgCl_3 (tetragonal) (revised)*

Sample

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_o=1.793, N_e=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]----------	4.20	7.96
NBS, sample at 25 °C-----	4.1977 ±.0001	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 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	4	106	75.25
1.2587	4	312	75.46
1.2366	2	303	77.05
1.2116	1	215	78.95
1.2081	3	116	79.22

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
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

References

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.

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution of $(NH_4)_2CrO_4$ 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", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.420 ±.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 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.31	16	020	14.03
6.04	12	001	14.66
5.45	40	011	16.26
5.28	7	$\bar{1}11$	16.78
5.18	25	120	17.11
4.530	25	200	19.58
4.358	18	021	20.36
4.269	95	$\bar{1}21$,210	20.79
4.227	100	111,$\bar{2}01$	21.00
4.003	8	$\bar{2}11$	22.19
3.811	75	130	23.32
3.657	19	121	24.32
3.508	4	$\bar{2}21$	25.37
3.449	18	031	25.81
3.406	16	$\bar{1}31$	26.14
3.226	10	201	27.63
3.152	14	040	28.29
3.124	14	211	28.55
3.041	40	$\bar{1}12$	29.35
2.977	8	$\bar{2}31$,140	29.99
2.936	10	310,012	30.42
2.908	8	$\bar{2}02$	30.72
2.872	18	221	31.12
2.805	15	$\bar{1}22$	31.88
2.772	7	$\bar{1}41$	32.27
2.753	8	$\bar{3}21$	32.50
2.722	6	320,022	32.88
2.638	3	$\bar{2}22$	33.96
2.597	6	112	34.51
2.579	6	141	34.75
2.556	8	231	35.08
2.525	4	$\bar{2}41$	35.53
2.470	20	$\bar{3}31$	36.34
2.451	7	330,032	36.64
2.427	2	150	37.01
2.399	3	311	37.45
2.388	3	$\bar{2}32$	37.64
2.326	3	$\bar{3}22$,051	38.67
2.280	3	321	39.49
2.252	15	241	40.01

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.230	4	410	40.41
2.202	6	250	40.95
2.193	7	$\bar{4}21,\bar{3}41$	41.12
2.178	16	340,042	41.43
2.163	6	$\bar{2}51$	41.72
2.131	12	420	42.39
2.112	2	222,331	42.77
2.079	2	$\bar{4}12$	43.49
2.061	2	$\bar{1}13,\bar{2}03$	43.90
2.033	3	$\bar{2}13$	44.54
2.011	4	003	45.05
2.001	3	$\bar{4}22$	45.29
1.984	5	061,$\bar{1}23$	45.70
1.976	5	$\bar{1}61$	45.88
1.944	6	$\bar{3}51$	46.68
1.934	7	350,052	46.93
1.914	9	$\bar{3}13$	47.47
1.903	6	$\bar{2}52,161$	47.75
1.880	3	$\bar{2}61,\bar{4}41$	48.37
1.863	4	$\bar{5}11$	48.85
1.849	7	$\bar{2}33$	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	$\bar{3}52$	51.37

References

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

Sample

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 $KZnF_3$ [Crocket and Haendler, 1960]

Lattice constants

	a(Å)
Crocket and Haendler[1960]	4.115
NBS, sample at 25°C	4.1162 ±.0001

Density

(calculated) 3.343 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.8$

References

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

CuKα_1 λ = 1.54056 Å; temp. 25 °C

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

Sample

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

Color

Colorless

Optical data

Biaxial (+) N_α=1.650, N_γ=1.738, 2V is small.

Structure

Monoclinic, I2/c (15), Z=4. The structure of $Ba(BrO_3)_2 \cdot H_2O$ was determined by Kartha [1953].

Lattice constants

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

Density

(calculated) 3.960 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 2.8$

Additional patterns

1. PDF card 16-247 [Weigel et al., 1962]. (In this reference and on the card, the formula was inadvertently given as $BaBrO_3 \cdot H_2O$).

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

d (Å)	I	hkl	2θ(°)
5.94	55	110	14.90
4.53	9	200	19.57
3.950	25	020	22.49
3.815	12	$\bar{1}12$	23.30
3.705	50	$\bar{2}11$	24.00
3.679	15	112	24.17
3.576	25	211	24.88
3.415	50	$\bar{1}21$	26.07
3.396	55	$\bar{2}02$	26.22
3.363	13	121	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	$\bar{2}22$	34.81
2.542	15	031	35.28
2.531	13	130	35.44
2.493	12	$\bar{3}12$,222	36.00
2.430	6	$\bar{1}23$	36.96
2.407	6	004	37.33
2.374	25	123	37.87
2.353	10	$\bar{3}21$	38.21
2.302	9	321	39.09
2.262	40	400,$\bar{1}14$	39.81
2.231	13	$\bar{2}31$	40.40
2.225	12	132	40.51
2.203	9	114,231	40.94
2.178	11	$\bar{2}04$	41.43
2.148	6	$\bar{4}11$	42.02
2.076	6	204	43.57
2.036	4	033	44.45
1.985	3	330	45.67
1.964	14	$\bar{3}23$,420	46.18
1.907	4	$\bar{2}24$	47.66
1.896	6	$\bar{1}41$	47.93
1.888	18	141	48.15
1.882	11	$\bar{2}33$,314	48.33
1.859	8	$\bar{3}32$	48.96
1.850	15	$\bar{4}22$	49.20
1.848	15	$\bar{4}13$	49.27

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 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	$\bar{1}34$,413	51.97
1.715	4	$\bar{1}25$	53.37
1.703	6	$\bar{4}31$	53.80
1.695	12	215	54.07
1.678	7	431	54.66
1.637	8	$\bar{3}41$,$\bar{5}21$	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	$\bar{3}25$	60.20
1.5267	4	044	60.60
1.5092	4	600	61.38
1.5032	5	334	61.65
1.4908	4	$\bar{2}35$	62.22
1.4848	8	$\bar{1}52$,206	62.50
1.4776	6	$\bar{6}11$,152	62.84
1.4644	8	$\bar{6}02$	63.47
1.4624	9	$\bar{2}44$,$\bar{5}14$	63.57
1.4526	6	611	64.05
1.4376	8	$\bar{4}42$	64.80
1.4340	7	$\bar{2}26$,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	$\bar{6}22$	68.26
1.3629	4	316,$\bar{2}53$	68.83
1.3534	5	$\bar{3}52$	69.38
1.3434	5	253	69.97
1.3348	5	352	70.49
1.3297	4	$\bar{5}41$	70.80

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.3170	4	060	71.58
1.3143	4	541	71.76
1.3094	7	$\bar{4}35$	72.07
1.3062	6	$\bar{6}31$	72.27
1.3010	6	154	72.61
1.2894	6	161,$\bar{4}51$	73.37
1.2784	4	451,217	74.10
1.2748	4	406	74.35
1.2545	4	435	75.76
1.2510	3	$\bar{7}12$,$\bar{5}43$	76.01
1.2339	4	$\bar{6}33$	77.26
1.2281	3	$\bar{7}21$,$\bar{2}62$	77.69
1.2244	5	$\bar{3}54$	77.97
1.2173	5	712,$\bar{3}27$	78.51
1.2139	4	$\bar{2}46$,543	78.77
1.2112	4	721,$\bar{1}63$	78.98
1.1992	4	640	79.93
1.1919	7	$\bar{2}37$,633,+	80.52
1.1887	6	624	80.78
1.1693	4	$\bar{7}23$	82.41
1.1658	5	$\bar{5}52$	82.71

References

Kartha, G.(1953). Structure of halogenates of the type $A(BO_3)_2 \cdot H_2O$, 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.

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

Color
Colorless

Optical data
Biaxial (+) N_α=1.564, N_β=1.58, N_γ=1.634, 2V is medium.

Structure
Monoclinic, I2/c (15), Z=4. The structure of $Ba(ClO_3)_2 \cdot H_2O$ 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 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	$\bar{1}12$	23.69
3.658	50	$\bar{2}11$	24.31
3.601	15	112	24.70
3.517	20	211	25.30
3.382	40	$\bar{1}21$	26.33
3.343	55	$\bar{2}02$	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	013	30.70
2.779	10	310	32.18
2.517	18	031	35.64
2.510	19	130,$\bar{2}$13	35.75
2.458	6	$\bar{3}12$	36.52
2.391	10	$\bar{1}23$	37.58
2.373	6	213	37.89
2.350	10	004	38.27
2.327	55	$\bar{3}21$	38.66
2.269	8	321	39.69
2.229	25	400,$\bar{1}$32	40.43
2.216	25	$\bar{1}14$	40.69
2.209	25	$\bar{2}31$	40.81
2.195	6	132	41.09
2.175	14	231	41.48
2.151	6	114	41.96
2.137	18	$\bar{2}04$	42.26
2.120	7	$\bar{4}11$	42.61
2.067	4	$\bar{4}02$	43.76
2.026	8	204	44.69
2.006	7	033	45.16
1.966	5	402	46.14
1.959	4	040	46.31
1.938	10	420,$\bar{3}$23	46.85
1.870	5	141	48.65

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.860	10	$\bar{2}33$	48.94
1.850	7	$\bar{3}14$	49.22
1.845	6	323	49.35
1.827	8	$\bar{4}22$,015	49.86
1.823	6	$\bar{4}13$	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	$\bar{1}34$,$\bar{2}15$	52.86
1.721	5	413	53.19
1.691	2	$\bar{2}42$	54.21
1.683	8	$\bar{4}31$,$\bar{1}25$	54.47
1.673	4	$\bar{4}04$	54.84
1.665	6	$\bar{5}12$	55.10
1.661	5	242	55.25
1.656	8	215,431	55.45
1.643	4	$\bar{1}43$	55.90
1.622	2	$\bar{3}41$	56.72
1.616	4	$\bar{5}21$	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	$\bar{3}34$,$\bar{4}24$	60.06
1.530	4	$\bar{1}16$	60.47
1.526	8	035	60.62
1.523	8	$\bar{4}33$	60.75
1.511	3	$\bar{3}25$	61.30
1.505	2	044	61.58
1.498	3	116	61.90
1.476	6	334	62.92

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.472	7	440,$\bar{3}43$,+	63.12
1.462	4	152,433	63.60
1.457	4	$\bar{6}11$	63.83
1.449	4	206	64.22
1.444	6	$\bar{6}02$,$\bar{2}44$	64.46
1.436	5	325	64.86
1.428	4	$\bar{5}32$	65.27
1.422	5	$\bar{4}42$,235	65.62
1.408	6	523,$\bar{2}26$,+	66.33
1.402	4	053,$\bar{3}16$	66.68
1.392	6	602	67.21
1.387	8	442	67.45
1.371	1	415	68.34
1.358	2	514,$\bar{6}13$	69.14
1.350	2	$\bar{1}45$	69.59
1.3408	2	$\bar{3}52$	70.13
1.3312	2	145,316	70.71
1.3234	6	017	71.19
1.3189	6	352	71.47
1.3062	2	060	72.27
1.2974	4	541,$\bar{1}54$	72.84
1.2910	6	$\bar{4}35$,$\bar{2}17$	73.26
1.2835	3	154	73.76
1.2784	4	161	74.10
1.2717	3	$\bar{4}44$	74.56
1.2681	4	$\bar{1}27$	74.81
1.2578	1	710	75.53

References

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

Kartha, G. (1952). Structure of barium chlorate monohydrate, $Ba(ClO_3)_2 \cdot H_2O$, Acta Cryst. **5**, 845 - 846.

Cadmium Imidazole Nitrate, $Cd(C_3H_4N_2)_6(NO_3)_2$ (hexagonal)

Sample
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, $R\bar{3}$ (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 °C	12.636 ±.001	15.044 ±.001

Density
(calculated) 1.544 g/cm³ 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 molecular structure of hexakis(imidazole) nickel(II) nitrate, $(C_3H_4N_2)_6Ni(NO_3)_2$, Acta Cryst. B25, 842-847.

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

d (Å)	I	hkl	2θ(°)
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	5	321	36.23
2.433	6	125	36.91
2.387	6	410	37.65
2.383	7	232	37.72
2.362	5	134	38.06
2.332	1	116	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	324	43.28
2.066	2	306	43.78
2.049	2	241	44.17
2.024	1	045	44.73
2.000	2	027	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 CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
1.907	1	217	47.65
1.901	1	152	47.80
1.853	1	018	49.13
1.824	1	600	49.95
1.811	1	244	50.33
1.787	1	431	51.07
1.779	2	208	51.30
1.771	2	505	51.57
1.753	3	137,520	52.12
1.741	2	514	52.51
1.730	2	416	52.89
1.712	2	128	53.47
1.690	1	407	54.23
1.659	1	161	55.33
1.654	1	523	55.50
1.633	1	327	56.30
1.616	1	119	56.92
1.599	<1	318	57.60
1.554	1	351	59.41
1.544	1	345	59.86
1.531	1	072	60.43
1.525	<1	164	60.68
1.519	<1	309	60.92
1.506	<1	443	61.50
1.490	<1	1·0·10,247	62.26
1.459	<1	615	63.71
1.450	1	0·2·10,517,+	64.16
1.437	<1	526	64.84
1.413	1	2·1·10	66.04
1.407	<1	624	66.40
1.392	1	713	67.18
1.369	<1	419	68.48
1.357	<1	0·1·11	69.18

Sample

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(Å)
Ludekens and Welch [1952]-------	4.523*
Klasens et al. [1953]----------	4.52
NBS, sample at 25 °C----------	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 ABF_3 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 ABF_3, Acta Cryst. **5**, 841.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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

Sample

The sample was prepared by treating Cs_2CO_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 Bergehoff [1956]	4.81*
NBS, sample at 25 °C	4.7990 ±.0002

* from kX

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
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
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	8	321	73.82
1.1996	1	400	79.90
1.1641	1	410	82.84
1.1314	3	330	85.82
1.0732	3	420	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.

Cesium Magnesium Chromium Oxide, $Cs_2Mg_2(CrO_4)_3$ (cubic)

Sample

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, $P2_13$ (198), Z=4, langbeinite type by analogy with langbeinite, $K_2Mg_2(SO_4)_3$, and similar sulfates. The structure of langbeinite was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
NBS, sample at 25 °C	10.5543 ±.0002

Density

(calculated) 3.742 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.2$

References

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409 - 413.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	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 CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*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	2	832	79.65
1.1952	2	752	80.25
1.1727	1	841	82.12
1.1657	2	910	82.72
1.1586	2	911	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	933	93.11
1.0555	1	10·0·0	93.73
1.0503	1	10·1·0	94.34
1.0452	1	10·1·1	94.94
1.0349	1	10·2·0	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

Cesium Magnesium Chromium Oxide Hydrate, $Cs_2Mg(CrO_4)_2 \cdot 6H_2O$ (monoclinic)

Sample

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_α=1.635, N_β=1.640, N_γ=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

$I/I_{corundum} = 2.2$

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. 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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
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	$\bar{1}11$	16.46
5.30	9	120	16.70
4.62	3	200	19.20
4.445	7	021	19.96
4.350	19	210	20.40
4.302	100	$\bar{2}01$,111	20.63
4.085	7	$\bar{2}11$	21.74
3.911	70	130	22.72
3.722	4	121	23.89
3.584	3	$\bar{2}21$	24.82
3.488	7	$\bar{1}31$	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	$\bar{1}12$	28.90
3.058	6	002,140	29.18
3.031	19	$\bar{3}11$	29.44
2.991	7	310	29.85
2.980	9	012	29.96
2.956	20	$\bar{2}02$	30.21
2.923	11	221	30.56
2.880	4	$\bar{2}12$	31.03
2.854	20	$\bar{1}22$	31.32
2.842	12	$\bar{1}41$	31.45
2.810	5	321	31.82
2.776	5	320	32.22
2.688	2	$\bar{2}22$	33.30
2.638	3	141	33.95
2.606	5	231	34.38
2.587	13	$\bar{2}41$	34.64
2.560	12	$\bar{1}32$	35.02
2.527	25	$\bar{3}31$	35.49
2.505	8	330,$\bar{3}12$	35.82
2.483	7	122	36.14

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.388	8	$\bar{4}01$,051	37.64
2.376	7	$\bar{3}22$,$\bar{1}51$	37.84
2.348	5	$\bar{4}11$	38.31
2.318	6	321	38.81
2.302	18	241	39.10
2.276	4	202	39.56
2.258	4	250	39.89
2.220	9	$\bar{2}51$	40.61
2.182	7	$\bar{2}42$	41.34
2.173	7	420	41.53
2.158	5	060	41.82
2.153	5	331,$\bar{4}02$	41.93
2.121	2	$\bar{4}12$	42.59
2.102	2	160	42.99
2.091	3	$\bar{1}13$,$\bar{4}31$	43.24
2.066	2	$\bar{2}13$	43.78
2.039	5	003	44.40
2.032	5	251	44.55
2.015	3	013,$\bar{1}23$,+	44.95
2.009	2	$\bar{1}52$	45.08
1.991	3	$\bar{3}51$,$\bar{2}23$	45.51
1.977	6	052	45.85
1.947	4	$\bar{2}52$,$\bar{3}13$,+	46.61
1.929	4	$\bar{2}61$	47.06
1.925	3	$\bar{4}32$	47.18
1.904	4	$\bar{1}33$	47.73
1.899	3	$\bar{5}11$,312,+	47.87
1.885	5	$\bar{3}23$	48.25
1.880	8	440	48.38
1.844	1	033	49.38
1.840	4	$\bar{5}21$,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,$\bar{3}33$	50.87
1.775	2	520,$\bar{3}61$,+	51.45
1.754	5	$\bar{5}31$,332	52.11
1.727	4	133,043	52.99
1.713	5	171	53.44
1.697	3	530	53.99
1.684	2	162,$\bar{3}43$,+	54.44
1.677	4	$\bar{5}32$	54.70
1.651	2	$\bar{5}41$,342	55.62
1.637	2	402	56.14

Copper Pyrazole Chloride, $Cu(C_3H_4N_2)_4Cl_2$ (monoclinic)

Sample

The sample was prepared by C. W. Reimann at NBS by evaporating an aqueous solution of $CuCl_2$ and pyrazole at room temperature.

Color

Unground: vivid purplish blue
Ground: brilliant purplish blue

Optical data

Biaxial(-) N_α=1.648, N_β=1.660, N_γ=1.670. 2V is large.

Structure

Monoclinic, C2/c (15), Z=4. Isostructural with $Ni(C_3H_4N_2)_4Cl_2$, the structure for which was determined by Reimann et al., [1967].

Lattice constants

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

Density

(calculated) 1.544 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 2.0$

References

Reimann, C.W., A.D. Mighell, and F.A.Mauer (1967). The crystal and molecular structure of tetrakispyrazole-nickel chloride $Ni(C_3H_4N_2)_4Cl_2$, Acta Cryst. **23**, 135-141.

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ (°)
7.30	70	$\bar{1}11$	12.12
6.58	20	002	13.45
6.10	12	$\bar{2}00$	14.52
6.03	9	$\bar{2}02$	14.69
5.78	40	111	15.32
4.60	5	020	19.30
4.348	4	112,021	20.41
4.314	6	$\bar{1}13$	20.57
4.035	5	$\bar{3}11$	22.01
3.813	14	$\bar{2}21$	23.31
3.770	8	022	23.58
3.663	100	$\bar{2}04,\bar{2}22$	24.28
3.413	6	$\bar{4}02$	26.09
3.245	6	$\bar{3}11$	27.46
3.201	1	$\bar{3}14$	27.85
3.171	1	023	28.12
3.046	3	400	29.30
3.015	2	$\bar{4}04$	29.60
2.888	4	222	30.94
2.830	4	$\bar{1}32$	31.59
2.781	5	312	32.16
2.741	6	$\bar{4}22$	32.64
2.722	2	$\bar{1}15$	32.88
2.690	2	$\bar{4}21$	33.28
2.674	6	024	33.49
2.609	5	$\bar{5}12$	34.34
2.603	8	$\bar{5}13,132$	34.42
2.534	19	$\bar{3}31$	35.40
2.520	14	$\bar{4}24,\bar{5}11$	35.59
2.444	10	$\bar{2}06$	36.75
2.439	5	$\bar{3}33$	36.82
2.389	4	313	37.62
2.384	5	402	37.70
2.352	9	$\bar{4}06$	38.23
2.346	10	133	38.34
2.337	9	421,$\bar{1}34$	38.49
2.311	3	$\bar{4}25$	38.94
2.296	4	331	39.20
2.239	2	$\bar{6}04$	40.25
2.173	3	224	41.52
2.159	3	$\bar{2}26$	41.81
2.150	3	240,$\bar{2}42$	41.98
2.094	2	134,$\bar{4}26$	43.16
2.054	3	$\bar{3}17$	44.06
2.033	6	$\bar{5}33$	44.52

Sample

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_2TiO_5 [Mumme and Wadsley, 1968]. The structure of Y_2TiO_5 was determined by Mumme and Wadsley [1968].

Lattice constants

	a(Å)	b(Å)	c(Å)
Mumme and Wadsley [1968]	10.48	11.33	3.76
NBS, sample at 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.]
2. 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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I *	hkl	2θ(°)
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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I* *	*hkl*	2θ(°)
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	3	550	60.10
1.5261	5	402,621	60.63
1.5188	5	361	60.95
1.5152	5	332	61.11
1.4863	2	640,071	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	811	77.60
1.2176	4	172,203	78.49
1.2111	4	632	78.99
1.1931	1	272,091	80.42
1.1880	3	033	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.

References

Mumme, W. G.,and A. D. Wadsley (1968). The structure of orthorhombic Y_2TiO_5, 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 Gd_2O_3-TiO_2, J.Res.NBS 69A,255-61.

Gallium Phosphate Hydrate, $GaPO_4 \cdot 2H_2O$ (monoclinic)

Sample

The sample was prepared by Alvin Perloff at NBS, from Ga_2O_3 dissolved in dilute H_3PO_4. This solution was then layered with water slightly alkaline with NH_4OH.

Color

Colorless

Optical data

Biaxial, N_α=1.605, N_γ=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, sample at 25 °C	9.77	9.64	9.68	102°42′
	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 $GaPO_4 \cdot 2H_2O$, Acta Cryst. **20**, 526-534.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ (°)
7.60	50	$\bar{1}01$	11.64
6.76	95	110,011	13.09
6.06	65	101	14.61
5.97	100	$\bar{1}11$	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	$\bar{1}12$	21.15
4.072	20	$\bar{1}21$	21.81
3.800	5	$\bar{2}02$	23.39
3.775	4	121	23.55
3.614	13	112	24.61
3.382	8	220	26.33
3.359	12	$\bar{2}21$	26.51
3.229	2	$\bar{3}01$	27.60
3.209	6	$\bar{1}03$	27.78
3.061	35	$\bar{3}11$	29.15
3.035	45	221,122	29.40
3.009	15	310	29.66
2.984	35	$\bar{2}22$	29.92
2.959	30	$\bar{1}31$	30.18
2.891	30	212	30.91
2.838	14	131	31.50
2.820	45	$\bar{3}12$,301	31.70
2.707	8	311	33.06
2.684	6	$\bar{3}21$	33.36
2.673	16	$\bar{1}23$	33.50
2.663	14	230	33.62
2.647	14	320,$\bar{1}32$	33.83
2.564	15	222	34.96
2.534	10	$\bar{3}03$	35.39
2.514	4	$\bar{2}23$	35.69
2.479	7	132	36.20
2.453	5	$\bar{2}32$,$\bar{3}13$	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	$\bar{1}41$	39.20
2.278	3	$\bar{3}31$,$\bar{4}12$	39.52
2.249	6	030	40.05

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.205	1	232	40.89
2.175	4	$\bar{4}21,\bar{3}32$	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	$\bar{4}22$	42.87
2.089	4	413	43.28
2.084	5	$\bar{3}14$	43.39
2.050	3	$241,\bar{1}42$	44.13
2.036	1	$\bar{2}42$	44.46
2.020	1	303	44.82
1.996	2	421	45.40
1.990	8	$\bar{3}33$	45.54
1.978	9	313	45.84
1.955	8	$\bar{4}23,402$	46.40
1.942	1	$\bar{4}31$	46.75
1.931	2	$\bar{3}41$	47.01
1.927	5	$\bar{1}43$	47.11
1.918	9	233,340	47.35
1.911	9	$\bar{5}11,430+$	47.53
1.901	6	$\bar{4}04,\bar{1}15$	47.81
1.887	7	$\bar{2}34,242$	48.18
1.881	6	$\bar{5}12$	48.34
1.866	4	$510,\bar{2}43+$	48.77
1.833	4	341	49.71
1.807	11	$\bar{5}21,224$	50.45
1.787	8	250	51.07
1.784	8	$\bar{5}13,052+$	51.16
1.779	7	$105,\bar{3}15+$	51.31
1.769	4	$520,\bar{4}24$	51.64
1.7587	3	025,511	51.95
1.7462	3	$\bar{3}43$	52.35
1.7278	2	$251,\bar{1}52$	52.95
1.7140	1	$\bar{4}41$	53.41
1.6944	10	$413,\bar{3}25$	54.08
1.6761	4	$521,\bar{2}44$	54.72
1.6549	6	$\bar{3}51$	55.48
1.6475	7	$\bar{5}32,350+$	55.75
1.6356	4	$530,\bar{4}34$	56.19
1.6211	6	441,423	56.74
1.6148	4	$\bar{6}02,\bar{3}52$	56.98
1.5997	1	$\bar{6}11,\bar{4}43$	57.57
1.5841	10	600,160+	58.19
1.5633	5	610,531	59.04
1.5547	10	522,016	59.40

Gold Potassium Cyanide, $AuK(CN)_2$ (hexagonal)

Sample

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_o=1.602, N_e=1.695

Structure

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

Lattice constants

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

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

d (Å)	I	hkl	2θ(°)
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	0·2·10	44.71
2.018	7	217	44.88
1.934	3	128	46.94
1.910	8	2·0·11	47.57
1.881	2	1·1·12	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 $CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
1.691	5	1·2·11	54.18
1.6857	14	226	54.38
1.6643	2	315	55.14
1.6177	7	2·0·14	56.87
1.5903	2	137	57.94
1.5786	4	401	58.41
1.5698	3	042	58.77
1.5495	3	229	59.62
1.5375	3	404	60.13
1.5143	2	045	61.15
1.5059	2	0·1·17	61.53
1.4646	3	0·0·18	63.46
1.4611	5	0·2·16,1·3·10	63.63
1.4577	4	407	63.80
1.4258	2	048	65.40
1.4160	2	3·1·11	65.91
1.4039	6	2·2·12	66.55
1.3798	1	410	67.87
1.3634	2	413	68.80
1.3553	3	4·0·10,1·0·9	69.27
1.3197	2	0·4·11	71.42

References

Rosenzweig, A.,and D.T. Cromer (1959). The crystal structure of $KAu(CN)_2$, Acta Cryst. **12**, 709-12.

Staritzky, E., and F. H. Ellinger (1956). Potassium gold dicyanide,$KAu(CN)_2$, Anal. Chem. (Crystallographic Data) **28**, 420-1.

Sample

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]*	15.33	6.50	20.08	104.26°
Keating & Berry [1953]	14.11	6.51	11.02	105°15'
Baur [1964]	14.072	6.503	11.041	105°34'
NBS, sample 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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ (°)
6.79	8	200	13.03
5.88	<2	110	15.06
5.56	8	011	15.94
5.49	11	$\bar{1}02$	16.14
5.41	3	$\bar{1}11$	16.36
5.33	7	002	16.62
4.90	100	$\bar{1}11$	18.10
4.87	50	$\bar{2}02$	18.19
4.56	9	102	19.44
4.20	<2	$\bar{1}12$	21.15
4.028	14	$\bar{2}11$	22.05
3.776	60	$\bar{3}11$	23.54
3.732	20	112,202	23.82
3.393	8	400	26.24
3.291	15	$\bar{4}02$,311	27.07
3.256	5	020	27.37
3.209	11	$\bar{1}13$	27.78
3.125	7	$\bar{2}13$	28.54
3.117	6	013,021	28.61
3.084	3	$\bar{1}21$	28.93
3.062	5	302	29.14
3.009	6	410	29.66
2.980	<2	121	29.96
2.937	4	$\bar{4}12$,220	30.41
2.905	<2	$\bar{3}13$	30.75
2.799	9	$\bar{1}22$	31.95
2.772	7	312	32.27
2.757	8	$\bar{1}04$	32.45
2.731	10	$\bar{5}02$,411	32.77
2.704	<2	$\bar{2}22$	33.10
2.665	3	$\bar{3}21$,004	33.60
2.649	7	122	33.81
2.643	9	320	33.89
2.625	8	$\bar{4}13$,$\bar{3}04$	34.13
2.564	<2	402	34.97
2.531	3	$\bar{3}22$	35.43
2.527	3	$\bar{2}14$	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 CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.434	5	$\bar{4}04,\bar{3}14$	36.90
2.399	4	023	37.46
2.346	2	420	38.33
2.336	2	$\bar{5}13$	38.50
2.314	11	$\bar{4}22,511$	38.89
2.277	2	204	39.54
2.190	<2	502	41.19
2.181	5	$\bar{6}12$	41.36
2.149	<2	$\bar{4}23,214$	42.00
2.117	<2	$\bar{1}31$	42.67
2.096	<2	$\bar{2}24$	43.12
2.081	7	$\bar{1}15$	43.44
2.063	2	413,304	43.84
2.054	2	$\bar{3}15$	44.06
2.023	5	015	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	$\bar{3}31$	46.18
1.951	8	$\bar{4}24$	46.51
1.931	6	115	47.03
1.913	5	$\bar{7}11,\bar{7}12$	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	$\bar{2}06,513$	49.48
1.826	2	$\bar{3}06,430+$	49.89
1.820	<2	$\bar{1}25$	50.08
1.804	2	$\bar{3}33$	50.55
1.800	3	133,$\bar{3}25$	50.66
1.780	<2	$\bar{4}06$	51.28
1.775	<2	006	51.44
1.758	<2	431,$\bar{8}02$	51.96
1.753	5	711	52.12
1.710	2	$\bar{5}06,\bar{6}24$	53.55
1.692	3	315	54.15

Additional patterns

1. Keating and Berry [1953]
2. 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 $FeSO_4 \cdot 7H_2O$ (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 $FeSO_4 \cdot 7H_2O$, Fortschr. Mineral. 26, 83 - 85.

Ness, I. (1940). Zum Gitterbau des monoklinen $FeSO_4 \cdot 7H_2O$ (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.

Lanthanum Nitrate Hydrate, $La(NO_3)_3 \cdot 6H_2O$ (triclinic)

Sample

The sample was obtained from Pfaltz and Bauer, Inc. Flushing, N.Y. The material was recrystallized from an aqueous solution at room temperature.

Color

Colorless

Optical data

Biaxial (-) N_α=1.458, N_β=1.552, N_γ=1.593
2V is small

Structure

Triclinic, $P\bar{1}$ (2),Z=2 [Iveronova et al., 1955].

Density

(calculated) 2.358 g/cm^3 at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.3

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

d (Å)	*I*	*hkl*	2θ(°)
8.71	25	100	10.15
6.70	100	$\bar{1}10$	13.20
6.389	45	001	13.85
5.985	60	011	14.79
5.749	40	$\bar{1}01$	15.40
5.443	40	$\bar{1}11$	16.27
5.254	40	020	16.86
5.046	40	$0\bar{1}1$	17.56
4.714	95	$\bar{1}\bar{1}1$,101	18.81
4.500	35	021,$\bar{1}$20	19.71
4.362	55	200	20.34
4.035	18	210	22.01
4.006	20	$\bar{2}01$	22.17
3.894	14	$\bar{2}11$	22.82
3.787	14	121	23.47
3.728	5	$0\bar{2}1$	23.85
3.591	4	$\bar{1}\bar{2}1$	24.77
3.508	4	030	25.37
3.383	20	$\bar{2}21$	26.32
3.355	20	031,$\bar{2}$20	26.55
3.256	35	$\bar{1}$12,130	27.37
3.232	25	012	27.58
3.191	10	002	27.94
3.062	14	$2\bar{1}1$	29.14
3.021	13	131,$\bar{2}\bar{2}$1	29.54
3.013	16	$\bar{1}22$	29.62
2.993	20	022	29.83
2.928	25	$\bar{1}\bar{1}2$	30.51
2.906	30	300,$0\bar{1}2$	30.74
2.872	8	$\bar{2}02$	31.11

Lattice constants

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

* from kX

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.849	20	$0\bar{3}1$	31.37
2.843	20	$11\bar{2}$	31.44
2.805	13	$3\bar{1}0,\bar{2}31$	31.88
2.797	8	$\bar{3}10$	31.97
2.722	13	$\bar{3}\bar{1}1,\bar{2}22$	32.88
2.677	8	$12\bar{2},2\bar{2}1$	33.45
2.660	25	$\bar{2}\bar{1}2$	33.66
2.626	19	040	34.12
2.617	25	$\bar{3}21$	34.24
2.612	20	$1\bar{1}2,041$	34.30
2.557	14	$\bar{1}41$	35.07
2.539	12	$\bar{1}\bar{2}2,\bar{3}20$	35.32
2.533	17	231	35.41
2.501	13	$\bar{2}31$	35.88
2.462	14	301	36.47
2.447	11	$141,\bar{3}\bar{2}1$	36.70
2.431	10	$\bar{2}32$	36.94
2.411	10	$\bar{3}02$	37.26
2.362	6	$\bar{2}\bar{2}2$	38.07
2.355	9	$3\bar{1}1,202$	38.18
2.323	16	$1\bar{2}2,\bar{2}41$	38.73
2.318	20	$\bar{3}31,\bar{3}22$	38.82
2.299	25	321	39.16
2.288	30	$2\bar{3}1$	39.35
2.274	12	222	39.60
2.254	20	$\bar{1}42,240$	39.96
2.231	7	$\bar{3}30,2\bar{1}2$	40.39
2.214	8	$\bar{1}13$	40.71
2.208	11	$\bar{4}01$	40.83
2.188	11	$\bar{4}11$	41.22

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.173	9	$\bar{1}\bar{3}2,\bar{1}03$	41.53
2.167	18	$1\bar{4}1,3\bar{2}1,+$	41.65
2.139	14	410	42.22
2.133	20	$\bar{4}10$	42.33
2.129	19	$\bar{3}32,003$	42.43
2.118	17	051,023	42.66
2.105	7	142	42.92
2.091	14	$\bar{2}03,\bar{2}41,+$	43.24
2.078	10	$\bar{2}23$	43.51
2.060	7	$\bar{2}\bar{3}2$	43.92
2.043	15	$2\bar{2}2$	44.30
2.011	6	$\bar{4}12,\bar{4}20$	45.04
2.008	9	113	45.12
2.004	10	$\bar{4}02$	45.20
1.994	5	$033,\bar{4}21$	45.46
1.982	6	$\bar{2}\bar{1}3$	45.73
1.967	4	$123,3\bar{1}2$	46.12
1.960	9	$\bar{2}33,2\bar{4}1$	46.28
1.947	7	$401,\bar{3}40,+$	46.62
1.933	8	052	46.98
1.929	5	$\bar{4}\bar{1}2$	47.07
1.915	5	$\bar{3}42$	47.44
1.890	6	$\bar{2}50$	48.11
1.884	9	$3\bar{1}2,\bar{1}\bar{2}3$	48.26
1.868	9	$133,\bar{3}\bar{4}1,+$	48.71

References

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

Sample

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_α=1.430, N_β=1.567, N_γ=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, sample at 25 °C	8.39	5.00	6.21	114.5°
	8.359 ±.001	4.9767 ±.0004	6.194 ±.001	114°43′ ±1′

Density

(calculated) 2.096 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 0.9

Additional patterns

1. PDF card 9-359, [Zemann, 1957].

References

Zemann, J. (1957). Die Kristallstruktur von Li_2CO_3, Acta Cryst. 10, 664-666.

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.164	85	110	21.32
3.797	19	200	23.41
3.029	25	111	29.46
2.918	80	$\bar{2}02$	30.61
2.812	100	002	31.80
2.627	30	$\bar{1}12$	34.10
2.488	18	020	36.07
2.431	40	$\bar{3}11$	36.95
2.276	20	021	39.57
2.256	12	310	39.92
2.116	4	112,$\bar{2}21$	42.69
2.081	7	220	43.44
2.012	2	$\bar{4}02$	45.02
1.910	2	202	47.56
1.893	2	$\bar{2}22$	48.02
1.867	17	311	48.74
1.8205	1	221	50.06
1.8121	4	$\bar{3}13$	50.31
1.6208	4	130	56.75
1.5959	7	$\bar{4}21$,$\bar{1}31$	57.72
1.5858	2	$\bar{2}23$	58.12
1.5804	4	113	58.34
1.5723	4	$\bar{5}12$	58.67
1.5652	8	$\bar{5}11$,$\bar{4}22$	58.96
1.5469	10	$\bar{2}04$	59.73
1.5154	6	222	61.10
1.5092	5	420	61.38
1.4980	1	023	61.89
1.4669	4	$\bar{5}13$	63.35
1.4622	3	$\bar{1}32$	63.58
1.4359	1	$\bar{1}14$	64.88
1.4250	5	$\bar{3}31$	65.44
1.4066	<1	004	66.41
1.3923	2	$\bar{6}02$	67.18
1.3879	1	330	67.42
1.3754	1	$\bar{3}32$	68.12
1.3529	1	132	69.41
1.3497	<1	421	69.60
1.3361	1	402	70.41
1.3132	1	$\bar{2}24$	71.83
1.3042	<1	$\bar{5}14$	72.40
1.2872	1	511	73.51
1.2842	3	$\bar{1}33$	73.71
1.2807	3	331	73.95
1.2655	3	600	74.99

Sample

The sample was prepared by dehydrating $MnCl_2 \cdot 4H_2O$ in vacuum above 650 °C.

Color

Unground: deep pink
Ground: light pink

Optical data

Uniaxial(-) N_o=1.708, N_e=1.622

Structure

Hexagonal, $R\bar{3}m$ (166), Z=3, isostructural with $CdCl_2$ and $NiCl_2$ [Ferrari et al., 1963]. The structure of $CdCl_2$ was determined by Pauling and Hoard [1930].

Lattice constants

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

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

d (Å)	I	hkl	2θ(°)
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
1.7663	13	113	51.71
1.5074	10	024	61.46
1.4638	10	0·0·12	63.50
1.4299	5	0·1·11	65.19
1.2959	6	208	72.94
1.1713	6	0·0·15	82.24
1.1488	8	1·1·12	84.21
1.0617	3	128	93.02
1.0390	3	1·0·16	95.70

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]

References

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 $CoCl_2$-$FeCl_2$ e $MnCl_2$-$FeCl_2$ anidri. Atti reale accad. naz. Lincei [6] **9**, 782 - 789.

Ferrari, A., A. Braibanti and G. Bigliardi (1963). Refinement of the crystal structure of $NiCl_2$ 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.

Nickel Pyrazole Chloride, $Ni(C_3H_4N_2)_4Cl_2$ (monoclinic)

Sample

The sample was prepared by C. W. Reimann at NBS by evaporating an aqueous solution of $NiCl_2$ and pyrazole at room temperature.

Color

Unground: deep blue
Ground: light greenish blue

Optical data

Biaxial, N_α=1.636, N_β=1.654, N_γ=1.670
2V is large.

Structure

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

Lattice constants

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

Density

(calculated) 1.613 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 1.9$

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

d (Å)	I	hkl	2θ(°)
7.40	100	110	11.95
6.43	16	002	13.75
6.18	14	200	14.31
6.02	18	$\bar{2}02$	14.70
5.78	8	111	15.33
5.679	30	$\bar{1}12$	15.59
4.624	8	020	19.18
4.362	5	021	20.34
4.320	8	112	20.54
4.249	5	$\bar{1}13$	20.89
4.103	3	$\bar{3}11$	21.64
4.066	7	$\bar{3}12$	21.84
3.849	18	$\bar{2}21$	23.09
3.762	10	022	23.63
3.703	70	220,202	24.01
3.670	45	$\bar{2}22$	24.23
3.597	10	$\bar{2}04$	24.73
3.466	9	$\bar{4}02$	25.68
3.346	4	113	26.62
3.270	5	311	27.25
3.181	3	$\bar{3}14$	28.03
3.149	5	023	28.32
3.010	4	$\bar{4}04$	29.65
2.992	3	130,$\bar{1}31$	29.84
2.891	2	222	30.90
2.839	4	$\bar{2}24$,$\bar{1}32$	31.49
2.788	5	312	32.08
2.708	5	$\bar{3}15$	33.05
2.637	6	$\bar{5}13$	33.97
2.593	4	$\bar{1}33$	34.56
2.572	7	420	34.85
2.550	16	$\bar{3}32$	35.17
2.524	7	$\bar{4}24$	35.54
2.491	3	223	36.02
2.448	6	$\bar{2}25$,$\bar{3}33$	36.68

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.440	6	204	36.81
2.398	8	402	37.48
2.359	10	421	38.11
2.324	8	$\bar{1}34,\bar{3}16,+$	38.72
2.281	6	$\bar{3}34,041$	39.48
2.261	3	$\bar{6}04$	39.83
2.161	5	$\bar{2}42$	41.76
2.124	4	$332,\bar{2}26,+$	42.52
2.077	5	$\bar{4}26$	43.54
2.064	6	600,314	43.82
2.034	7	$\bar{6}24$	44.51
1.996	4	$\bar{5}34$	45.40
1.979	4	512	45.81
1.948	4	$026,\bar{2}44$	46.58
1.928	6	333,714,+	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	$\bar{7}11,150$	49.70
1.796	3	$\bar{7}16$	50.80
1.763	4	$\bar{2}08,621$	51.80
1.736	3	710	52.67
1.732	2	152	52.82
1.714	2	$\bar{3}37,\bar{3}52$	53.42
1.689	3	$\bar{8}02$	54.28
1.677	3	$\bar{4}28$	54.69
1.672	4	226	54.87
1.662	4	$\bar{2}46$	55.21

References

Reimann, C.W., A.D. Mighell, and F.A.Mauer (1967). The crystal and molecular structure of tetrakispyrazole-nickel chloride $Ni(C_3H_4N_2)_4Cl_2$, Acta Cryst. **23**, 135-141.

Sample

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

Color

Colorless

Optical data

Isotropic, N=1.528

Structure

Cubic, Fm3m (225), NaCl type, Z=4. This 1:1 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

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

d (Å)	*I*	*hkl*	2θ(°)
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

Potassium Cadmium Fluoride, $KCdF_3$ (orthorhombic)

Sample

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 ≅ 1.464

Structure

Orthorhombic, Pnma (62) Z=4, distorted perovskite, by analogy with $RbCaCl_3$ and other ABX_3 compounds. $KCdF_3$ 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]-----	4.293*		
Klasens et al. [1953]-----------	4.33**		
Martin et al. [1956]-----------	4.33**		
NBS, sample at 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 $KCdF_3$ e $KCaF_3$, Ann. Chim. Rome **42**, 356-60.

Klasens, H. A., P. Zalm, and F. O. Huysman (1953). The manganese emission in ABF_3 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

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

d (Å)	I	hkl	2θ(°)
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	231,132	45.65
1.936	20	141,301	46.90
1.933		222	46.96
1.7669	30	321,042	51.69
1.7638	30	123	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	2	404	90.91
1.0508	3	181,460,+	94.28
1.0485	3	064,424	94.55
1.0209	4	082,600	97.97
1.0182	5	325	98.31
.9932	1	462	101.71
.9685	2	282	105.38
.9673	2	444	105.56
.9449	3	622,183	109.22
.9431	3	345	109.52
.9229	2	561,640	113.16
.9216	2	165	113.40

Additional patterns

1. Brisi [1952]

Sample

The sample was prepared by melting an equimolar mixture of K_2CO_3 and $CaCO_3$ at about 900 °C. The sample was slightly unstable.

Color

Colorless

Optical data

Uniaxial (-) N_O=1.532, N_e=1.478

Structure

Hexagonal, $P6_3/mmc$ (194), $P6_3mc$ (186) or $P\bar{6}2c$ (190), Z=2, [Mrose et al., 1967]

Lattice constants

	a(Å)	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 ±.001	13.355 ±.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 buetschliite, $K_2Ca(CO_3)_2$ [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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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.) $K_2CO_3 \cdot CaCO_3$, buetschliite(n.sp.) $3K_2CO_3 \cdot 2CaCO_3 \cdot 6H_2O$ and calcite, $CaCO_3$, 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.

Potassium Calcium Fluoride, $KCaF_3$ (orthorhombic)

Sample

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 $NaMnF_3$ and $CaZrO_3$. $KCaF_3$ has been reported as cubic [Brisi, 1952], as pseudocubic [Klasens et al., 1953] and as monoclinic [Ludekens and Welch, 1952].

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
Brisi [1952]-----	8.742*		
Ludekens and Welch [1952]-----	8.82**	8.82**	8.82**
Klasens et al. [1953]----------	4.37		
NBS, sample at 25 °C----------	6.209 ±.001	8.757 ±.001	6.164 ±.001

* as published

** from kX and with β=92°36′

Density

(calculated) 2.699 g/cm³ 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 cristallina dei composti $KCdF_3$ e $KCaF_3$, Ann. Chim. Rome **42**, 356-360.

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

Klasens, H. A., P. Zalm, and F. O. Huysman (1953). The manganese emission in ABF_3 compounds, Philips Res. Rept. **8**,441-451.

Internal standard W, a = 3.16516 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
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

Sample

The sample was obtained by using the first crystals formed by evaporation of a water solution of KCl and an excess of $MgCl_2$.

Color

Colorless

Optical data

Biaxial(+) N_α=1.468, N_β=1.47, N_γ=1.495, 2V is large.

Structure

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

Lattice constants

	a(Å)	b(Å)	c(Å)
Leonhardt [1928]- Andress and Saffe [1939]	16.08	22.25	9.53
	16.02	22.52	9.54
Fischer [1965]	16.141	22.519	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

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.76	7	111	11.40
5.56	5	131	15.93
5.49	4	230	16.12
4.79	17	002	18.49
4.691	30	301	18.90
4.650	20	141	19.07
4.616	14	240	19.21
4.057	8	212	21.89
3.980	8	331,410	22.32
3.954	8	151	22.47
3.865	40	222	22.99
3.800	35	420	23.39
3.751	70	060	23.70
3.614	65	232	24.61
3.603		341	24.69
3.562	70	142	24.98
3.553		430	25.04
3.324	100	242	26.80
3.281	70	440	27.16
3.229	3	332	27.60
3.103	3	441,113	28.75
3.061	8	501,412	29.15
3.049	12	071	29.27
3.038	65	252	29.38
3.013	25	123	29.62
3.004	30	450	29.72
2.977	25	422	29.99
2.935	80	033	30.43
2.929		361	30.49
2.887	8	133	30.95
2.855	30	432,271	31.30
2.837	8	531	31.51
2.747	12	460,303	32.57
2.736	12	143	32.70
2.728	10	313	32.80
2.694	35	600	33.23
2.663	11	181	33.63
2.643	6	461	33.89
2.633	8	172	34.02
2.578	3	333	34.77

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
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	8	082	37.03
2.399	8	182	37.45
2.393	25	191,372,+	37.56
2.346	35	602,353	38.34
2.324	20	282	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	18	671,064	44.89
2.011	18	810	45.04
1.990	40	662	45.55
1.985		434,633,+	45.67
1.974	13	473,2•10•2	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 $KCl \cdot MgCl_2 \cdot 6H_2O$, Deut. Mineral. Ges. Sektion für Kristallk., Marburg Program, October 1965.

Leonhardt, J. (1928). Das Raumgitter des Carnallits, Z. Krist. **66**, 506-507.

Sample

The sample was made by heating a mixture of K_2CrO_4 and $MgCrO_4$ at 510 °C for one half hour in nitrogen.

Color

Vivid yellow

Optical data

Isotropic, N=1.864

Structure

Cubic, $P2_13$ (198), Z=4, langbeinite type by analogy with langbeinite, $K_2Mg_2(SO_4)_3$, and similar sulfates. The structure of langbeinite was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	10.3684 ±.0002

Density

(calculated) 2.829 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.4

References

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409-413.

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

d (Å)	I	hkl	2θ(°)
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	5	511	45.40
1.926	5	420	47.15
1.893	3	521	48.03
1.8051	11	522	50.52
1.7778	3	530	51.35
1.7524	6	531	52.15
1.7278	6	600	52.95
1.7046	6	610	53.73
1.6820	16	611	54.51
1.6394	4	620	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 CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ (°)
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

Sample

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 (+) N_α=1.460, N_β=1.462, N_γ=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].

Lattice constants

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

* 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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	$\bar{2}01$	21.85
3.859	7	$\bar{2}11$	23.03
3.706	100	130	23.99
3.583	9	121	24.83
3.383	5	$\bar{2}21$	26.32
3.362	12	031	26.49
3.307	12	$\bar{1}31$	26.94
3.164	40	201	28.18
3.063	70	211,040	29.13
2.995	20	230	29.81
2.964	60	$\bar{1}12$,002	30.13
2.895	7	140	30.86
2.882	10	$\bar{2}31$,012	31.00
2.863	30	$\bar{3}11$	31.22
2.853	11	310	31.33
2.813	40	221,$\bar{2}02$	31.78
2.740	25	$\bar{2}12$	32.65
2.733	12	$\bar{1}22$	32.74
2.690	9	$\bar{1}41$	33.28
2.668	4	022	33.56
2.654	9	$\bar{3}21$	33.75
2.555	2	$\bar{2}22$,112	35.09
2.516	8	141,240	35.66
2.503	15	231	35.85
2.446	12	$\bar{2}41$,$\bar{1}32$	36.71
2.398	10	032	37.47
2.388	45	$\bar{3}31$	37.64
2.265	8	051	39.77
2.248	6	$\bar{1}51$,$\bar{3}22$	40.07
2.220	5	$\bar{4}11$	40.61
2.199	25	132,400	41.00
2.175	5	212	41.49
2.165	4	410,$\bar{1}42$	41.68

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.129	12	042	42.42
2.122	11	$\bar{3}41$	42.56
2.118	11	$\bar{4}21,340$	42.66
2.098	5	$\bar{2}51$	43.07
2.070	19	$\bar{2}42,420$	43.69
2.015	2	$\bar{1}13$	44.96
2.004	3	$\bar{4}12,\bar{2}03$	45.22
1.987	3	142	45.62
1.975	11	$\bar{4}31,003$	45.90
1.936	8	$\bar{1}23,430$	46.89
1.912	2	$\bar{1}52$	47.52
1.896	4	$\bar{3}42$	47.95
1.888	9	052,341	48.17
1.883	9	$\bar{3}51$	48.30
1.879	7	350,023	48.41
1.854	9	$161,\bar{3}13$	49.09
1.824	10	$\bar{2}61$	49.95
1.799	9	$\bar{2}33,\bar{5}11$	50.70
1.786	9	440	51.09
1.753	3	123	52.13
1.741	8	510	52.53
1.729	2	431	52.91
1.717	3	170,261	53.32

Additional patterns

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

References

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 $MgK_2(SO_4)_2 \cdot 6H_2O$, 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 $R_2M(SO_4)_2 \cdot 6H_2O$, J. Chem. Soc.,63, 337-423.

Sample

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_α= 1.77, N_β= 2.27, N_γ= 2.34
2V= 26° [Evans and Block, 1966]

Structure

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

Lattice constants

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

Density

(calculated) 3.349 g/cm³ at 25° C.

Additional patterns

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

References

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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	$\bar{2}01$,021	27.86
2.993	14	$\bar{2}11$	29.83

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

d (Å)	I	hkl	2θ(°)
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	$\bar{2}21$	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	$\bar{3}01$,012	37.91
2.356	9	221	38.16
2.281	5	$\bar{3}11$,131	39.47
2.251	4	230	40.03
2.197	17	$\bar{2}02$	41.05
2.166	5	320	41.67
2.149	5	301	42.01
2.124	7	$\bar{2}12$	42.53
2.064	7	$\bar{3}21$	43.83
1.996	20	122,231	45.41
1.946	7	$\bar{2}22$	46.64
1.913	4	212,321	47.50
1.897	4	400	47.91
1.886	5	$\bar{3}02$	48.22
1.848	7	$\bar{4}01$	49.27
1.804	6	$\bar{4}11$	50.54
1.778	7	222	51.33
1.728	4	420,$\bar{2}32$	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	3	500,$\bar{2}42$	61.01
1.5028	5	$\bar{5}01$	61.67
1.4934	5	510	62.10
1.4797	5	$\bar{5}11$	62.74
1.4270	7	213,520	65.34
1.4037	7	501,412	66.56
1.3870	8	$\bar{4}41$	67.47
1.3706	5	$\bar{3}51$,133	68.39
1.3476	4	422	69.72
1.3310	5	521	70.72

Rubidium Calcium Fluoride, $RbCaF_3$ (cubic)

Sample

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]-------	4.452*
Klasens el al. [1953]----------	4.46
NBS, sample at 25 °C----------	4.4560 ±.0001

* from kX

Density

(calculated) 3.426 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 4.5$

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
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 ABF_3, Acta Cryst. **5**, 841.

Klasens, H. A., P. Zalm and F. O. Huysman (1953). The manganese emission in ABF_3 compounds, Philips Res. Rept. **8**, 441-451.

Sample

The sample was prepared by adding an aqueous solution of $CoCl_2$ 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]----------	4.062
Crocket and Haendler [1960]-----	4.141
NBS, sample at 25 °C----------	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
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.132	1	100	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
.8812	2	332	121.88

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.

Rubidium Cobalt Sulfate, $Rb_2Co_2(SO_4)_3$ (cubic)

Sample

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, $P2_13$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The structure of langbeinite, $K_2Mg_2(SO_4)_3$ 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

$I/I_{corundum} = 3.4$

References

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

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. **10**, 409-413.

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	2	444	64.35
1.4313	2	632	65.12
1.4168	2	710	65.87
1.4030	1	711	66.60
1.3894	1	640	67.34

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
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	811	77.28
1.2243	1	733	77.98
1.2150	1	820	78.69
1.2063	3	821	79.37
1.1976	2	653	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	2	930	93.65
1.0505	<1	931	94.30
1.0391	1	852	95.68
1.0336	1	932	96.36
1.0174	<1	940	98.42
1.0125	1	941	99.07
1.0073	1	933	99.76

Rubidium Copper Sulfate Hydrate, $Rb_2Cu(SO_4)_2 \cdot 6H_2O$ (monoclinic)

Sample

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 (+) N_α=1.488, N_β=1.491, N_γ=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

$I/I_{corundum} = 1.6$

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 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 $R_2M(SO_4)_2 \cdot 6H_2O$, J. Chem. Soc. **63**, 337-423.

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.24	5	110	12.21
6.18	2	020	14.31
5.21	3	$\bar{1}11$	17.00
4.47	13	200	19.86
4.31	25	021	20.58
4.20	100	111,210,+	21.12
4.149	95	$\bar{2}01$	21.40
3.928	5	$\bar{2}11$	22.62
3.745	100	130	23.74
3.625	10	121,220	24.54
3.350	18	$\bar{1}31$	26.59
3.205	35	201	27.81
3.094	40	040	28.83
3.029	40	131,230	29.46
3.013	50	$\bar{1}12$	29.62
2.920	12	012,$\bar{3}11$,+	30.59
2.895	15	310	30.86
2.869	25	$\bar{2}02$	31.15
2.845	25	221	31.42
2.792	6	$\bar{2}12$	32.03
2.775	20	$\bar{1}22$	32.23
2.749	4	041	32.54
2.723	12	$\bar{1}41$	32.87
2.702	12	022,$\bar{3}21$	33.13
2.683	6	320	33.37
2.603	6	$\bar{2}22$	34.43
2.542	7	141,240	35.28
2.531	8	231	35.44
2.480	12	$\bar{1}32$,$\bar{2}41$	36.19
2.426	45	$\bar{3}31$,032	37.03
2.301	7	$\bar{4}01$	39.11
2.288	16	$\bar{3}22$,051	39.34
2.265	5	$\bar{4}11$	39.76
2.258	9	321	39.90
2.233	15	400,202	40.35
2.224	30	132,241	40.52
2.197	3	410,212	41.04
2.163	5	250,151	41.73
2.155	10	$\bar{3}41$,042	41.88
2.123	10	$\bar{2}51$	42.54

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.100	25	420,222	43.03
2.074	<2	$\bar{4}02$	43.61
2.061	2	060	43.90
2.047	5	$\bar{4}12,\bar{1}13$	44.21
2.039	5	$\bar{2}03$	44.39
2.009	6	142,160,+	45.09
2.002	13	003	45.26
1.976	<2	013	45.89
1.966	3	$\bar{4}22,\bar{1}23$	46.13
1.957	3	251	46.36
1.928	3	$\bar{3}42$	47.11
1.909	12	$\bar{3}51,052,+$	47.59
1.903	8	350,023	47.74
1.889	8	$\bar{3}13$	48.13
1.874	2	$\bar{2}52$	48.54
1.854	10	$\bar{4}32,\bar{1}33$	49.11
1.847	10	$\bar{4}41,\bar{2}61,+$	49.31
1.827	5	$\bar{2}33,\bar{3}23$	49.87
1.810	10	440,242	50.36
1.800	4	033,322	50.67
1.775	8	$\bar{5}21,123$	51.44
1.770	10	510	51.60
1.745	2	$\bar{3}52$	52.38
1.7315	3	351	52.83
1.7111	7	332	53.51
1.6895	3	$\bar{5}31,133,+$	54.25
1.6866	5	$\bar{5}22,\bar{4}51$	54.35
1.6730	2	$\bar{2}62,\bar{4}23$	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,$\bar{2}71$	56.57
1.6131	3	$\bar{5}32,223$	57.05

Sample

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 [Goldschmidt, 1926].

Lattice constants

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

*as published.

Density

(calculated) 3.844 g/cm³ at 25° C.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ (°)
3.262	65	111	27.32
2.823	100	200	31.67
1.998	50	220	45.36
1.703	25	311	53.77
1.6311	13	222	56.36
1.4130	6	400	66.07
1.2967	7	331	72.89
1.2637	11	420	75.11
1.1536	6	422	83.78
1.0876	4	511	90.18
0.9990	4	440	100.90
.9553	1	531	107.47
.9420	4	600	109.72
.8937	2	620	119.07
.8619	2	533	126.69
.8520	3	622	129.39
.8156	1	444	141.60
.7914	2	551	153.48
.7837	<1	640	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.

Sample

The sample was prepared at room temperature by slow evaporation of a 1:3 molar solution of Rb_2SO_4 and $FeSO_4$. The first crystals formed were used.

Color

Pale green

Optical data

Biaxial (+) N_α=1.480, N_β=1.489, N_γ=1.501
2V is large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2
$Rb_2Fe(SO_4)_2 \cdot 6H_2O$ 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	9.218 ±.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

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.21	8	110	12.26
6.25	2	020	14.17
6.02	2	001	14.71
5.24	2	$\bar{1}11$	16.90
5.11	2	120	17.35
4.44	10	200	19.99
4.33	15	021	20.49
4.19	85	111,210	21.20
4.15	100	$\bar{2}01$	21.40
3.771	80	130	23.57
3.616	7	220	24.60
3.424	2	031	26.00
3.374	14	$\bar{1}31$	26.39
3.182	25	201	28.02
3.124	25	040	28.55
3.082	20	211	28.95
3.040	50	131,230	29.36
3.027		$\bar{1}12$	29.48
2.945	2	140	30.33
2.913	13	$\bar{3}11$	30.67
2.877	30	310	31.06
2.837	17	221	31.51
2.806	13	$\bar{2}12$	31.87
2.794	18	$\bar{1}22$	32.01
2.747	8	$\bar{1}41$	32.57
2.701	2	$\bar{3}21$	33.14
2.674	2	320	33.48
2.614	3	$\bar{2}22$	34.28
2.556	6	141,240	35.08
2.528	6	231	35.48
2.495	12	$\bar{2}41,\bar{1}32$	35.96
2.434	45	122,$\bar{3}31$	36.90
2.308	10	051	38.99
2.300	12	$\bar{3}22$	39.14
2.255	9	$\bar{4}11$	39.95

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
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	$\bar{2}51$	42.16
2.117	11	$\bar{2}42$	42.67
2.089	11	420	43.27
2.049	4	$\bar{2}03$	44.16
2.008	10	$\bar{4}31$,003	45.12
1.967	5	251	46.12
1.938	3	$\bar{3}42$	46.84
1.923	10	052	47.23
1.912	5	023	47.52
1.897	7	$\bar{3}13$,411	47.91
1.863	13	$\bar{1}33$,$\bar{2}61$	48.85
1.835	2	$\bar{3}23$,421	49.64
1.824	3	$\bar{5}11$	49.96
1.8088	10	440,033	50.41
1.7922	1	322	50.91
1.7756	4	123	51.42
1.7575	6	$\bar{3}52$,510	51.99
1.7437	3	$\bar{3}33$,431,+	52.43
1.7345	5	351,$\bar{5}12$	52.73
1.7072	7	520,332	53.64
1.6923	4	133	54.15

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 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 $R_2M(SO_4)_2 \cdot 6H_2O$, J. Chem. Soc. 63, 337-423.

Sample

The sample was made by heating a 1:2 mixture of Rb_2CrO_4 and $MgCrO_4$ at 500 °C for 45 minutes in nitrogen.

Color

Vivid greenish yellow

Optical data

Isotropic, N=1.885

Structure

Cubic, $P2_13$ (198), Z=4, langbeinite type by analogy with langbeinite, $K_2Mg_2(SO_4)_3$, 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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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 CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
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

References

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409-413.

Sample

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_α=1.635, N_β=1.630, N_γ=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", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.474 ±.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

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.40	35	110	11.95
6.28	4	020	14.09
6.03	9	001	14.67
5.24	7	$\bar{1}11$	16.89
4.58	10	200	19.35
4.36	9	021	20.34
4.263	50	$\bar{1}11$	20.82
4.213	85	$\bar{2}01$	21.07
3.810	100	130	23.33
3.702	9	220	24.02
3.673	4	$\bar{1}21$	24.21
3.501	5	$\bar{2}21$	25.42
3.445	5	031	25.84
3.388	12	$\bar{1}31$	26.28
3.266	20	201	27.28
3.161	35	211	28.21
3.142		040	28.38
3.095	25	230	28.82
3.077	25	$\bar{1}31$	28.99
3.026	40	$\bar{1}12$	29.49
2.975	40	$\bar{3}11$, 140	30.01
2.936	8	012	30.42
2.897	9	$\bar{2}21$	30.84
2.887	35	$\bar{2}02$	30.95
2.813	8	$\bar{2}12$	31.78
2.793	20	$\bar{1}22$	32.02
2.761	13	$\bar{1}41$	32.40
2.746	8	320	32.58
2.623	5	$\bar{2}22$	34.15
2.590	6	240	34.60
2.577	8	$\bar{2}31$	34.79
2.518	17	$\bar{2}41$	35.62
2.503	20	$\bar{1}32$	35.85
2.471	35	$\bar{3}31$	36.33
2.460	12	122	36.50
2.321	20	051	38.76
2.317	20	322	38.84
2.310	13	$\bar{4}11$	38.96
2.289	15	400	39.33
2.264	25	241	39.78

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.232	10	212	40.37
2.204	12	250	40.91
2.193	9	$\bar{3}41$	41.13
2.180	12	042	41.39
2.160	12	$\bar{2}51$	41.79
2.149	19	420	42.00
2.134	18	331,222	42.32
2.126	13	$\bar{2}42$	42.48
2.095	5	060	43.14
2.076	5	$\bar{4}12$	43.55
2.050	6	$\bar{4}31,\bar{2}03$	44.15
2.015	11	003	44.95
1.992	5	251	45.50
1.978	4	$\bar{1}23,401$	45.84
1.953	6	411,$\bar{3}42$	46.47
1.942	8	$\bar{3}51$	46.74
1.933	7	052	46.98
1.903	10	$\bar{3}13,161$	47.76
1.876	7	$\bar{2}61$	48.49
1.866	8	$\bar{1}33$	48.75
1.850	12	440,113	49.21
1.841	6	$\bar{2}33,\bar{3}23$	49.48
1.812	8	$\bar{5}21,510$	50.32
1.792	6	123	50.92
1.764	10	261,170	51.79
1.753	6	$\bar{4}03$	52.14
1.742	9	332	52.49
1.717	7	$\bar{4}51,\bar{2}43$	53.32
1.707	8	133	53.64
1.677	10	530	54.67
1.673	12	441	54.82
1.669	6	171	54.96
1.641	10	$\bar{3}43,\bar{5}32$	56.00
1.621	6	$\bar{5}41$	56.76
1.617	5	$\bar{4}33$	56.88

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. 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.

Rubidium Magnesium Sulfate Hydrate, $Rb_2Mg(SO_4)_2 \cdot 6H_2O$ (monoclinic)

Sample

The sample was prepared at room temperature by slow evaporation of an equimolar aqueous solution of Rb_2SO_4 and $MgSO_4$.

Color

Colorless

Optical data

Biaxial(+) N_α=1.467, N_β=1.469, N_γ=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", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

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

Density

(calculated) 2.385 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 1.8$

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 $R_2M(SO_4)_2 \cdot 6H_2O$ J. Chem. Soc. 63, 337-423.

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.25	25	110	12.20
5.99	6	001	14.77
5.104	6	120	17.36
4.442	6	200	19.97
4.323	9	021	20.53
4.235	9	$\bar{1}21$	20.96
4.174	100	111	21.27
4.156		$\bar{2}01$	21.36
3.770	85	130	23.58
3.614	3	220,121	24.61
3.460	4	$\bar{2}21$	25.73
3.418	4	031	26.05
3.369	12	$\bar{1}31$	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	$\bar{1}12$	29.60
2.945	6	140	30.32
2.916	25	$\bar{3}11$	30.63
2.874	30	$\bar{2}02$	31.09
2.826	13	221	31.63
2.802	8	$\bar{2}12$	31.91
2.779	20	$\bar{1}22$	32.18
2.743	7	$\bar{1}41$	32.62
2.703	4	$\bar{3}21$	33.12
2.674	4	320	33.49
2.611	2	$\bar{2}22$	34.32
2.569	2	112	34.90
2.552	6	240,141	35.13
2.523	8	$\bar{2}31$	35.56
2.497	16	$\bar{2}41$	35.94
2.489	18	$\bar{1}32$	36.05
2.433	35	$\bar{3}31$	36.91
2.426	19	$\bar{3}12$	37.02
2.412	8	330	37.24
2.304	13	051	39.07
2.298	11	$\bar{3}22,\bar{4}01$	39.17
2.259	7	$\bar{4}11$	39.88
2.242	6	321	40.19
2.225	19	241	40.51
2.219	17	132,400	40.62
2.182	6	212	41.35
2.177	6	250,151	41.45
2.159	7	042	41.80

Internal standard Ag, a = 4.08641 Å $CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.142	8	$\bar{2}51$	42.16
2.114	9	$\bar{2}42$	42.73
2.092	9	420	43.22
2.083	5	060,331	43.40
2.049	3	$\bar{4}12$	44.17
2.026	2	$\bar{1}60$	44.69
2.012	4	$\bar{4}31$	45.02
1.994	8	003	45.45
1.968	4	013,$\bar{1}$23	46.09
1.961	6	251	46.26
1.945	2	$\bar{1}52$	46.65
1.938	4	$\bar{3}42$	46.84
1.916	9	052,401	47.40
1.908	5	350	47.61
1.894	6	$\bar{3}13$,411	47.99
1.884	2	260,161,+	48.26
1.860	8	$\bar{2}61$	48.93
1.855	8	$\bar{1}33$	49.08
1.831	4	$\bar{3}23$,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,$\bar{3}$52	51.99
1.739	6	261	52.58
1.729	5	$\bar{4}42$,$\bar{1}62$	52.91
1.708	3	062,520	53.62
1.700	5	332	53.87
1.688	3	$\bar{5}22$,$\bar{5}31$	54.31
1.683	4	133	54.49
1.676	3	$\bar{4}23$	54.71
1.658	3	450,252	55.37
1.654	5	270,171	55.50
1.639	3	$\bar{2}71$	56.08
1.633	4	530,$\bar{3}$43,+	56.28
1.616	5	$\bar{5}32$	56.95
1.598	2	$\bar{4}52$	57.65
1.580	3	$\bar{2}53$	58.35

Sample

The sample was made by heating Rb_2SO_4 and $NiSO_4$ in nitrogen at 540 °C for 10 minutes. It was then ground and reheated at 450 °C for 15 minutes.

Color

Light yellow

Optical data

Isotropic, N=1.636

Structure

Cubic, $P2_13$ (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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	7	541	60.39
1.513	2	533	61.19
1.495	2	622	62.01
1.479	8	630	62.77
1.463	5	631	63.55
1.432	4	444	65.09
1.418	3	632	65.83
1.402	3	710	66.63
1.3894	1	711	67.35
1.3757	1	640	68.10

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ (°)
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	2	811	78.20
1.2123	2	733	78.90
1.2034	2	820	79.60
1.1945	4	821	80.31
1.1859	1	653	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

References

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

Zemann,A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. **10**, 409 - 413.

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

Sample
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_α=1.488, N_β=1.496, N_γ=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", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25 °C	9.138 ±.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 $R_2M(SO_4)_2 \cdot 6H_2O$ J. Chem. Soc. 63, 337-423.

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

d (Å)	*I*	*hkl*	2*θ*(°)
7.18	6	110	12.31
6.20	1	020	14.27
5.98	1	001	14.81
5.21	2	$\bar{1}11$	16.99
5.072	3	120	17.47
4.390	9	200	20.21
4.310	16	021	20.59
4.209	6	$\bar{1}21$	21.09
4.151	100	111	21.39
4.122		$\bar{2}01$	21.54
3.745	85	130	23.74
3.586	6	220	24.81
3.400	2	031	26.19
3.356	15	$\bar{1}31$	26.54
3.148	20	201	28.33
3.104	25	040	28.74
3.052	20	211	29.24
3.013	65	$\bar{1}12$,230	29.62
2.992	12	002	29.84
2.925	4	140,$\bar{2}31$	30.54
2.906	7	012	30.74
2.893	12	$\bar{3}11$	30.88
2.868	19	$\bar{2}02$	31.16
2.849	13	310	31.37
2.807	18	221	31.85
2.796	13	$\bar{2}12$	31.98
2.778	18	$\bar{1}22$	32.20
2.755	4	041	32.47
2.730	9	$\bar{1}41$	32.78
2.695	1	022	33.22
2.682	2	$\bar{3}21$	33.38
2.649	2	320	33.81
2.603	3	$\bar{2}22$	34.42
2.536	7	141,240	35.36
2.506	6	231	35.80
2.483	14	$\bar{1}32$,$\bar{2}41$	36.14
2.422	45	032	37.09
2.414		$\bar{3}31$,$\bar{3}12$,+	37.21
2.390	2	330,150	37.61
2.358	1	$\bar{2}32$	38.13

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

d (Å)	*I*	*hkl*	2θ(°)
2.339	1	311	38.46
2.293	14	051	39.26
2.286	13	$\bar{3}22$	39.38
2.237	7	$\bar{4}11$	40.29
2.225	6	321	40.51
2.210	20	241	40.79
2.197	6	400,$\bar{1}42$	41.05
2.170	2	212	41.59
2.163	8	151,410,+	41.73
2.154	10	042	41.91
2.128	7	340,$\bar{2}51$	42.45
2.106	10	$\bar{2}42$	42.91
2.069	12	420,060	43.72
2.062	7	$\bar{4}02$	43.88
2.040	2	$\bar{2}03$	44.37
2.034	3	$\bar{4}12$	44.51
2.013	2	160,$\bar{2}13$	45.00
1.994	10	003,$\bar{4}31$	45.46
1.965	1	$\bar{1}23$	46.15
1.949	5	251	46.55
1.927	3	$\bar{3}42$	47.11
1.910	8	052	47.56
1.906	7	$\bar{3}51$	47.68
1.895	6	350	47.98
1.890	10	$\bar{3}13$,341	48.09
1.854	14	$\bar{1}33$	49.11
1.849		$\bar{2}61$	49.24
1.829	2	$\bar{2}33$	49.82
1.807	2	$\bar{5}11$	50.45
1.793	9	440	50.90

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

d (Å)	*I*	*hkl*	2θ(°)
1.775	2	322	51.45
1.761	3	$\bar{1}23$	51.87
1.753	2	$\bar{5}21$	52.13
1.748	2	$\bar{3}52$	52.29
1.739	6	510,170	52.57
1.7248	3	431	53.05
1.7188	5	351,$\bar{4}42$	53.25
1.7049	1	$\bar{2}43$	53.72
1.6900	5	332,520,+	54.23
1.6792	4	133,$\bar{2}62$	54.62
1.6750	3	$\bar{5}22$	54.76
1.6699	2	$\bar{4}23$	54.94
1.6451	6	450,270,+	55.84
1.6293	1	$\bar{2}71$	56.43
1.6195	2	530	56.90
1.6030	7	$\bar{5}32$	57.44
1.5988	5	$\bar{4}33$	57.61
1.5954		223	57.74
1.5762	3	$\bar{2}53$	58.51
1.5616	2	361,412	59.11
1.5530	4	$\bar{2}04$,080	59.47
1.5401	5	$\bar{2}14$,$\bar{1}72$	60.02
1.5279	4	540,180	60.55
1.5231	4	521,$\bar{3}71$	60.76
1.5163	3	$\bar{5}42$,370	61.06
1.5052	3	$\bar{2}24$,460	61.56
1.5013	3	$\bar{5}23$,$\bar{3}14$,+	61.74
1.4869	1	$\bar{6}02$	62.40

Sample

The sample was prepared from a 1:1 molar mixture of KCl and RbCl by melting, quenching, and annealing for 3 days at 400 °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(Å)
NBS, sample at 25 °C----------	6.4481 ±.0002

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

d (Å)	*I*	*hkl*	*2θ(°)*
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	422	71.65
1.2410	1	511	76.73
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

Density

(calculated) 2.421 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 5.3

Samarium Tin Oxide, $Sm_2Sn_2O_7$ (cubic)

Sample

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]	10.507
NBS, sample at 25 °C	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
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
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	12·4·0	136.01
.8013	20	10·6·6	148.03

Additional patterns

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

Sample
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_o=1.492, N_e=1.602

Structure
Hexagonal, P31c (159), Z=6 [Staritzky, 1956]. The structure was determined by Hoard [1933], assuming $P\bar{3}1c$ to be the space group.

Lattice constants

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

References
Hoard, J.L. (1933). The crystal structure of potassium silver cyanide, Z. Krist. **84**, 231-255.
Staritzky, E. (1956). Potassium silver dicyanide $KAg(CN)_2$, Anal.Chem. **28**, 419-20.

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	59.88

Silver Sodium Chloride, $Ag_{0.5}Na_{0.5}Cl$ (cubic)

Sample

A 1:1 molar mixture of NaCl and AgCl was melted, ground, and then annealed at 400 °C overnight. It was reground and annealed at 400 °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.

Lattice constants

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

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
3.24	14	111	27.49
2.807	100	200	31.85
1.984	55	220	45.69
1.692	4	311	54.17
1.620	15	222	56.79
1.4028	6	400	66.61
1.2868	2	331	73.54
1.2545	11	420	75.76
1.1451	6	422	84.55
.9919	1	440	101.90
.9483	1	531	108.63
.9351	3	600	110.93
.8870	2	620	120.55
.8457	2	622	131.23

Density

(calculated) 3.795 g/cm^3 at 25° C.

Reference intensity

$I/I_{corundum}$ = 3.3

Sample

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=1.90, material was very fine grained.

Structure

Cubic, $P2_13$ (198) or $P4_232$ (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*
Megaw [1946]	4.0337**
Naray-Szabo [1947]	8.05***
Smith and Welch [1960]	8.070
NBS, sample at 25 °C	8.0682 ±.0001

* as published
** from kX
*** as published, and considered to be monoclinic

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
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 CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	*2θ(°)*
1.0330	1	650	96.43
1.0086	3	800	99.59
1.0008	1	810	100.63
0.9784	2	820	103.87
.9713	1	821	104.92
.9509	9	822	108.21
.9317	<1	751	111.53
.9255	1	662	112.65
.9195	1	832	113.79
.9022	5	840	117.26
.8965	1	841	118.46
.8803	2	842	122.09
.8601	4	664	127.15
.8551	1	922	128.48
.8567	1	852	134.03
.8235	6	844	138.59
.8068	2	10·0·0	145.40
.8028	1	10·1·0	147.28
.7912	11	10·2·0	153.61

Density

(calculated) 6.432 g/cm^3 at 25° 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.

Sample

The sample of TlN_3 was obtained from Picatinny Arsenal, Dover, N.J.

Color

Yellowish white

Structure

Tetragonal, I4/mcm (140), Z=4. Isostructural with KN_3 [Krause, 1963]

Lattice constants

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

Density

(calculated) 5.763 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 3.2

Additional patterns

1. 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 TlN_3, J.Chem.Phys. 39,1706-13.

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

d (Å)	I	hkl	2θ(°)
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	5	402	65.21
1.4118	5	224	66.13
1.3872	5	420	67.46
1.3593	4	332	69.04
1.3441	6	314	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

Thallium Cadmium Sulfate, $Tl_2Cd_2(SO_4)_3$ (cubic)

Sample
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, $P2_13$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The structure of langbeinite, $K_2Mg_2(SO_4)_3$ 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
$I/I_{corundum} = 6.0$

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	2	530	51.26
1.7556	1	531	52.05
1.7303	1	600	52.87
1.7072	3	610	53.64
1.6846	16	611	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 CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
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	2	752	81.86
1.1537	1	841	83.77
1.1467	1	910	84.40
1.1398	1	911	85.03
1.1331	1	842	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

References

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

Zemann,A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409 - 413.

Thallium Cobalt Sulfate, $Tl_2Co_2(SO_4)_3$ (cubic)

Sample

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, $P2_13$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The structure of langbeinite, $K_2Mg_2(SO_4)_3$ was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
Gattow and Zemann [1958]	10.033 ±.005
NBS, sample at 25 °C	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 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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
2.302	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	2	530	53.17
1.696	2	531	54.02
1.672	2	600	54.85
1.649	6	610	55.69
1.628	17	611	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

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ (°)
1.4049	1	711	66.50
1.3910	1	640	67.25
1.3780	3	720	67.97
1.3653	8	721	68.69
1.3404	1	642	70.15
1.3286	4	722	70.87
1.3173	3	730	71.57
1.3061	4	731	72.28
1.2844	3	650	73.70
1.2737	4	732	74.42
1.2539	1	800	75.80
1.2442	3	810	76.50
1.2347	2	811	77.20
1.2252	1	733	77.91
1.2167	1	820	78.56
1.2077	5	821	79.26
1.1991	2	653	79.94
1.1820	2	822	81.34
1.1741	1	830	82.00
1.1660	7	831	82.69
1.1583	2	751	83.37
1.1509	<1	662	84.02
1.1431	1	832	84.73
1.1358	3	752	85.40
1.1144	2	841	87.45
1.1076	1	910	88.13
1.1010	3	911	88.79
1.0945	2	842	89.46
1.0878	1	920	90.16

References

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

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409-413.

Thallium Iron Sulfate Hydrate, $Tl_2Fe(SO_4)_2 \cdot 6H_2O$ (monoclinic)

Sample

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(-) N_α=1.590, N_β=1.605, N_γ=1.615, 2V is large

Structure

Monoclinic, $P2_1/a$ (14), Z=2. Isostructural with other "Tutton" salts [Tutton, 1928]. 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	9.264 ±.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 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
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	$\bar{1}21$	20.96
4.174	100	111,$\bar{2}$01	21.27
3.959	6	$\bar{2}$11	22.44
3.771	50	130	23.57
3.623	2	220	24.55
3.469	1	$\bar{2}21$	25.66
3.377	6	$\bar{1}31$	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	$\bar{1}12$	29.54
2.927	16	$\bar{3}11$	30.52
2.883	30	$\bar{2}02$,310	30.99
2.828	7	221	31.61
2.809	5	$\bar{2}12$	31.83
2.784	13	$\bar{1}22$	32.12
2.773	8	041	32.25
2.745	7	$\bar{1}41$	32.59
2.678	6	$\bar{3}20$	33.43
2.617	3	$\bar{2}22$	34.23
2.558	2	240	35.05
2.525	4	231	35.52
2.495	14	$\bar{1}32$	35.96
2.440	30	$\bar{3}31$	36.80
2.418	12	330	37.15
2.307	25	051,$\bar{3}22$	39.01
2.268	7	$\bar{4}11$	39.70
2.244	9	321	40.15

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.225	18	241,400	40.50
2.180	10	250	41.39
2.145	6	$\bar{2}51$	42.10
2.119	11	$\bar{2}42$	42.63
2.095	5	420	43.14
2.056	5	$\bar{4}12$	44.00
2.020	5	$\bar{2}13$	44.84
1.997	6	003	45.38
1.963	6	251,430	46.21
1.959	6	$\bar{1}61$	46.31
1.942	2	$\bar{3}42$	46.73
1.9190	10	052,401	47.33
1.9061	2	341	47.67
1.8993	5	$\bar{3}13$	47.85
1.8635	6	$\bar{4}32,\bar{2}61$	48.83
1.8578	10	$\bar{1}33$	48.99
1.8364	4	$\bar{3}23,\bar{2}33$	49.60
1.8111	9	152	50.34
1.7762	5	$\bar{5}21$	51.40
1.7616	6	510,$\bar{3}52$	51.86

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.(1928). The hexahydrated double sulphates containing thallium, Proc. Roy. Soc. London, Ser. A **118**, 367-392.

Sample

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, $K_2Mg_2(SO_4)_3$, and similar sulfates. The structure of langbeinite was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	10.4174 ±.0003

Density

(calculated) 4.731 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 4.5$

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

d (Å)	I	hkl	2θ(°)
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	25	510	44.30
2.0052	8	511	45.18
1.9341	8	520	46.94
1.9016	3	521	47.79
1.8135	5	522	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 $CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
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

References

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. **10**, 409 - 413.

4-Acetyl-2′-fluorobiphenyl, $C_{14}H_{11}OF$ (monoclinic)

Structure

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

Lattice parameters

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

Density

(calculated) 1.313 g/cm^3 [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^0, C^0, H^0 [3.3.1A]

Scale factor

(integrated intensities) 3.465 × 10^4

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)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
12.27	5	1 0 0	7.20
6.62	50	0 0 2	13.36
6.14	14	2 0 0	14.42
6.01	6	-2 0 2	14.72
5.44	71	0 1 1	16.28
5.35	9	-1 1 1	16.56
4.98	7	1 0 2	17.78
4.63	51	-1 1 2	19.14
4.50	4	-2 1 1	19.72
4.48	6	-3 0 2	19.82
4.44	6	0 1 2	20.00
4.28	6	2 1 0	20.74
4.10	8	3 0 0	21.68
3.828	3	1 1 2	23.22
3.693	70	-3 1 3	24.08
3.669	100	-2 0 4	24.24
3.627	6	-1 0 4	24.52
3.601	5	-3 1 1	24.70
3.581	8	-3 1 2	24.84
3.550	16	0 1 3	25.06

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
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	29.06
3.009	1	-4 0 4	29.66
2.965	26	-3 1 4 +	30.12
2.910	2	-4 1 1	30.70
2.897	11	0 1 4 +	30.84
2.884	6	-4 1 3	30.98
2.766	1	-1 2 2	32.34
2.736	2	-2 2 1	32.70
2.730	2	-5 0 2	32.78
2.685	2	-4 1 4 +	33.34
2.647	5	-2 1 5 +	33.84
2.605	2	1 1 4	34.40
2.596	3	-5 0 4	34.52
2.583	1	-1 1 5	34.70
2.490	2	-3 2 1	36.04
2.473	1	-5 1 3 +	36.30
2.457	5	5 0 0	36.54
2.439	1	-4 1 5	36.82
2.423	1	0 1 5	37.08
2.412	3	3 2 0	37.24
2.309	1	3 1 3	38.98
2.272	4	3 2 1	39.64
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
2.056	1	-5 1 6	43.96
2.030	3	5 0 2	44.60
2.009	2	-5 2 3	45.10
1.982	2	0 2 5	45.74
1.956	4	-4 1 7	46.38
1.946	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 6 +	53.50
1.640	1	1 3 4	56.02

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
12.28	4	1 0 0	7.19
6.63	44	0 0 2	13.35
6.14	13	2 0 0	14.41
6.02	5	-2 0 2	14.71
5.44	68	0 1 1	16.27
5.37	2	1 1 0	16.49
5.35	6	-1 1 1	16.56
4.99	6	1 0 2	17.78
4.63	51	-1 1 2	19.15
4.50	3	-2 1 1	19.72
4.48	5	-3 0 2	19.82
4.44	6	0 1 2	20.00
4.28	6	2 1 0	20.73
4.09	9	3 0 0	21.69
3.827	3	1 1 2	23.22
3.694	69	-2 1 3	24.07
3.670	100	-2 0 4	24.23
3.626	3	-1 0 4	24.53
3.601	3	-3 1 1	24.70
3.582	7	-3 1 2	24.84
3.551	17	0 1 3	25.05
3.421	3	-4 0 2	26.03
3.129	3	1 1 3	28.51
3.099	30	-1 1 4	28.78
3.071	3	4 0 0	29.05
3.009	1	-4 0 4	29.66
2.986	1	0 2 0	29.90
2.968	1	-4 1 2	30.08
2.965	27	-3 1 4	30.12
2.950	5	3 0 2	30.27
2.910	1	-4 1 1	30.70
2.898	5	-1 2 1	30.83
2.897	7	0 1 4	30.84
2.894	1	1 0 4	30.87
2.883	5	-4 1 3	30.99
2.765	1	-1 2 2	32.35
2.736	2	-2 2 1	32.70
2.729	1	-5 0 2	32.79
2.687	1	-4 1 4	33.32
2.685	1	2 2 0	33.34

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.647	4	-2 1 5	33.83
2.645	2	3 1 2	33.87
2.604	3	1 1 4	34.41
2.596	3	-5 0 4	34.52
2.583	1	-1 1 5	34.70
2.490	2	-3 2 1	36.04
2.474	1	0 2 3	36.29
2.472	1	-5 1 3	36.32
2.457	5	5 0 0	36.54
2.439	1	-4 1 5	36.81
2.423	1	0 1 5	37.08
2.412	4	3 2 0	37.24
2.308	1	3 1 3	38.99
2.272	4	3 2 1	39.64
2.249	1	-4 2 2	40.05
2.209	1	0 0 6	40.82
2.111	2	-6 1 2	42.80
2.101	1	5 1 1	43.01
2.078	2	1 2 4	43.51
2.058	1	-5 1 6	43.96
2.030	4	5 0 2	44.59
2.009	3	-5 2 3	45.10
1.982	2	0 2 5	45.74
1.956	4	-4 1 7	46.38
1.946	1	-7 0 4	46.64
1.937	1	6 1 0	46.87
1.919	2	-7 0 2	47.34
1.893	1	2 3 0	48.01
1.847	1	-4 2 6	49.30
1.840	1	2 3 1	49.51
1.792	1	3 1 5	50.90
1.791	1	4 1 4	50.95
1.790	1	3 3 0	50.97
1.762	2	-3 1 8	51.84
1.758	2	2 3 2	51.96
1.723	2	-3 2 7	53.13
1.712	2	-5 1 8	53.49
1.710	1	-2 2 7	53.53
1.640	1	1 3 4	56.03

ℓ-Alanine, $C_3H_7O_2N$ (orthorhombic)

Structure

Orthorhombic, $P2_12_12_1$ (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/cm^3 [ibid.]

Thermal parameters

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

Polymorphism

The d form has the same powder pattern given here, but the dℓ 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

1. PDF 5-0306 [Institute of Physics, University College, Cardiff]
2. 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.

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
6.171	5	0 2 0	14.34
5.420	11	1 1 0	16.34
5.236	22	0 1 1	16.92
4.312	100	1 2 0	20.58
4.219	3	0 2 1	21.04
3.955	4	1 1 1	22.46
3.458	3	1 2 1	25.74
3.399	2	1 3 0	26.20
3.353	6	0 3 1	26.56
3.085	20	0 4 0	28.92
2.930	14	1 3 1	30.48
2.891	10	0 0 2	30.90
2.815	3	0 1 2	31.76
2.748	9	1 4 0	32.56
2.709	9	2 2 0	33.04
2.608	16	1 0 2	34.36
2.482	1	1 4 1	36.16
2.453	2	2 2 1	36.60
2.433	2	2 3 0	36.92
2.403	5	1 2 2	37.40
2.2851	1	1 5 0	39.40
2.2425	3	2 3 1	40.18
2.2026	1	1 3 2	40.94
2.1253	2	1 5 1	42.50
2.0580	2	2 1 2	43.96
2.0205	1	2 4 1	44.82
1.9919	5	1 4 2	45.50
1.9771	4	2 2 2	45.86
1.9380	1	0 6 1	46.84
1.8776	2	0 5 2 +	48.44
1.8136	2	2 5 1 +	50.26
1.7245	1	3 3 1	53.06
1.6996	2	2 6 0	53.90
1.6846	1	3 4 0	54.42
1.6354	1	0 4 3	56.20
1.6242	1	1 7 1	56.62
1.5711	1	2 2 3	58.72

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.172	4	0 2 0	14.34
5.419	10	1 1 0	16.34
5.237	21	0 1 1	16.91
4.314	100	1 2 0	20.57
4.220	3	0 2 1	21.03
3.955	4	1 1 1	22.46
3.458	3	1 2 1	25.74
3.399	2	1 3 0	26.20
3.353	6	0 3 1	26.57
3.086	22	0 4 0	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	0 2 2	34.21
2.608	17	1 0 2	34.36
2.481	1	1 4 1	36.17
2.454	3	2 2 1	36.59
2.432	2	2 3 0	36.92
2.402	6	1 2 2	37.41
2.2847	1	1 5 0	39.41
2.2422	3	2 3 1	40.18
2.2026	1	1 3 2	40.94
2.1249	3	1 5 1	42.51
2.1101	1	0 4 2	42.82
2.0582	2	2 1 2	43.96
2.0209	1	2 4 1	44.81
1.9918	6	1 4 2	45.50
1.9774	5	2 2 2	45.85
1.9382	1	0 6 1	46.83
1.8992	1	3 0 1	47.86
1.8776	1	0 5 2	48.44
1.8771	1	3 1 1	48.45
1.8165	1	1 1 3	50.18
1.8139	2	2 5 1	50.26
1.7602	1	1 2 3	51.90
1.7243	1	3 3 1	53.07
1.6995	3	2 6 0	53.90
1.6846	1	3 4 0	54.42
1.6351	1	0 4 3	56.21
1.6243	1	1 7 1	56.62
1.5709	1	2 2 3	58.72
1.5109	1	2 3 3	61.30
1.2876	1	3 6 2	73.49

Ammonium Acetate, $NH_4 \cdot CH_3CO_2$ (monoclinic)

Structure

Monoclinic, $P2_1/c$ (14), Z=4 [Nahringbauer, 1967]

Lattice parameters

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

Density

(calculated) 1.169 g/cm³ [ibid.]

Thermal parameters

Isotropic

H 7.0 [ibid.]

O(1)	4.20	N	3.66	C(1)	3.49
O(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^0, C^0, N^0, O^0 [3.3.1A]

Scale factor

(integrated intensities) 0.3776×10^4

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)	I	hkl	2θ(°) λ = 1.54056 Å
6.468	28	0 1 1	13.68
5.901	3	0 0 2	15.00
4.691	65	0 1 2	18.90
4.066	100	-1 0 2	21.84
4.019	94	1 1 0 +	22.10
3.870	94	0 2 0	22.96
3.678	14	0 2 1	24.18
3.630	33	1 1 1	24.50
3.599	19	-1 1 2	24.72
3.506	1	0 1 3	25.38
3.383	8	1 0 2	26.32
3.236	9	0 2 2	27.54
3.099	25	1 1 2	28.78
3.066	29	-1 1 3	29.10
2.982	6	-1 2 1	29.94

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.951	8	0 0 4	30.26
2.803	46	-1 2 2	31.90
2.758	22	0 1 4 +	32.44
2.741	4	-1 0 4	32.64
2.611	8	1 1 3	34.32
2.583	3	-1 1 4	34.70
2.528	7	-1 2 3	35.48
2.521	17	0 3 1	35.58
2.365	2	0 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
2.186	7	1 3 1	41.26
2.179	6	-1 3 2	41.40
2.141	1	2 1 1	42.18
2.042	6	-1 3 3	44.32
2.036	6	-2 2 1	44.46
1.987	3	2 1 2 +	45.62
1.967	3	0 0 6 +	46.10
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	-1 1 6 +	48.10
1.8791	2	-1 3 4	48.40
1.8392	1	0 4 2	49.52
1.7998	2	-2 2 4	50.68
1.7899	1	1 4 0	50.98
1.7540	4	1 2 5 +	52.10
1.7478	2	-1 4 2	52.30
1.7336	3	-2 3 2	52.76
1.6915	1	2 0 4	54.18
1.6863	2	2 3 1	54.36
1.6749	1	-1 4 3	54.76
1.6671	1	-2 2 5	55.04
1.5495	1	-1 2 7	59.62
1.5457	1	0 2 7	59.78
1.5355	1	0 5 1	60.22
1.4943	1	2 4 0	62.06
1.4780	2	-3 1 4	62.82
1.4556	1	-2 4 3	63.90
1.4495	2	3 0 2	64.20

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
6.474	26	0	1	1	13.67
5.902	2	0	0	2	15.00
4.694	64	0	1	2	18.89
4.067	100	-1	0	2	21.84
4.019	92	1	1	0	22.10
4.005	8	-1	1	1	22.18
3.871	97	0	2	0	22.96
3.678	14	0	2	1	24.18
3.632	37	1	1	1	24.49
3.600	19	-1	1	2	24.71
3.508	1	0	1	3	25.37
3.383	9	1	0	2	26.32
3.237	10	0	2	2	27.53
3.100	28	1	1	2	28.78
3.067	33	-1	1	3	29.09
2.983	7	-1	2	1	29.93
2.951	9	0	0	4	30.26
2.819	2	1	2	1	31.72
2.804	54	-1	2	2	31.89
2.759	12	0	2	3	32.42
2.757	15	0	1	4	32.44
2.741	3	-1	0	4	32.65
2.611	10	1	1	3	34.32
2.583	4	-1	1	4	34.69
2.529	6	-1	2	3	35.47
2.521	17	0	3	1	35.58
2.364	2	0	3	2	38.02
2.351	3	2	0	0	38.24
2.340	2	-2	0	2	38.44
2.313	3	1	0	4	38.91
2.287	2	-2	1	1	39.37
2.262	10	1	3	0	39.81
2.255	3	1	2	3	39.95
2.250	4	2	1	0	40.04
2.240	23	-2	1	2	40.23
2.237	3	-1	2	4	40.29
2.216	5	1	1	4	40.68
2.186	8	1	3	1	41.27
2.179	5	-1	3	2	41.40
2.141	2	2	1	1	42.17

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
2.042	8	-1	3	3	44.32
2.036	4	-2	2	1	44.47
1.987	3	2	1	2	45.51
1.985	2	1	2	4	45.66
1.967	2	0	0	6	46.10
1.967	1	-2	1	4	46.12
1.949	1	-1	0	6	46.56
1.943	1	0	3	4	46.72
1.918	4	-2	2	3	47.36
1.9100	1	0	4	1	47.57
1.9067	1	0	1	6	47.66
1.8901	7	-1	1	6	48.10
1.8833	5	1	3	3	48.12
1.8788	2	-1	3	4	48.41
1.8391	1	0	4	2	49.52
1.8001	3	-2	2	4	50.67
1.7898	1	1	4	0	50.98
1.7541	4	1	2	5	52.10
1.7538	1	0	2	6	52.11
1.7476	2	-1	4	2	52.30
1.7334	4	-2	3	2	52.77
1.6915	1	2	0	4	54.18
1.6864	3	2	3	1	54.36
1.6747	1	-1	4	3	54.77
1.6672	2	-2	2	5	55.03
1.6325	1	-2	1	6	56.31
1.5494	1	-1	2	7	59.62
1.5459	1	0	2	7	59.77
1.5353	1	0	5	1	60.23
1.4944	1	2	4	0	62.06
1.4781	3	-3	1	4	62.82
1.4555	1	-2	4	3	63.91
1.4494	1	3	0	2	64.21
1.4019	1	-2	4	4	66.66
1.3798	1	1	4	5	67.87
1.2714	1	0	4	7	74.58
1.1437	1	2	1	8	84.68

Ammonium Yttrium Oxalate Hydrate, $NH_4Y(C_2O_4)_2 \cdot H_2O$ (monoclinic)

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

Lattice parameters
a=9.18±0.01, b=6.09±0.01, c=7.89±0.01Å, β=90.2±0.1° [ibid.]

Density
(calculated) 2.27 g/cm³ [ibid.]

Thermal parameters
Anisotropic [ibid.]

Scattering factors
N^0, O^0, C^0 [Berghuis et al., 1955]
Y^0 [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, $NH_4Y(C_2O_4)_2 \cdot H_2O$, Acta Cryst. 23, 944-949.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
6.09	100	0 1 0	14.54
5.97	93	1 0 1 +	14.82
5.08	16	1 1 0	17.46
4.82	17	0 1 1	18.40
4.59	3	2 0 0	19.32
4.26	38	-1 1 1 +	20.82
3.94	2	0 0 2	22.52
3.32	16	2 1 1	26.82
3.12	18	-1 1 2	28.62
3.00	9	-2 0 2	29.80
2.99	14	2 0 2	29.88
2.89	3	1 2 0	30.92
2.86	3	-3 0 1	31.30
2.85	4	3 0 1	31.36
2.84	5	0 2 1	31.46

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.73	2	3 1 0	32.72
2.72	1	-1 2 1	32.96
2.69	2	-2 1 2	33.30
2.68	4	2 1 2	33.38
2.59	6	-3 1 1	34.66
2.58	4	3 1 1	34.74
2.54	6	2 2 0	35.34
2.53	7	-1 0 3	35.44
2.53	5	1 0 3	35.50
2.414	14	2 2 1 +	37.22
2.333	19	-1 2 2 +	38.56
2.295	5	4 0 0	39.22
2.244	9	3 1 2	40.16
2.158	6	3 2 0	41.82
2.147	3	4 1 0	42.04
2.140	10	-2 1 3 +	42.20
2.134	7	2 2 2	42.32
2.083	3	-3 2 1	43.40
2.071	4	4 1 1 +	43.68
2.030	4	0 3 0	44.60
1.998	1	-3 0 3	45.36
1.990	5	0 2 3 +	45.54
1.987	6	-4 0 2	45.62
1.981	4	4 0 2	45.76
1.972	3	0 0 4	45.98
1.967	3	0 3 1	46.12
1.944	1	1 2 3	46.68
1.922	2	1 3 1 +	47.24
1.892	6	3 2 2 +	48.06
1.876	2	0 1 4	48.48
1.840	1	-1 1 4	49.50
1.833	2	4 2 0	49.70
1.828	5	-2 2 3	49.84
1.814	2	-2 0 4	50.24
1.807	6	2 3 1 +	50.46
1.789	4	-5 0 1	51.00
1.785	4	4 2 1 +	51.14
1.771	5	1 3 2 +	51.56
1.735	1	2 1 4	52.72
1.717	2	-5 1 1	53.32
1.714	1	5 1 1	53.40
1.691	3	3 3 0	54.18
1.661	1	4 1 3	55.26
1.630	1	-1 2 4 +	56.40
1.607	2	0 3 3 +	57.28
1.556	1	-3 3 2	59.36
1.554	1	1 0 5	59.42
1.518	1	-2 3 3	61.00
1.516	1	2 3 3	61.08
1.508	1	-5 0 3	61.44
1.506	1	-4 2 3	61.54

Ammonium Yttrium Oxalate Hydrate, $NH_4Y(C_2O_4)_2 \cdot H_2O$ (monoclinic) – continued

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.09	100	0 1 0	14.53
5.99	58	-1 0 1	14.77
5.97	62	1 0 1	14.82
5.07	17	1 1 0	17.46
4.82	20	0 1 1	18.39
4.59	3	2 0 0	19.32
4.27	28	-1 1 1	20.78
4.26	23	1 1 1	20.81
3.94	2	0 0 2	22.52
3.32	20	2 1 1	26.83
3.12	23	-1 1 2	28.61
3.00	10	-2 0 2	29.79
2.99	15	2 0 2	29.89
2.89	4	1 2 0	30.91
2.86	3	-3 0 1	31.29
2.85	2	3 0 1	31.37
2.84	5	0 2 1	31.47
2.73	3	3 1 0	32.73
2.71	1	-1 2 1	32.97
2.69	2	-2 1 2	33.29
2.68	4	2 1 2	33.39
2.59	7	-3 1 1	34.66
2.58	1	3 1 1	34.73
2.54	8	2 2 0	35.34
2.53	4	-1 0 3	35.44
2.53	3	1 0 3	35.51
2.417	4	-2 2 1	37.17
2.414	1	0 1 3	37.21
2.414	15	2 2 1	37.21
2.410	3	0 2 2	37.27
2.337	2	-1 1 3	38.49
2.333	6	1 1 3	38.55
2.333	19	-1 2 2	38.56
2.330	3	1 2 2	38.61
2.295	6	4 0 0	39.22
2.251	1	-3 1 2	40.03
2.244	12	3 1 2	40.15
2.158	8	3 2 0	41.82
2.148	2	4 1 0	42.04
2.140	13	-2 1 3	42.20
2.136	2	-2 2 2	42.28
2.132	2	2 2 2	42.36
2.083	4	-3 2 1	43.40
2.074	2	-4 1 1	43.61
2.070	4	4 1 1	43.68
2.030	5	0 3 0	44.60
1.998	1	-3 0 3	45.35
1.991	3	3 0 3	45.52
1.990	3	0 2 3	45.54
1.987	6	-4 0 2	45.62

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.981	3	4 0 2	45.77
1.972	4	0 0 4	45.97
1.966	2	0 3 1	46.13
1.944	2	1 2 3	46.68
1.923	1	-1 3 1	47.23
1.922	2	1 3 1	47.25
1.898	1	-3 1 3	47.88
1.896	2	-3 2 2	47.95
1.893	2	3 1 3	48.03
1.892	6	3 2 2	48.06
1.889	2	-4 1 2	48.14
1.877	2	0 1 4	48.47
1.840	2	-1 1 4	49.51
1.833	1	4 2 0	49.71
1.828	7	-2 2 3	49.85
1.815	3	-2 0 4	50.24
1.810	3	2 0 4	50.37
1.808	4	-2 3 1	50.44
1.807	5	2 3 1	50.47
1.790	5	-5 0 1	50.99
1.787	1	5 0 1	51.07
1.786	2	-4 2 1	51.09
1.784	3	4 2 1	51.16
1.772	5	-1 3 2	51.54
1.771	5	1 3 2	51.58
1.735	1	2 1 4	52.72
1.717	2	-5 1 1	53.31
1.715	1	5 1 1	53.39
1.692	4	3 3 0	54.18
1.679	1	2 3 2	54.62
1.661	1	4 1 3	55.27
1.630	1	-1 2 4	56.40
1.628	1	1 2 4	56.46
1.608	1	-5 1 2	57.26
1.607	3	0 3 3	57.28
1.572	1	5 2 0	58.67
1.556	1	-3 3 2	59.35
1.554	1	1 0 5	59.42
1.518	1	-2 3 3	61.00
1.516	1	2 3 3	61.09
1.508	1	-5 0 3	61.44
1.506	1	-4 2 3	61.54
1.503	1	5 0 3	61.66
1.502	1	4 2 3	61.72
1.494	1	-4 3 1	62.09
1.492	1	4 3 1	62.15
1.476	1	-1 4 1	62.93
1.475	1	1 4 1	62.95
1.464	1	-5 1 3	63.50
1.462	1	-5 2 2	63.58

ℓ-Ascorbic Acid, $C_6H_8O_6$ (monoclinic)

Structure

Monoclinic, $P2_1$ (4), Z=4, [Hvoslef,1968]

Lattice parameters

a=17.300±.008,b=6.353±.003,c=6.411±.003Å
β=102°11′±08′,(published value,a=17.299) [ibid.]

Density

(calculated) 1.699 g/cm^3 [ibid.]

Thermal parameters

Isotropic:O(1) 1.94;O(2) 1.70;O(3) 1.85; O(4) 1.85;O(5) 2.04;O(6) 2.38;O(1)*1.98; O(2)*1.77;O(3)*2.16;O(4)*1.55;O(5)*1.80; O(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 × 10^4

Additional patterns

1. 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.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
8.45	40	2	0	0		10.46
6.32	8	-1	0	1		14.00
6.27	14	0	0	1		14.12
5.63	17	-2	0	1		15.72
5.51	15	1	0	1		16.08
5.08	40	2	1	0		17.46
4.480	65	-1	1	1		19.80
4.462	68	0	1	1		19.88
4.215	18	-2	1	1		21.06
4.160	7	1	1	1		21.34
3.786	12	-3	1	1		23.48
3.720	1	2	1	1		23.90
3.520	38	4	1	0		25.28
3.329	15	-4	1	1		26.76
3.281	10	-5	0	1		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	-1	1	2		31.24
2.838	2	-1	2	1		31.50
2.832	2	0	2	1		31.56
2.819	1	6	0	0		31.72
2.801	3	-6	0	1		31.92
2.768	1	-2	2	1		32.32
2.751	2	1	2	1		32.52
2.730	2	-3	1	2		32.78
2.692	5	1	1	2		33.26
2.635	3	-3	2	1		34.00
2.612	2	2	2	1		34.30
2.586	10	-5	0	2		34.66
2.576	10	6	1	0		34.80
2.563	4	-6	1	1		34.98
2.539	8	4	2	0		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	-1	2	2	+	39.92
2.236	9	6	1	1		40.30
2.169	11	1	2	2		41.60
2.136	3	-2	0	3		42.28
2.109	7	7	0	1	+	42.84
2.103	5	-6	2	1		42.98
2.089	4	5	0	2		43.28
2.054	4	2	3	0		44.04
2.032	2	-7	1	2		44.56
2.018	2	-1	1	3		44.88

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.005	5	8 1 0 +	45.18
2.002	9	-3 1 3 +	45.26
1.975	6	3 2 2	45.90
1.953	1	-4 1 3	46.46
1.932	2	-7 2 1	47.00
1.893	2	4 3 0	48.02
1.886	2	8 0 1 +	48.22
1.879	2	-6 0 3	48.40
1.851	1	2 1 3	49.18
1.808	1	8 1 1	50.44
1.802	1	-6 1 3	50.62
1.786	1	-9 0 2	51.10
1.778	3	-7 2 2 +	51.36
1.772	2	-2 2 3	51.52
1.764	1	3 1 3	51.78
1.757	1	7 2 1	52.00
1.745	1	0 2 3	52.38
1.693	2	6 3 0	54.14
1.689	3	-6 3 1 +	54.26
1.681	1	7 1 2	54.54
1.639	1	-5 3 2	56.08
1.634	2	10 1 0	56.24
1.588	3	0 4 0	58.02
1.584	3	6 3 1	58.18
1.582	2	-4 0 4	58.28
1.561	4	2 4 0	59.14
1.557	3	-9 2 2	59.30
1.535	1	-4 1 4	60.24
1.501	1	9 2 1	61.74
1.494	1	-3 3 3	62.06
1.441	1	9 1 2	64.62
1.437	1	-10 1 3	64.82
1.409	2	-9 2 3 +	66.30
1.401	1	1 4 2	66.72
1.395	1	10 2 1	67.04

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
8.46	29	2 0 0	10.45
6.33	6	-1 0 1	13.99
6.27	10	0 0 1	14.12
5.64	13	-2 0 1	15.71
5.51	12	1 0 1	16.07
5.08	35	2 1 0	17.45
4.483	52	-1 1 1	19.79
4.461	46	0 1 1	19.88
4.216	15	-2 1 1	21.06
4.162	6	1 1 1	21.33
3.786	11	-3 1 1	23.48
3.722	1	2 1 1	23.89
3.520	36	4 1 0	25.28
3.329	14	-4 1 1	26.76
3.280	9	-5 0 1	27.17
3.205	1	4 0 1	27.81
3.204	2	-1 0 2	27.82
3.176	100	0 2 0	28.07
3.023	7	-3 0 2	29.53
2.974	51	2 2 0	30.03
2.971	19	1 0 2	30.06
2.914	1	-5 1 1	30.65
2.861	2	-1 1 2	31.24
2.839	1	-1 2 1	31.49
2.833	1	0 2 1	31.55
2.818	1	6 0 0	31.72
2.801	2	-6 0 1	31.92
2.767	1	-2 2 1	32.32
2.752	2	1 2 1	32.51
2.730	2	-3 1 2	32.78
2.691	5	1 1 2	33.27
2.634	3	-3 2 1	34.00
2.612	1	2 2 1	34.30
2.587	10	-5 0 2	34.65
2.576	8	6 1 0	34.79
2.563	3	-6 1 1	34.98
2.540	7	4 2 0	35.31
2.522	23	3 0 2	35.57
2.519	1	5 1 1	35.61
2.440	1	3 2 1	36.81
2.433	1	-7 0 1	36.91
2.396	11	-5 1 2	37.51
2.272	3	-7 1 1	39.63
2.256	1	4 2 1	39.93
2.256	2	-1 2 2	39.93
2.236	9	6 1 1	40.30
2.170	13	1 2 2	41.59
2.136	4	-2 0 3	42.29
2.110	4	7 0 1	42.83
2.108	4	6 2 0	42.86

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.101	3	-6 2 1	43.02
2.089	4	5 0 2	43.27
2.054	4	2 3 0	44.05
2.032	1	-7 1 2	44.56
2.022	1	1 0 3	44.79
2.018	2	-1 1 3	44.87
2.008	2	-1 3 1	45.11
2.006	1	0 3 1	45.16
2.006	2	-5 2 2	45.17
2.006	2	8 1 0	45.17
2.002	2	7 1 1	45.25
2.002	6	-3 1 3	45.26
1.975	6	3 2 2	45.91
1.953	1	-4 1 3	46.45
1.932	2	-7 2 1	47.01
1.893	2	4 3 0	48.01
1.886	2	8 0 1	48.21
1.884	1	-5 1 3	48.26
1.879	1	-6 0 3	48.42
1.851	1	2 1 3	49.18
1.808	1	8 1 1	50.43
1.801	1	-6 1 3	50.63
1.786	1	-9 0 2	51.09
1.779	2	-5 3 1	51.31
1.777	2	-7 2 2	51.37
1.772	1	-2 2 3	51.52
1.764	1	3 1 3	51.77
1.757	1	7 2 1	51.99
1.745	1	0 2 3	52.38
1.693	2	6 3 0	54.13
1.691	1	10 0 0	54.20
1.689	2	-6 3 1	54.26
1.681	1	7 1 2	54.53
1.639	1	-5 3 2	56.08
1.634	1	10 1 0	56.25
1.588	3	0 4 0	58.02
1.585	2	6 3 1	58.17
1.582	1	-4 0 4	58.28
1.561	5	2 4 0	59.14
1.557	1	-9 2 2	59.30
1.535	1	-4 1 4	60.24
1.501	1	9 2 1	61.74
1.494	1	-3 3 3	62.06
1.441	1	9 1 2	64.63
1.437	1	-10 1 3	64.82
1.409	1	-9 2 3	66.30
1.408	1	8 3 1	66.31
1.401	1	1 4 2	66.73
1.395	1	10 2 1	67.05

Structure

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(1) 1.704; N(1) 1.625; O(1) 2.248; H(1) 1.50; H(1′) 3.0

Scattering factors

H^0, C^0, N^0, O^0 [3.3.1A]

Scale factor

(integrated intensities) 0.1436 × 10^4

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)	*I*	*hkl*	2θ(°) λ = 1.54056 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	25.92
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	68	1 1 1	31.92
2.74	7	0 0 4	32.70
2.58	10	-1 1 2	34.68
2.55	20	1 1 2	35.14
2.26	5	-1 0 4	39.94
2.21	1	1 0 4	40.74
2.05	2	0 2 2	44.22
1.92	3	1 2 0	47.38
1.89	2	0 2 3	48.16
1.88	3	1 2 1	48.24
1.84	3	-2 0 2	49.64
1.82	6	0 0 6	49.94
1.82	2	-1 2 2	50.22
1.77	3	2 1 0	51.56
1.76	5	-1 1 5	51.84
1.75	5	-2 1 1	52.12
1.74	2	1 1 5	52.66
1.69	4	1 2 3	54.24
1.68	2	2 1 2	54.72
1.61	1	-2 1 3	57.36
1.58	3	2 1 3	58.28
1.56	4	1 2 4	59.06
1.56	2	-1 1 6	59.32
1.458	2	0 3 1	63.78
1.454	3	2 2 0	63.96
1.439	3	2 2 1	64.74
1.400	1	2 2 2	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	73.16
1.227	1	3 1 1	77.78
1.148	1	-2 3 2	84.30
1.095	1	1 3 6 +	89.46

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
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	81	-1 0 2	27.95
3.13	19	1 0 2	28.51
2.91	36	1 1 0	30.71
2.82	2	-1 1 1	31.68
2.81	47	0 1 3	31.79
2.80	62	1 1 1	31.93
2.74	6	0 0 4	32.70
2.59	10	-1 1 2	34.67
2.55	22	1 1 2	35.13
2.26	5	-1 0 4	39.93
2.21	1	1 0 4	40.74
2.05	2	0 2 2	44.21
1.92	4	1 2 0	47.39
1.89	2	0 2 3	48.14
1.88	3	1 2 1	48.24
1.83	3	-2 0 2	49.64
1.82	8	0 0 6	49.95
1.81	1	-1 2 2	50.23
1.77	4	2 1 0	51.56
1.76	6	-1 1 5	51.84
1.75	5	-2 1 1	52.11
1.74	2	1 1 5	52.67
1.69	6	1 2 3	54.23
1.68	2	2 1 2	54.72
1.61	1	-2 1 3	57.36
1.58	4	2 1 3	58.28
1.56	5	1 2 4	59.07
1.56	3	-1 1 6	59.33
1.458	3	0 3 1	63.77
1.454	3	2 2 0	63.96
1.439	4	2 2 1	64.74
1.400	2	2 2 2	66.75
1.375	1	1 3 0	68.13
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	-1 0 8	72.78
1.293	1	-2 2 4	73.16
1.227	1	3 1 1	77.78
1.183	1	-2 1 7	81.23
1.148	1	-2 3 2	84.29
1.129	1	2 2 6	86.06
1.098	1	0 4 1	89.11
1.095	1	-3 2 2	89.46
1.094	1	1 3 6	89.48

Structure
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± 0.015Å, β= 90.1±0.1° [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
O° [3.3.1A]
I° [3.3.1B]

Scale factor
(integrated intensities) 25.00 × 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, HI_3O_8, Acta Cryst. **20**, 769-777.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(^{\circ})$ λ = 1.54056 Å
6.37	12	0 1 1	13.90
6.28	11	1 0 1 +	14.08
4.87	11	1 1 1 +	18.22
4.58	1	0 1 2	19.38
3.91	13	-1 1 2 +	22.70
3.84	15	0 2 0	23.14
3.77	60	2 0 0	23.56
3.64	7	0 2 1	24.44
3.39	62	-1 0 3 +	26.24
3.28	100	1 2 1 +	27.18
3.25	8	-2 1 1 +	27.44
3.18	20	0 2 2	28.00
3.14	11	2 0 2 +	28.36
3.10	6	1 1 3	28.74
2.934	3	-1 2 2 +	30.44
2.914	7	-2 1 2 +	30.66
2.850	10	0 0 4	31.36
2.701	1	0 2 3	33.14
2.692	3	2 2 0	33.26
2.620	4	2 2 1 +	34.20
2.543	14	-1 2 3 +	35.26
2.531	5	-2 1 3	35.44
2.520	10	-1 1 4 +	35.60
2.457	2	-3 0 1 +	36.54
2.435	15	-2 2 2	36.88
2.428	9	1 3 0	37.00
2.371	1	-1 3 1 +	37.92
2.339	7	3 1 1 +	38.46
2.288	7	0 2 4	39.34
2.273	4	2 0 4 +	39.62
2.231	1	-1 3 2	40.40
2.204	2	3 1 2 +	40.92
2.183	10	-2 1 4 +	41.32
2.179	10	2 1 4	41.40
2.123	1	0 3 3	42.54
2.119	2	2 3 0	42.64
2.099	5	-3 0 3 +	43.06
2.082	1	2 3 1	43.42
2.069	13	3 2 1 +	43.72
2.045	4	-1 3 3	44.26
2.025	6	-3 1 3	44.72
2.022	6	3 1 3	44.78
1.975	2	-3 2 2	45.90
1.956	7	2 2 4 +	46.38
1.920	5	0 4 0	47.30
1.904	2	0 3 4	47.72
1.900	3	0 0 6 +	47.84
1.893	3	-2 1 5	48.02
1.890	3	2 1 5	48.10
1.887	3	4 0 0	48.18

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.861	6	1 4 0	48.90
1.850	2	2 3 3	49.22
1.845	3	0 1 6 +	49.36
1.842	3	-3 2 3	49.44
1.836	4	1 4 1	49.60
1.832	5	3 1 4 +	49.74
1.809	1	4 1 1	50.40
1.791	3	4 0 2 +	50.96
1.772	5	3 3 1 +	51.52
1.768	3	1 4 2	51.66
1.745	7	-4 1 2 +	52.38
1.711	7	2 4 0 +	53.50
1.703	8	0 2 6 +	53.78
1.699	9	2 3 4 +	53.92
1.695	4	-2 4 1	54.06
1.691	3	-3 0 5	54.18
1.671	7	-1 4 3 +	54.90
1.662	3	-1 3 5 +	55.24
1.658	2	-2 1 6 +	55.38
1.652	4	-3 1 5 +	55.60
1.649	5	3 1 5 +	55.70
1.639	1	2 4 2 +	56.06
1.624	6	-3 3 3 +	56.64
1.592	8	-1 0 7 +	57.86
1.560	3	-2 4 3 +	59.18
1.559	3	1 1 7 +	59.24
1.553	7	-2 2 6 +	59.46
1.549	4	-3 2 5	59.64
1.546	2	3 2 5	59.78
1.540	3	4 1 4	60.02
1.526	2	3 4 0	60.62
1.519	2	4 3 0	60.94
1.513	1	3 4 1	61.22
1.496	1	5 0 1 +	61.98
1.493	1	-1 5 1	62.14
1.487	1	3 1 6	62.42
1.474	1	3 4 2	63.02
1.468	5	5 1 1 +	63.28
1.415	2	-2 3 6 +	65.94
1.412	2	2 5 1	66.14
1.399	3	1 5 3	66.80
1.395	1	5 2 1	67.02
1.381	2	-2 5 2	67.82
1.368	1	-3 0 7	68.52
1.366	1	3 0 7	68.64
1.351	1	0 4 6 +	69.50
1.345	1	3 1 7	69.86
1.340	4	4 3 4	70.20
1.336	4	0 2 8 +	70.40
1.320	1	-4 1 6	71.38

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.37	13	0 1 1	13.89
6.30	2	-1 0 1	14.05
6.29	11	1 0 1	14.07
5.70	1	0 0 2	15.53
4.87	6	-1 1 1	18.20
4.87	8	1 1 1	18.22
4.58	1	0 1 2	19.37
3.92	11	-1 1 2	22.69
3.91	7	1 1 2	22.71
3.84	18	0 2 0	23.14
3.77	79	2 0 0	23.55
3.64	9	0 2 1	24.44
3.41	15	0 1 3	26.14
3.40	50	-1 0 3	26.21
3.39	41	1 0 3	26.25
3.39	13	2 1 0	26.29
3.28	41	-1 2 1	27.17
3.28	100	1 2 1	27.19
3.25	5	-2 1 1	27.43
3.25	1	2 1 1	27.46
3.18	27	0 2 2	27.99
3.15	4	-2 0 2	28.31
3.14	12	2 0 2	28.36
3.10	7	1 1 3	28.75
2.935	2	-1 2 2	30.43
2.933	2	1 2 2	30.45
2.914	9	-2 1 2	30.66
2.910	1	2 1 2	30.70
2.851	14	0 0 4	31.36
2.701	1	0 2 3	33.14
2.692	4	2 2 0	33.26
2.620	2	-2 2 1	34.19
2.619	5	2 2 1	34.21
2.544	14	-1 2 3	35.25
2.542	9	1 2 3	35.27
2.531	3	-2 1 3	35.44
2.527	3	2 1 3	35.50
2.520	10	-1 1 4	35.59
2.518	3	1 1 4	35.63
2.458	3	-3 0 1	36.53
2.456	1	3 0 1	36.56
2.435	22	-2 2 2	36.88
2.424	2	1 3 0	37.05
2.372	1	-1 3 1	37.91
2.371	1	1 3 1	37.91
2.339	10	3 1 1	38.45
2.335	3	0 3 2	38.52
2.269	10	0 2 4	39.33
2.277	2	-2 0 4	39.55
2.273	5	2 0 4	39.62

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.731	2	-1 3 2	40.39
2.706	1	-3 1 2	40.87
2.704	2	3 1 2	40.92
2.191	1	-1 2 4	41.16
2.189	3	1 2 4	41.20
2.186	5	0 1 5	41.26
2.184	4	-1 0 5	41.30
2.183	6	-2 1 4	41.33
2.179	8	2 1 4	41.40
2.123	1	0 3 3	42.54
2.119	3	2 3 0	42.64
2.101	1	-1 1 5	43.02
2.100	4	-3 0 3	43.04
2.099	3	1 1 5	43.06
2.096	1	3 0 3	43.12
2.083	1	2 3 1	43.42
2.070	3	-3 2 1	43.69
2.069	19	3 2 1	43.71
2.044	6	-1 3 3	44.27
2.025	8	-3 1 3	44.71
2.022	6	3 1 3	44.78
1.985	1	2 3 2	45.66
1.975	3	-3 2 2	45.91
1.958	1	-2 2 4	46.33
1.956	11	2 2 4	46.39
1.920	8	0 4 0	47.30
1.905	3	0 3 4	47.71
1.900	2	0 0 6	47.82
1.897	1	1 2 5	47.91
1.893	2	-2 1 5	48.02
1.890	2	2 1 5	48.10
1.887	4	4 0 0	48.18
1.861	10	1 4 0	48.91
1.850	2	2 3 3	49.22
1.847	1	-1 3 4	49.29
1.845	2	0 1 6	49.36
1.842	3	-3 2 3	49.43
1.836	4	1 4 1	49.60
1.833	3	-3 1 4	49.69
1.832	3	4 1 0	49.71
1.830	4	3 1 4	49.77
1.809	1	4 1 1	50.41
1.793	2	-1 1 6	50.90
1.791	2	1 1 6	50.94
1.790	3	4 0 2	50.96
1.773	1	-3 3 1	51.50
1.772	7	3 3 1	51.52
1.769	1	1 4 2	51.64
1.745	11	-4 1 2	52.37
1.744	4	4 1 2	52.43

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.714	4	0 4 3	53.42
1.712	3	-3 3 2	53.47
1.711	8	2 4 0	53.50
1.703	12	0 2 6	53.78
1.703	1	0 3 5	53.79
1.700	9	2 3 4	53.90
1.698	2	-2 0 6	53.94
1.693	1	-2 4 1	54.14
1.691	2	-3 0 5	54.19
1.675	2	4 2 1	54.76
1.671	8	-1 4 3	54.88
1.671	5	1 4 3	54.90
1.662	2	-1 2 6	55.22
1.662	2	-1 3 5	55.24
1.661	1	1 3 5	55.27
1.658	1	-2 1 6	55.35
1.656	1	2 1 6	55.43
1.652	2	-4 1 3	55.59
1.652	3	-3 1 5	55.60
1.650	1	4 1 3	55.67
1.649	5	3 1 5	55.70
1.639	1	-2 4 2	56.05
1.639	1	2 4 2	56.08
1.624	4	-4 2 2	56.62
1.623	8	-3 3 3	56.65
1.593	7	-1 0 7	57.84
1.592	3	0 4 4	57.86
1.592	6	1 0 7	57.89
1.561	2	-2 4 3	59.14
1.560	2	2 4 3	59.18
1.559	1	1 1 7	59.24
1.558	1	-1 4 4	59.24
1.553	9	-2 2 6	59.46
1.553	2	-2 3 5	59.48
1.552	2	2 2 6	59.53
1.551	1	2 3 5	59.54
1.548	1	-3 2 5	59.70
1.545	2	3 2 5	59.79
1.540	5	4 1 4	60.01
1.526	3	3 4 0	60.62
1.519	2	4 3 0	60.94
1.513	1	3 4 1	61.23
1.496	1	5 0 1	61.97
1.495	1	1 3 6	62.02
1.492	1	-1 5 1	62.15
1.486	1	3 1 6	62.42
1.474	1	3 4 2	63.01
1.470	2	1 2 7	63.19
1.469	2	-5 1 1	63.24
1.469	5	5 1 1	63.27

Hydroquinone, gamma, $C_6H_6O_2$ (monoclinic)

Structure
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/cm^3 [ibid.]

Thermal parameters
Anisotropic (ibid.)

Scattering factors
H^0, C^0, O^0 [3.3.1A]

Scale factor
(integrated intensities) 1.294×10^4

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

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.31	13	0 0 2	14.02
4.30	79	-1 1 1	20.64
4.01	2	0 1 2	22.14
3.89	54	1 1 1	22.84
3.86	100	2 0 0	23.04
3.29	11	-1 1 3	27.06
3.19	2	-2 1 1	27.96
3.10	31	2 1 0	28.78
3.08	17	-2 1 2	28.94
2.93	2	2 0 2	30.46
2.86	2	2 1 1	31.28
2.79	7	1 1 3	32.02
2.60	2	0 2 0	34.46
2.55	7	2 1 2	35.10
2.46	1	-1 2 1	36.46
2.40	14	0 2 2	37.38
2.38	5	-3 1 1	37.74
2.35	1	-1 1 5	38.22
2.29	4	-3 1 3	39.30
2.17	2	3 1 1	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	-1 3 3	57.36
1.57	1	1 1 7	58.58
1.55	2	4 2 0	59.62
1.54	1	1 3 3	60.22
1.18	1	-2 2 10	81.80

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
6.31	11	0 0 2	14.02
4.30	76	-1 1 1	20.63
4.01	1	0 1 2	22.13
3.89	49	1 1 1	22.84
3.86	100	2 0 0	23.03
3.29	12	-1 1 3	27.06
3.19	2	-2 1 1	27.97
3.10	33	2 1 0	28.79
3.08	14	-2 1 2	28.94
2.93	2	2 0 2	30.46
2.86	2	2 1 1	31.27
2.79	8	1 1 3	32.03
2.60	2	0 2 0	34.47
2.55	8	2 1 2	35.10
2.46	1	-1 2 1	36.47
2.40	16	0 2 2	37.38
2.38	6	-3 1 1	37.75
2.35	1	-1 1 5	38.22
2.29	4	-3 1 3	39.30
2.17	2	3 1 1	41.58
2.16	6	2 2 0	41.86
2.15	6	-2 2 2	41.97
2.13	3	-2 0 6	42.47
2.10	3	0 0 6	42.95
2.04	1	1 2 3	44.26
2.02	2	-4 0 2	44.89
1.95	2	2 2 2	46.65
1.88	2	-4 1 2	48.35
1.87	2	-3 2 1	48.77
1.86	1	-4 1 1	48.82
1.83	2	3 1 3	49.78
1.81	2	4 1 0	50.41
1.77	4	-1 1 7	51.60
1.76	1	3 2 1	51.95
1.71	1	4 0 2	53.53
1.64	2	-3 1 7	55.84
1.64	1	-2 0 8	56.11
1.61	3	-1 3 3	57.35
1.57	1	1 1 7	58.57
1.55	3	4 2 0	59.62
1.54	2	1 3 3	60.22
1.43	1	-3 3 3	64.99
1.23	1	2 4 0	77.40
1.18	2	-2 2 10	81.81

Lead Uranium Oxide, Pb_3UO_6 (orthorhombic)

Structure

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/cm^3

Thermal parameters

Average isotropic, [ibid.]

U: 0.12

Pb: 0.62

O: 0.90

Atomic positions

Positions used from table 3 [ibid.]

Scattering factors

O° [3.3.1A]

Pb° and U° [3.3.1B]

Scale factor

(integrated intensities) 536.6 x 10^4

Reference

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

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
6.18	2	0 2 0	14.32
6.12	6	1 1 1	14.46
6.00	2	2 1 0	14.76
4.643	1	1 2 1 +	19.10
4.005	2	2 2 1	22.18
3.945	3	1 3 0	22.52
3.556	6	1 3 1	25.02
3.523	7	2 0 2	25.26
3.427	3	4 0 0	25.98
3.386	62	2 1 2	26.30
3.353	4	3 2 1	26.56
3.302	23	4 1 0	26.98
3.243	1	2 3 1	27.48
3.089	51	0 4 0	28.88
3.060	100	2 2 2 +	29.16
2.998	44	4 2 0	29.78
2.965	3	3 1 2	30.12
2.829	4	1 4 1	31.60
2.815	5	4 2 1	31.76
2.738	1	3 2 2	32.68
2.677	22	2 3 2 +	33.44
2.635	11	4 3 0	34.00
2.627	7	1 1 3	34.10

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
2.545	3	5 1 1	35.24
2.490	1	2 1 3	36.04
2.453	1	3 3 2	36.60
2.350	1	2 2 3	38.26
2.322	5	2 4 2	38.74
2.306	2	3 1 3	39.02
2.295	2	4 4 0	39.22
2.242	1	5 1 2	40.18
2.202	3	6 0 1	40.96
2.163	1	2 3 3	41.72
2.053	16	0 0 4 +	44.08
2.040	3	3 3 3	44.36
2.023	14	2 5 2 +	44.76
2.005	4	4 5 0	45.18
1.997	20	6 0 2	45.38
1.991	12	5 4 1	45.52
1.977	1	1 6 1	45.86
1.922	1	3 5 2	47.26
1.900	1	6 2 2	47.84
1.836	3	5 5 0	49.62
1.831	5	3 6 1	49.76
1.819	2	1 5 3	50.12
1.793	3	6 4 1 +	50.90
1.778	13	2 6 2	51.34
1.765	7	4 6 0	51.74
1.754	4	6 0 3	52.10
1.750	5	7 1 2 +	52.24
1.743	6	4 1 4	52.44
1.726	1	4 6 1	53.00
1.710	14	0 4 4 +	53.56
1.705	8	3 5 3	53.72
1.697	5	8 1 0	53.98
1.693	13	4 2 4	54.12
1.677	17	6 4 2	54.68
1.663	1	8 1 1	55.20
1.652	3	8 2 0	55.60
1.628	1	5 1 4	56.46
1.624	4	7 3 2	56.62
1.619	7	4 3 4 +	56.82
1.615	4	1 1 5	56.96
1.582	2	8 3 0	58.26
1.578	4	2 7 2 +	58.42
1.570	3	4 7 0	58.78
1.549	2	3 6 3	59.66
1.545	4	0 8 0	59.82
1.525	2	6 4 3	60.66
1.516	2	1 3 5	61.08
1.512	2	9 1 0	61.26
1.509	2	1 8 1	61.38
1.486	1	7 3 3	62.46
1.476	1	8 3 2	62.90

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
6.18	1	0 2 0	14.32
6.12	5	1 1 1	14.46
5.99	2	2 1 0	14.76
4.841	1	2 1 1	18.31
4.645	1	1 2 1	19.09
4.006	2	2 2 1	22.17
3.946	3	1 3 0	22.52
3.556	6	1 3 1	25.02
3.522	6	2 0 2	25.27
3.428	2	4 0 0	25.97
3.387	64	2 1 2	26.29
3.354	2	3 2 1	26.56
3.303	23	4 1 0	26.97
3.244	1	2 3 1	27.47
3.090	53	0 4 0	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
2.816	5	4 2 1	31.75
2.738	1	3 2 2	32.68
2.677	20	2 3 2	33.44
2.677	4	5 1 0	33.45
2.635	12	4 3 0	34.00
2.623	3	1 1 3	34.16
2.545	3	5 1 1	35.23
2.490	1	2 1 3	36.05
2.453	1	3 3 2	36.60
2.351	1	2 2 3	38.26
2.323	5	2 4 2	38.74
2.307	2	3 1 3	39.02
2.295	1	4 4 0	39.22
2.242	1	5 1 2	40.18
2.201	4	6 0 1	40.96
2.163	1	2 3 3	41.72
2.053	19	0 0 4	44.08
2.051	1	5 4 0	44.12
2.040	3	3 3 3	44.37
2.026	3	1 4 3	44.69
2.023	15	2 5 2	44.75
2.005	4	4 5 0	45.19
1.997	24	6 0 2	45.39
1.990	1	5 4 1	45.55
1.977	1	1 6 1	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	49.76
1.818	3	1 5 3	50.13

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.793	2	6 4 1	50.89
1.792	2	5 5 1	50.92
1.778	17	2 6 2	51.34
1.766	8	4 6 0	51.73
1.754	3	6 0 3	52.10
1.751	1	1 7 0	52.19
1.750	3	7 1 2	52.23
1.743	8	4 1 4	52.44
1.726	1	4 6 1	53.00
1.713	1	1 7 1	53.45
1.710	16	0 4 4	53.56
1.708	2	3 6 2	53.62
1.702	1	3 5 3	53.80
1.698	4	8 1 0	53.97
1.693	15	4 2 4	54.11
1.677	22	6 4 2	54.69
1.662	1	8 1 1	55.21
1.651	3	8 2 0	55.61
1.629	1	5 1 4	56.45
1.624	4	7 3 2	56.61
1.619	6	4 3 4	56.81
1.619	2	8 2 1	56.82
1.616	2	1 1 5	56.92
1.582	2	8 3 0	58.26
1.580	1	7 1 3	58.37
1.578	4	2 7 2	58.42
1.570	3	4 7 0	58.78
1.548	2	3 6 3	59.66
1.545	4	0 8 0	59.81
1.525	3	6 4 3	60.66
1.516	2	1 3 5	61.08
1.512	1	9 1 0	61.26
1.509	2	1 8 1	61.38
1.486	1	7 3 3	62.46
1.476	1	8 3 2	62.69
1.440	1	4 2 5	64.67
1.434	2	4 5 4	64.97
1.429	1	9 3 0	65.25
1.411	1	3 7 3	66.16
1.408	2	8 5 0	66.31
1.400	2	5 1 5	66.78
1.388	1	8 5 1	67.41
1.368	2	5 5 4	68.51
1.339	1	1 8 3	70.24
1.339	5	4 6 4	70.27
1.334	4	2 1 6	70.54
1.332	1	1 7 4	70.65

Structure

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/cm^3

Thermal parameters

Anisotropic [ibid.]

Scattering factors

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

Scale factor

(integrated intensities) 1.383 × 10^4

Polymorphism

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

Reference

Burns, J.H., A.C. Tennissen, and G.D.Brunton (1968). The crystal structure of α-Li_3AlF_6, Acta Cryst. B24, 225-230.

Garton, G. and B.M. Wanklyn (1965). Polymorphism in Li_3AlF_6, J. Inorg.Nucl.Chem. 27, 2466-2469.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
6.223	6	1 1 0	14.22
4.195	42	0 1 1	21.16
4.115	100	2 1 0 +	21.58
3.837	2	1 1 1	23.16
3.404	21	2 0 1	26.16
2.959	2	3 1 0	30.18
2.623	17	2 2 1	34.16
2.529	1	3 1 1	35.46
2.4377	2	0 0 2	36.84
2.3902	4	0 3 1	37.60
2.3768	18	4 0 0 +	37.82
2.3190	6	1 3 1	38.80
2.1691	50	2 0 2	41.60
2.1358	97	2 3 1 +	42.28
2.0980	3	2 1 2	43.08
2.0687	2	4 1 1	43.72
1.9088	5	3 3 1	47.60
1.8968	5	4 2 1	47.92

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.8813	1	3 1 2	48.34
1.8532	1	5 1 0	49.12
1.7609	1	2 4 1	51.88
1.7019	21	4 0 2 +	53.82
1.6857	25	4 3 1	54.38
1.6671	3	4 1 2	55.04
1.6269	1	3 4 1	56.52
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 2	62.12
1.4887	2	5 3 1	62.32
1.4818	3	4 4 1 +	62.64
1.4463	1	4 3 2	64.36
1.4407	6	2 2 3	64.64
1.4154	6	6 2 1	65.94
1.3982	13	0 3 3	66.86
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	5	6 3 1	71.34
1.3117	6	6 1 2 +	71.92
1.3039	1	4 5 1	72.42
1.2723	1	2 6 1	74.52
1.2320	1	2 4 3	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
1.1566	2	0 5 3	83.52
1.1430	1	0 7 1 +	84.74
1.1348	1	6 0 3	85.50
1.1186	1	3 6 2	87.04
1.1119	1	8 2 1	87.70
1.0848	2	4 0 4 +	90.48
1.0679	2	4 6 2	92.32
1.0596	1	8 1 2	93.26
1.0488	1	0 4 4	94.52
1.0339	2	6 5 2	96.32
.9596	1	6 1 4 +	106.78
.9448	1	10 1 0	109.24
.8057	2	8 3 3	116.52
.9022	1	2 3 5	117.24
.8969	1	4 1 5	118.38

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.223	4	1 1 0	14.22
4.195	34	0 1 1	21.16
4.117	73	2 1 0	21.57
4.115	16	0 2 0	21.58
3.838	2	1 1 1	23.15
3.404	19	2 0 1	26.15
2.958	2	3 1 0	30.19
2.623	16	2 2 1	34.16
2.529	1	3 1 1	35.46
2.4381	2	0 0 2	36.83
2.3908	3	0 3 1	37.59
2.3775	18	4 0 0	37.81
2.3761	1	2 3 0	37.83
2.3187	6	1 3 1	38.81
2.1695	53	2 0 2	41.59
2.1370	1	4 0 1	42.26
2.1360	100	2 3 1	42.28
2.0978	3	2 1 2	43.08
2.0684	2	4 1 1	43.73
1.9088	5	3 3 1	47.60
1.8965	6	4 2 1	47.93
1.8814	1	3 1 2	48.34
1.8531	1	5 1 0	49.12
1.7608	1	2 4 1	51.88
1.7022	22	4 0 2	53.81
1.7017	2	2 3 2	53.83
1.6858	29	4 3 1	54.36
1.6669	3	4 1 2	55.05
1.6269	1	3 4 1	56.52
1.5729	6	4 2 2	58.64
1.5724	1	0 4 2	58.67
1.5595	1	0 5 1	59.20
1.5557	3	4 4 0	59.36
1.5554	6	2 5 0	59.37
1.5118	2	2 1 3	61.26
1.4929	1	2 4 2	62.13
1.4884	2	5 3 1	62.33
1.4821	2	4 4 1	62.63
1.4818	1	2 5 1	62.64
1.4463	1	4 3 2	64.36
1.4407	7	2 2 3	64.64
1.4154	7	6 2 1	65.94
1.3984	18	0 3 3	66.65
1.3835	2	1 3 3	67.67
1.3724	2	6 3 0	68.29
1.3716	6	0 6 0	68.33
1.3575	2	1 6 0	69.14
1.3289	3	6 0 2	70.85
1.3243	2	4 1 3	71.13
1.3211	6	6 3 1	71.33

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.3119	4	6 1 2	71.91
1.3115	2	4 4 2	71.94
1.3113	2	2 5 2	71.95
1.3040	1	4 5 1	72.42
1.2722	1	2 6 1	74.52
1.2319	2	2 4 3	77.41
1.2159	2	6 4 1	78.62
1.2053	1	4 3 3	79.44
1.1959	1	6 3 2	80.19
1.1887	2	8 0 0	80.78
1.1881	1	4 6 0	80.84
1.1861	1	1 6 2	81.00
1.1809	3	2 0 4	81.43
1.1689	1	2 1 4	82.45
1.1688	1	0 2 4	82.45
1.1593	3	2 6 2	83.28
1.1565	1	0 5 3	83.52
1.1437	1	8 1 1	84.67
1.1429	1	0 7 1	84.75
1.1348	1	6 0 3	85.50
1.1185	1	3 6 2	87.05
1.1120	1	8 2 1	87.69
1.0848	2	4 0 4	90.48
1.0846	1	2 3 4	90.50
1.0680	3	4 6 2	92.31
1.0596	1	8 1 2	93.26
1.0488	1	0 4 4	94.52
1.0339	2	6 5 2	96.32
1.0121	1	5 6 2	99.12
1.0071	1	8 4 1	99.79
.9663	1	6 0 4	105.72
.9597	1	6 1 4	106.76
.9595	1	2 5 4	106.80
.9544	1	6 6 2	107.62
.9447	2	10 1 0	109.25
.9306	1	2 2 5	111.73
.9057	3	8 3 3	116.53
.9022	1	2 3 5	117.25
.8983	1	8 6 0	118.07
.8969	1	4 1 5	118.37
.8949	1	2 6 4	118.80
.8843	2	4 7 3	121.16
.8831	1	2 9 1	121.44
.8805	1	6 7 2	122.04
.8804	1	4 8 2	122.07
.8743	1	6 6 3	123.53

Lithium Azide, LiN_3 (monoclinic)

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

Lattice parameters
a=5.627,b=3.319, c=4.979Å,β=107.4°[ibid.]

Density
(calculated) 1.832 g/cm^3

Thermal parameters
Anisotropic [ibid.]

Scattering factors
Li^0 [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)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
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	0 2 0	55.32
1.629	15	-3 1 1	56.44
1.587	1	-2 0 3	58.06
1.508	3	-3 1 2	61.42
1.415	4	-2 2 1	65.96
1.412	4	2 2 0	66.14
1.407	1	-4 0 1	66.40
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	-1 1 4	83.04
1.070	1	-1 3 1	92.04
1.054	1	-5 1 2	93.94
1.050	1	-4 2 2	94.42
.994	1	3 1 3	101.62

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
4.75	25	0 0 1	18.66
2.82	91	1 1 0	31.67
2.71	60	-2 0 1	33.02
2.68	26	2 0 0	33.35
2.61	100	-1 1 1	34.27
2.38	2	0 0 2	37.84
2.12	4	-2 0 2	42.58
2.09	4	2 0 1	43.35
1.977	2	-1 1 2	45.85
1.691	2	1 1 2	54.18
1.660	10	0 2 0	55.31
1.629	18	-3 1 1	56.44
1.588	1	-2 0 3	58.05
1.567	1	0 2 1	58.90
1.508	4	-3 1 2	61.41
1.415	5	-2 2 1	65.95
1.412	3	2 2 0	66.14
1.407	1	-4 0 1	66.41
1.355	4	-4 0 2	69.28
1.307	1	-2 2 2	72.21
1.297	2	1 1 3	72.87
1.214	1	2 0 3	78.74
1.188	1	0 0 4	80.86
1.162	1	-1 1 4	83.03
1.084	1	1 3 0	90.61
1.071	1	-1 3 1	92.03
1.054	2	-5 1 2	93.94
1.050	2	-4 2 2	94.42
1.038	1	1 1 4	95.81
.998	1	-5 1 3	101.10
.994	1	-2 0 5	101.58
.994	1	3 1 3	101.63
.966	1	0 2 4	105.78
.952	1	-3 3 1	108.00
.947	1	-1 1 5	108.91
.929	1	-3 1 5	112.03
.903	1	-6 0 3	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.

Structure
Tetragonal, $I4_1cd$ (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) 7.114×10^4

Reference
Krogh-Moe, J. (1968). Refinement of the crystal structure of lithium diborate, $Li_2O \cdot 2B_2O_3$, Acta Cryst. **B24**, 179-181.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
4.736	5	2 0 0	18.72
4.077	100	1 1 2	21.78
3.917	12	2 1 1	22.68
3.485	30	2 0 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 0 0	37.94
2.259	1	2 0 4	39.88
2.244	7	4 1 1	40.16
2.152	1	4 0 2	41.94
2.120	2	4 2 0	42.62
2.086	6	3 2 3	43.34
2.049	14	3 3 2	44.16

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.040	9	2 2 4	44.38
1.959	6	4 2 2	46.30
1.951	6	3 1 4	46.50
1.909	5	4 1 3	47.60
1.865	1	4 3 1	48.80
1.850	3	2 1 5	49.22
1.748	2	5 1 2	52.28
1.742	2	4 0 4	52.48
1.735	6	5 2 1	52.72
1.659	7	4 3 3 +	55.32
1.635	4	4 2 4	56.20
1.620	3	3 2 5	56.80
1.611	1	2 0 6	57.12
1.566	1	5 2 3	58.94
1.550	1	5 3 2	59.60
1.541	2	6 1 1	60.00
1.533	1	4 1 5	60.34
1.493	2	6 2 0	61.86
1.487	1	3 1 6	62.38
1.465	1	5 4 1	63.44
1.400	1	6 3 1	66.76
1.388	2	4 0 6	67.40
1.337	1	5 2 5	70.34
1.295	2	6 2 4	73.02
1.260	1	5 1 6	75.38
1.2420	1	6 1 5	76.66
1.2376	1	4 1 7	76.98
1.2097	2	7 3 2	79.10
1.2054	1	6 5 1	79.44
1.1680	1	7 4 1	82.52
1.1616	1	6 0 6	83.08
1.1275	1	5 2 7	86.18
1.0986	1	4 2 8	89.02
1.0774	1	7 5 2	91.28
1.0761	1	8 0 4	91.42
1.0598	1	8 4 0	93.24
1.0570	1	5 1 8	93.56
1.0258	1	9 1 2	97.34
1.0245	1	6 6 4	97.50
1.0230	2	4 1 9	97.70

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
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	34.61
2.570	6	0 0 4	34.88
2.547	4	3 2 1	35.21
2.370	3	4 0 0	37.94
2.259	1	2 0 4	39.87
2.244	8	4 1 1	40.16
2.152	2	4 0 2	41.95
2.120	2	4 2 0	42.62
2.086	8	3 2 3	43.34
2.049	17	3 3 2	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	2 1 5	49.21
1.748	2	5 1 2	52.29
1.742	2	4 0 4	52.48
1.735	8	5 2 1	52.72
1.660	5	1 1 6	55.30
1.659	6	4 3 3	55.34
1.635	6	4 2 4	56.21
1.620	5	3 2 5	56.80
1.611	1	2 0 6	57.12
1.580	1	6 0 0	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	3 1 6	62.37
1.465	1	5 4 1	63.43
1.400	1	6 3 1	66.77
1.388	3	4 0 6	67.39
1.374	1	5 3 4	68.20
1.341	1	7 1 0	70.14
1.337	1	5 2 5	70.35
1.315	1	6 4 0	71.75
1.295	3	6 2 4	73.02
1.260	2	5 1 6	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)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.1811	1	3 1 8	81.42
1.1793	1	5 3 6	81.56
1.1703	1	6 4 4	82.32
1.1681	1	7 4 1	82.51
1.1645	1	6 3 5	82.82
1.1614	1	6 0 6	83.09
1.1276	2	5 2 7	86.17
1.1202	1	7 3 4	86.89
1.1121	1	7 4 3	87.68
1.0986	1	4 2 8	89.01
1.0774	2	7 5 2	91.27
1.0760	2	8 0 4	91.43
1.0598	1	8 4 0	93.24
1.0571	1	5 1 8	93.56
1.0257	3	9 1 2	97.35
1.0245	1	6 6 4	97.50
1.0229	2	4 1 9	97.70
1.0070	1	7 3 6	99.80
.8806	1	3 2 11	122.03
.8616	1	6 0 10	126.75
.8431	1	6 6 8	132.03
.8294	1	8 6 6	136.46
.8237	1	3 1 12	138.51
.8230	1	10 5 3	138.76
.8207	1	11 3 2	139.62
.7926	1	7 3 10	152.74
.7888	1	9 3 8	155.13
.7838	1	10 5 5	158.68

Magnesium Selenite Hydrate, $MgSeO_3 \cdot 6H_2O$ (hexagonal)

Structure
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/cm^3 [ibid.]

Thermal parameters
Isotropic [ibid.]

Scattering factors
Mg^0 and O^{-1} [3.3.1A]
Se^0 [3.3.1B]

Scale factor
(integrated intensities) 6.841 x 10^4

Additional patterns
1. PDF card 20-687[Leshchinskaya and Selivanova,1966]

Reference

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)	*I*	*hkl*	2θ(°) λ = 1.54056 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 0 3	29.98
2.927	29	2 0 2	30.52
2.783	32	2 1 1	32.14
2.582	6	3 0 0	34.72
2.479	9	1 1 3 +	36.20
2.449	21	2 1 -2 +	36.66
2.236	2	2 2 0	40.30
2.146	1	1 0 4	42.06
2.089	5	1 3 1	43.28
1.951	4	3 0 3 +	46.50
1.936	17	1 3 -2 +	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	4 1 3 +	63.20
1.463	3	4 0 4 +	63.52
1.445	1	4 2 -1 +	64.44
1.413	2	1 1 6 +	66.06
1.391	5	3 2 4 +	67.26
1.374	1	1 3 -5	68.20
1.328	2	1 5 2 +	70.88
.290	2	6 0 0 +	73.30
1.260	1	3 4 -1	75.34
1.240	2	2 2 6 +	76.84
1.225	2	3 4 2 +	77.96
1.185	1	0 6 3	81.12
1.170	1	1 2 -7	82.32
1.142	1	1 6 -2	84.82
1.117	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

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
5.85	27	1 0 1	15.12
4.47	100	1 1 0	19.84
3.870	69	0 1 2	22.96
3.553	12	0 2 1	25.04
2.979	19	0 0 3	29.97
2.926	34	2 0 2	30.52
2.782	38	2 1 1	32.15
2.582	7	3 0 0	34.72
2.479	10	1 1 3	36.20
2.479	1	1 1 -3	36.20
2.449	3	1 2 2	36.67
2.449	24	2 1 -2	36.67
2.236	3	2 2 0	40.30
2.147	2	1 0 4	42.06
2.089	6	1 3 1	43.28
1.951	1	0 3 3	46.51
1.951	4	3 0 3	46.51
1.936	5	3 1 2	46.89
1.936	13	1 3 -2	46.89
1.935	6	0 2 4	46.91
1.893	2	4 0 1	48.03
1.788	4	2 2 3	51.03
1.788	1	2 2 -3	51.03
1.777	2	0 4 2	51.38
1.776	13	2 1 4	51.41
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	8	1 4 0	54.22
1.651	3	2 3 2	55.61
1.651	3	3 2 -2	55.61
1.623	1	2 0 5	56.68
1.548	3	1 3 4	59.66
1.548	2	3 1 -4	59.66
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
1.470	1	1 4 3	63.20
1.470	1	1 4 -3	63.20
1.470	1	4 1 -3	63.20
1.464	2	5 0 2	63.51
1.463	2	4 0 4	63.53
1.445	1	2 4 1	64.45
1.445	1	4 2 -1	64.45
1.413	2	1 1 6	66.07
1.413	1	1 1 -6	66.07
1.391	2	4 2 2	67.25

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.391	2	2 4 -2	67.25
1.391	3	3 2 4	67.27
1.391	2	2 3 -4	67.27
1.374	1	1 3 -5	68.20
1.328	2	1 5 2	70.89
1.328	1	5 1 -2	70.89
1.291	3	6 0 0	73.26
1.290	1	0 3 6	73.32
1.290	1	3 0 6	73.32
1.261	2	3 4 -1	75.33
1.240	1	5 2 0	76.78
1.240	2	2 5 0	76.78
1.240	2	2 2 6	76.84
1.225	2	3 4 2	77.95
1.224	1	4 2 -4	77.97
1.184	1	0 6 3	81.13
1.170	1	1 2 -7	82.34
1.142	1	1 6 -2	84.83
1.117	1	4 1 6	87.15
1.117	1	4 1 -6	87.15
1.106	1	3 4 -4	88.26
1.097	1	3 1 -7	89.16
1.044	1	6 2 -2	95.05
.926	1	2 7 -2	112.67

Structure

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

Lattice parameters

a=8.949±.002Å [ibid.]

Density

(calculated) 6.827 g/cm^3 [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 × 10^4

Additional patterns

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

Reference

Aurivillius, K. (1967). An x-ray single crystal study of $Hg_3S_2Cl_2$, Arkiv Kemi 26(6), 497-505.

Carlson, E.H. (1967). The growth of HgS and $Hg_3S_2Cl_2$ 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 $Hg_3S_2Cl_2$, Acta Cryst. B24, 156-157.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
6.330	43	1	1	0		13.98
4.476	14	2	0	0		19.82
3.654	100	2	1	1		24.34
3.164	1	2	2	0		28.18
2.829	47	0	1	3		31.60
2.583	36	2	2	2		34.70
2.391	24	1	2	3	+	37.58
2.237	24	4	0	0		40.28
2.109	20	4	1	1	+	42.84
2.001	8	4	2	0		45.28
1.908	3	3	3	2		47.62
1.827	1	4	2	2		49.88
1.7553	22	1	3	4	+	52.06
1.6338	10	5	2	1	+	56.26
1.5819	5	4	4	0		58.28
1.5345	8	4	3	3	+	60.26
1.4917	1	4	4	2		62.18
1.4516	9	2	3	5	+	64.10
1.4151	2	0	2	6		65.96
1.3807	2	5	4	1	+	67.82
1.3490	2	6	2	2		69.64
1.3194	2	6	3	1	+	71.44
1.2656	5	0	1	7	+	74.98
1.2177	2	6	3	3		78.48
1.1959	2	2	4	6		80.20
1.1365	3	1	5	6	+	85.34
1.1015	3	7	4	1	+	88.74
1.0852	1	8	2	0		90.44
1.0695	1	3	5	6	+	92.14
1.0403	3	1	3	8	+	95.54
.9434	1	7	5	4		109.48
.9230	1	9	3	2	+	113.14
.8775	1	8	6	2	+	122.76
.8382	1	1	7	8		133.56
.8102	1	9	5	4	+	143.88
.7972	1	3	6	9	+	150.12

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.328	38	1 1 0	13.98
4.475	13	2 0 0	19.83
3.653	100	2 1 1	24.34
3.164	1	2 2 0	28.18
2.830	53	0 1 3	31.59
2.583	40	2 2 2	34.70
2.392	7	3 2 1	37.58
2.392	20	1 2 3	37.58
2.237	28	4 0 0	40.28
2.109	11	3 3 0	42.84
2.109	13	4 1 1	42.84
2.001	9	4 2 0	45.28
1.908	3	3 3 2	47.62
1.827	1	4 2 2	49.88
1.7550	6	4 3 1	52.07
1.7550	24	1 3 4	52.07
1.6339	12	5 2 1	56.26
1.6339	1	1 2 5	56.26
1.5820	7	4 4 0	58.28
1.5347	1	5 3 0	60.25
1.5347	9	4 3 3	60.25
1.5347	1	0 3 5	60.25
1.4915	1	4 4 2	62.19
1.4517	5	6 1 1	64.09
1.4517	3	5 3 2	64.09
1.4517	5	2 3 5	64.09
1.4150	2	0 2 6	65.96
1.3809	2	5 4 1	67.81
1.3809	2	1 4 5	67.81
1.3491	3	6 2 2	69.63
1.3195	3	6 3 1	71.43
1.3195	1	1 3 6	71.43
1.2917	1	4 4 4	73.22
1.2656	2	5 4 3	74.98
1.2656	2	0 1 7	74.98
1.2656	1	5 5 0	74.98
1.2656	1	7 1 0	74.98
1.2656	2	3 4 5	74.98
1.2410	1	6 4 0	76.73
1.2178	1	6 3 3	78.47
1.1959	2	2 4 6	80.20
1.1751	1	0 3 7	81.92
1.1365	1	7 3 2	85.34
1.1365	3	1 5 6	85.34
1.1015	1	5 5 4	88.74
1.1015	3	7 4 1	88.74
1.1015	2	1 4 7	88.74
1.0852	2	8 2 0	90.44
1.0696	1	6 5 3	92.13
1.0696	2	3 5 6	92.13

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.0546	1	8 2 2	93.83
1.0403	1	7 5 0	95.54
1.0403	2	7 4 3	95.54
1.0403	2	1 3 8	95.54
.9883	1	8 3 3	102.42
.9764	1	2 4 8	104.16
.9433	2	7 5 4	109.49
.9230	1	9 3 2	113.13
.9230	1	3 6 7	113.13
.8949	1	0 6 8	118.80
.8775	1	0 2 10	122.75
.8775	2	8 6 2	122.75
.8382	1	1 7 8	133.57
.8309	1	4 6 8	135.96
.8169	1	2 4 10	141.09
.8169	1	10 4 2	141.09
.8102	1	9 5 4	143.88
.8102	1	3 7 8	143.88
.7972	1	1 5 10	150.11
.7972	2	11 2 1	150.11
.7972	2	3 6 9	150.11

Structure
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/cm^3

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]
Nb^0 [3.3.1A]
F^0 [Cromer and Waber,1965]

Scale factor
(integrated intensities) 7.495×10^4

Additional patterns
1. PDF card 18-1013 [Mukhtar and Winand, 1965]

Reference
Brown, G.M. and L.A. Walker(1966). Refinement of the structure of potassium heptafluoroniobate, K_2NbF_7, from neutron-diffraction 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 $KF-K_2NbF_7$, Compt. Rend. 260, 3674-3676.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ λ = 1.54056 Å
7.06	2	0	1	1		12.52
6.35	2	0	2	0		13.94
5.85	2	1	0	0		15.14
5.31	58	1	1	0		16.68
5.09	100	0	2	1		17.42
4.50	42	1	1	1	+	19.70
4.26	38	0	0	2		20.84
4.04	1	0	1	2		22.00
3.837	6	1	2	1	+	23.16
3.789	6	0	3	1		23.46
3.537	3	0	2	2		25.16
3.440	34	-1	0	2	+	25.88
3.427	67	1	3	0		25.98
3.321	64	1	1	2	+	26.82
3.180	41	-1	3	1	+	28.04
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	16	2	0	0		30.56
2.789	1	1	4	0		32.06
2.701	3	-2	1	1	+	33.14
2.670	4	1	3	2		33.54
2.654	2	2	2	0		33.74
2.650	2	-1	4	1		33.80
2.590	2	0	2	3		34.60
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	-2	1	2		37.98
2.328	6	1	5	0		38.64
2.314	8	-2	3	1	+	38.88
2.253	12	-2	2	2	+	39.98
2.247	8	1	5	1		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	+	43.16
2.085	6	2	4	1	+	43.36
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	5	-1	4	3	+	45.56
1.976	4	1	1	4	+	45.88
1.939	17	2	2	3	+	46.82
1.919	13	2	4	2	+	47.32
1.908	4	1	2	4	+	47.62

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.878	2	-3 1 1	48.42
1.835	1	-2 3 3	49.64
1.820	2	-3 2 1	50.08
1.808	3	1 3 4	50.42
1.800	4	1 5 3	50.66
1.770	9	3 3 0 +	51.60
1.755	4	3 1 2 +	52.08
1.748	2	-2 5 2	52.30
1.732	4	1 7 0 +	52.80
1.721	5	2 0 4 +	53.18
1.714	2	2 6 0	53.42
1.705	2	-2 1 4 +	53.70
1.697	8	-1 7 1 +	53.98
1.693	6	-1 4 4 +	54.14
1.688	3	0 1 5	54.30
1.680	9	-2 6 1 +	54.58
1.645	1	0 2 5	55.84
1.634	3	-3 3 2 +	56.24
1.630	3	-1 6 3	56.42
1.622	3	-1 1 5 +	56.72
1.604	1	1 7 2	57.40
1.594	3	3 1 3 +	57.80
1.590	3	2 6 2	57.96
1.586	2	0 8 0	58.10
1.583	4	-1 2 5 +	58.22
1.580	3	0 3 5	58.36
1.571	2	1 5 4 +	58.72
1.558	1	-3 2 3	59.28
1.547	3	-3 4 2 +	59.72
1.528	1	0 7 3	60.54
1.525	2	1 3 5 +	60.68
1.513	4	2 4 4 +	61.22
1.502	1	3 3 3	61.72
1.487	1	0 8 2	62.42
1.478	4	-1 7 3 +	62.80
1.467	3	2 6 3 +	63.34
1.461	3	4 0 0	63.62
1.453	2	3 5 2	64.02
1.433	2	2 2 5	65.02
1.414	2	-3 6 1 +	66.04
1.410	2	0 1 6	66.22
1.405	1	4 2 1	66.50
1.402	2	-3 2 4 +	66.66
1.390	1	-2 3 5	67.32
1.382	1	4 0 2	67.74
1.379	4	-1 0 6 +	67.90
1.371	1	1 9 0	68.36
1.363	1	-4 3 1	68.80
1.361	1	3 3 4	68.94
1.358	2	3 5 3 +	69.14

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
7.07	2	0 1 1	12.51
6.35	2	0 2 0	13.94
5.85	2	1 0 0	15.14
5.31	58	1 1 0	16.68
5.09	100	0 2 1	17.41
4.51	28	1 1 1	19.69
4.51	18	-1 1 1	19.69
4.26	43	0 0 2	20.85
4.04	2	0 1 2	22.00
3.838	5	1 2 1	23.15
3.838	1	-1 2 1	23.15
3.789	7	0 3 1	23.46
3.536	3	0 2 2	25.17
3.442	11	1 0 2	25.67
3.442	21	-1 0 2	25.87
3.428	68	1 3 0	25.97
3.322	45	1 1 2	26.82
3.322	28	-1 1 2	26.82
3.180	18	1 3 1	28.04
3.180	27	-1 3 1	28.04
3.173	9	0 4 0	28.10
3.025	1	-1 2 2	29.50
3.001	3	0 3 2	29.74
2.973	1	0 4 1	30.03
2.923	19	2 0 0	30.56
2.789	1	1 4 0	32.07
2.701	1	2 1 1	33.14
2.701	2	-2 1 1	33.14
2.670	5	1 3 2	33.54
2.655	1	2 2 0	33.73
2.650	1	-1 4 1	33.79
2.591	3	0 2 3	34.59
2.544	2	0 4 2	35.25
2.535	3	-2 2 1	35.38
2.503	9	1 1 3	35.84
2.503	1	-1 1 3	35.84
2.433	2	0 5 1	36.92
2.410	2	2 0 2	37.28
2.410	5	-2 0 2	37.28
2.367	1	-2 1 2	37.98
2.333	1	1 4 2	38.56
2.329	7	1 5 0	38.63
2.314	2	2 3 1	38.88
2.314	8	-2 3 1	38.88
2.253	7	2 2 2	39.99
2.253	10	-2 2 2	39.99
2.246	1	1 5 1	40.11
2.186	2	1 3 3	41.26
2.150	4	2 4 0	41.99
2.129	3	0 0 4	42.43

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.116	5	0 4 3	42.71
2.116	3	0 6 0	42.71
2.099	18	0 1 4	43.05
2.094	4	2 3 2	43.17
2.094	13	-2 3 2	43.17
2.084	4	2 4 1	43.37
2.084	2	-2 4 1	43.37
2.053	22	0 6 1	44.07
2.043	1	-1 5 2	44.30
2.018	1	0 2 4	44.87
2.000	3	1 0 4	45.30
2.000	2	-1 0 4	45.30
1.989	3	1 4 3	45.56
1.989	4	-1 4 3	45.56
1.976	3	1 1 4	45.89
1.976	2	-1 1 4	45.89
1.939	14	2 2 3	46.82
1.939	6	-2 2 3	46.82
1.937	2	1 6 1	46.86
1.937	5	-1 6 1	46.86
1.919	11	2 4 2	47.33
1.919	7	-2 4 2	47.33
1.908	4	1 2 4	47.63
1.908	1	-1 2 4	47.63
1.879	2	-3 1 1	48.41
1.835	1	-2 3 3	49.64
1.820	3	-3 2 1	50.08
1.808	3	1 3 4	50.42
1.800	4	1 5 3	50.67
1.772	1	3 0 2	51.54
1.772	6	-3 0 2	51.54
1.770	9	3 3 0	51.60
1.755	3	3 1 2	52.07
1.755	2	-3 1 2	52.07
1.748	2	-2 5 2	52.30
1.733	2	3 3 1	52.73
1.733	3	-3 3 1	52.78
1.732	3	1 7 0	52.82
1.721	4	2 0 4	53.18
1.721	2	-2 0 4	53.18
1.714	1	2 6 0	53.42
1.707	1	3 2 2	53.66
1.705	2	-2 1 4	53.71
1.697	6	-1 7 1	53.98
1.697	4	1 7 1	53.98
1.696	1	0 6 3	54.02
1.692	2	1 4 4	54.16
1.692	2	-1 4 4	54.16
1.688	2	0 1 5	54.31
1.680	8	-2 6 1	54.58

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.680	5	2 6 1	54.58
1.645	1	0 2 5	55.85
1.634	2	3 3 2	56.24
1.634	3	-3 3 2	56.24
1.629	1	-1 6 3	56.44
1.622	2	1 1 5	56.72
1.622	3	-1 1 5	56.72
1.604	1	1 7 2	57.39
1.594	1	-2 3 4	57.79
1.594	2	3 1 3	57.80
1.590	1	2 6 2	57.96
1.587	2	0 8 0	58.09
1.583	1	1 2 5	58.22
1.583	2	-1 2 5	58.22
1.580	2	0 3 5	58.36
1.571	2	1 5 4	58.72
1.571	1	-1 5 4	58.72
1.557	2	-3 2 3	59.29
1.547	3	-3 4 2	59.72
1.546	2	3 5 0	59.78
1.528	1	0 7 3	60.54
1.525	1	1 3 5	60.67
1.525	1	-1 3 5	60.67
1.513	5	2 4 4	61.22
1.513	2	-2 4 4	61.22
1.502	2	3 3 3	61.71
1.487	2	0 8 2	62.41
1.478	3	1 7 3	62.60
1.478	3	-1 7 3	62.80
1.467	3	2 6 3	63.34
1.467	1	-2 6 3	63.34
1.462	4	4 0 0	63.61
1.453	1	3 5 2	64.03
1.433	2	2 2 5	65.01
1.414	1	0 5 5	66.00
1.413	2	-3 6 1	66.05
1.410	1	0 1 6	66.21
1.405	1	4 2 1	66.51
1.402	1	3 2 4	66.66
1.402	1	-3 2 4	66.66
1.390	1	-2 3 5	67.32
1.382	1	4 0 2	67.73
1.380	1	0 7 4	67.84
1.379	2	1 0 6	67.91
1.379	3	-1 0 6	67.91
1.371	2	1 3 0	68.37
1.364	1	-4 3 1	68.79
1.361	1	3 3 4	68.94
1.358	1	3 5 3	69.14
1.358	1	-3 5 3	69.14

Reserpine, $C_{33}H_{40}N_2O_9$ (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) 4.708×10^4

Additional patterns

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

Reference

Karle, I.L. and J. Karle (1968). The crystal structure of the alkaloid reserpine, $C_{33}H_{40}N_2O_9$, Acta Cryst. B24 81-91.

Rose, H.A. (1954). Crystallographic Data. 83.Reserpine, Anal. Chem. 26 1245.

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
13.06	47	1 0 0	6.76
12.10	44	0 0 1	7.30
11.68	10	-1 0 1	7.56
7.43	36	1 0 1 +	11.90
7.20	100	0 1 1 +	12.28
6.68	5	-1 0 2	13.24
6.53	5	2 0 0	13.54
6.05	5	0 0 2	14.64
5.73	45	1 1 1	15.46
5.60	3	-2 1 1	15.82
5.36	33	-1 1 2	16.54
5.29	9	2 1 0	16.76
5.02	69	0 1 2	17.66
4.90	13	-2 1 2	18.08
4.77	60	1 0 2	18.58
4.58	5	-3 0 2	19.36
4.49	63	0 2 0	19.76
4.42	4	-1 0 3	20.08
4.36	3	-2 0 3	20.36
4.33	5	2 1 1	20.50
4.25	38	1 2 0 +	20.90
4.21	22	0 2 1 +	21.08
4.19	35	-1 2 1	21.18
4.08	7	-3 1 2	21.76
4.03	13	0 0 3	22.02
3.97	1	-1 1 3	22.40
3.92	4	-2 1 3	22.66
3.90	3	-3 0 3	22.78
3.84	16	1 2 1	23.12
3.80	16	-2 2 1	23.36
3.73	27	-1 2 2 +	23.86
3.68	4	0 1 3	24.18
3.64	2	3 0 1	24.46
3.60	4	0 2 2	24.68
3.58	18	-3 1 3 +	24.86
3.46	13	1 0 3	25.72
3.44	12	2 1 2	25.90
3.37	3	3 1 1	26.42
3.33	4	-4 1 2 +	26.76
3.31	3	-4 1 1	26.92
3.27	8	4 0 0 +	27.26
3.23	7	1 1 3	27.60
3.20	6	-3 0 4	27.82
3.13	3	3 2 0 +	28.52
3.12	4	-4 1 3	28.60
3.07	2	-1 1 4	29.06
3.02	1	0 0 4	29.52
3.02	1	-3 1 4	29.58
3.00	2	0 2 3	29.76
2.90	2	-1 3 1 +	30.80

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
2.86	4	4 0 1 +	31.20
2.81	2	-5 0 3	31.86
2.80	2	-4 2 2	31.92
2.78	2	1 3 1 +	32.20
2.76	8	-2 3 1	32.38
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	33.10
2.68	6	-5 1 3 +	33.42
2.67	3	-2 3 2	33.60
2.64	2	-1 2 4	33.90
2.62	1	5 0 0	34.26
2.59	2	1 1 4	34.62
2.58	2	-1 0 5	34.68
2.56	1	-2 1 5	35.04
2.48	1	-1 3 3	36.22
2.47	1	-2 3 3	36.38
2.39	2	3 1 3	37.60
2.38	4	4 1 2	37.76
2.36	1	5 0 1	38.14
2.31	1	-6 1 3	38.98
2.30	1	-4 3 2	39.18
2.29	1	-2 2 5	39.24
2.28	1	-3 2 5	39.48
2.27	1	-5 1 5	39.76
2.25	5	-5 2 4 +	40.04
2.216	2	1 0 5 +	40.68
2.213	2	1 4 0	40.74
2.161	2	-3 1 6	41.76
2.151	2	1 1 5	41.96
2.143	3	-2 4 1 +	42.14
2.136	2	-1 0 6	42.28
2.119	2	-4 1 6	42.64
2.109	3	-6 2 3	42.84
2.105	3	0 4 2 +	42.94
2.064	2	-6 2 1	43.82
2.046	2	3 1 4	44.24
2.040	2	5 1 2 +	44.36
2.028	1	-5 1 6	44.64
1.996	1	-2 4 3	45.40
1.962	2	-4 2 6	46.24
1.900	1	5 2 2	47.84
1.867	1	-3 1 7	48.72
1.813	1	-6 3 4	50.12
1.775	1	-1 5 1	51.44

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
13.07	41	1 0 0	6.75
12.10	40	0 0 1	7.30
11.71	9	-1 0 1	7.55
7.44	34	1 0 1	11.89
7.40	3	1 1 0	11.95
7.21	100	0 1 1	12.26
7.17	10	-2 0 1	12.34
7.12	6	-1 1 1	12.41
6.68	5	-1 0 2	13.24
6.54	5	2 0 0	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	20.95
4.21	8	1 1 2	21.07
4.21	10	0 2 1	21.09
4.19	34	-1 2 1	21.18
4.08	8	-3 1 2	21.77
4.03	15	0 0 3	22.02
3.97	1	-1 1 3	22.40
3.92	4	-2 1 3	22.65
3.90	3	-3 0 3	22.77
3.84	18	1 2 1	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

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.33	4	-4 1 2	26.76
3.32	2	2 2 1	26.81
3.31	2	-4 1 1	26.92
3.28	1	-3 2 1	27.16
3.27	2	1 2 2	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	0 2 3	29.75
2.91	2	0 3 1	30.74
2.90	2	-1 3 1	30.81
2.87	2	0 1 4	31.18
2.86	1	2 2 2	31.20
2.86	3	4 0 1	31.21
2.81	1	-5 0 3	31.86
2.80	1	-4 2 2	31.92
2.78	1	2 1 3	32.20
2.78	1	1 3 1	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
2.64	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	37.68
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)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.28	1	-3 2 5	39.49
2.27	1	-5 1 5	39.76
2.25	5	-5 2 4	40.04
2.250	1	-6 1 1	40.04
2.219	1	-6 1 4	40.63
2.216	2	1 0 5	40.68
2.213	1	1 4 0	40.75
2.161	2	-3 1 6	41.76
2.152	2	1 1 5	41.95
2.146	1	-2 1 6	42.07
2.142	4	-2 4 1	42.14
2.134	1	-1 0 6	42.31
2.119	1	-4 1 6	42.64
2.109	3	-6 2 3	42.84
2.106	1	2 2 4	42.90
2.105	2	0 4 2	42.94
2.064	3	-6 2 1	43.82
2.046	1	3 1 4	44.24
2.042	1	5 1 2	44.32
2.040	1	-6 2 4	44.37
2.028	1	-5 1 6	44.64
1.996	1	-2 4 3	45.40
1.961	2	-4 2 6	46.25
1.900	1	5 2 2	47.83
1.867	1	-3 1 7	48.73
1.819	1	-6 3 4	50.11
1.786	1	-3 3 6	51.08
1.775	1	-1 5 1	51.43

Silver Arsenic Sulfide, xanthoconite, Ag_3AsS_3 (monoclinic)

Structure
Monoclinic, C2/c (15),Z=8 [Engel and Nowacki, 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^0 [3.3.1A]
As^0, Ag^0 [3.3.1B]

Scale factor
(integrated intensities) 61.68× 10^4

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

Reference

Engel,P. and W. Nowacki (1968). Die Kristallstruktur von Xanthokon,Ag_3AsS_3, 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)	*I*	*hkl*				$2\theta(^\circ)$ λ = 1.54056 Å
5.60	1	-2	0	2		15.82
5.47	25	1	1	0	+	16.20
4.92	3	-1	1	2		18.02
4.19	8	-1	1	3		21.20
4.01	28	0	0	4	+	22.14
3.54	4	1	1	3		25.12
3.53	4	-1	1	4		25.22
3.35	25	-3	1	2	+	26.60
3.22	7	3	1	0		27.66
3.13	55	0	2	0		28.50
3.07	30	0	2	1		29.04
3.01	82	1	1	4		29.68
2.974	100	-3	1	4		30.02
2.841	4	2	0	4		31.46
2.819	70	4	0	0	+	31.72
2.801	10	-4	0	4		31.92
2.774	13	-2	2	1		32.24
2.727	26	3	1	2		32.82
2.674	5	0	0	6		33.48
2.620	12	-2	2	3		34.20
2.579	9	-1	1	6		34.76
2.468	9	2	2	2		36.38
2.461	6	-2	2	4		36.48
2.439	7	-3	1	6		36.82
2.414	3	4	0	2		37.22
2.391	5	-4	0	6		37.58
2.277	2	-2	2	5		39.54
2.260	2	1	1	6		39.86
2.237	12	-5	1	2	+	40.28
2.197	1	-3	1	7		41.04
2.148	22	-4	2	1	+	42.02
2.135	19	-2	0	8		42.30
2.104	2	2	2	4		42.96
2.094	15	4	2	0	+	43.16
2.052	2	-1	3	1		44.10
2.033	2	0	2	6		44.52
2.020	2	1	3	1	+	44.84
2.006	12	4	0	4	+	45.16
2.000	8	1	1	7		45.30
1.994	7	-1	1	8		45.46
1.987	7	-4	0	8	+	45.62
1.982	8	-6	0	4	+	45.74
1.957	5	-1	3	3	+	46.36
1.922	13	-2	2	7		47.26
1.912	4	4	2	2		47.52
1.906	5	5	1	2		47.68
1.901	5	-4	2	6		47.82
1.877	12	1	3	3	+	48.46
1.867	8	-6	0	6		48.72
1.847	4	-3	3	2	+	49.30

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.824	3	3 3 0	49.96
1.821	4	-3 3 3	50.04
1.801	2	4 2 3	50.64
1.782	11	1 3 4 +	51.22
1.776	15	-3 3 4	51.42
1.771	12	2 2 6 +	51.56
1.763	7	-2 2 8	51.80
1.719	1	3 3 2	53.26
1.714	2	2 0 8	53.42
1.705	1	-2 0 10	53.72
1.690	6	-6 0 8 +	54.24
1.686	6	-6 2 3	54.38
1.675	4	4 0 6 +	54.74
1.667	3	5 1 4	55.04
1.660	1	-4 0 10	55.28
1.650	3	-7 1 4	55.64
1.646	3	3 3 3 +	55.82
1.636	6	-7 1 2	56.16
1.630	5	2 2 7	56.42
1.623	1	-2 2 9	56.68
1.614	4	-1 1 10	57.00
1.603	4	-6 2 6 +	57.42
1.569	1	-4 2 9	58.82
1.560	2	7 1 0	59.18
1.558	2	6 2 1 +	59.26
1.549	2	-6 2 7	59.62
1.541	2	-5 1 10	60.00
1.527	1	-5 3 5	60.58
1.515	1	-2 4 1	61.14
1.503	1	2 2 8	61.64
1.500	1	-6 0 10	61.80
1.492	1	5 3 1	62.16
1.487	3	-6 2 8 +	62.38
1.477	2	4 2 6	62.88
1.475	3	1 1 10	62.94
1.472	3	-8 0 6	63.12
1.444	1	7 1 2 +	64.46
1.437	2	-5 3 7	64.82
1.409	1	-4 0 12	66.26
1.389	2	5 3 3 +	67.34
1.383	2	-4 4 1	67.70
1.368	2	-7 1 10	68.54
1.343	1	-5 1 12	69.98

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.60	1	-2 0 2	15.81
5.47	13	1 1 0	16.18
5.46	11	-1 1 1	16.21
4.92	3	-1 1 2	18.02
4.21	2	1 1 2	21.09
4.19	7	-1 1 3	21.19
4.01	10	2 0 2	22.13
4.01	15	0 0 4	22.14
3.54	3	1 1 3	25.11
3.53	3	-1 1 4	25.23
3.36	8	-3 1 1	26.55
3.35	19	-3 1 2	26.59
3.22	7	3 1 0	27.66
3.13	56	0 2 0	28.49
3.07	30	0 2 1	29.04
3.01	86	1 1 4	29.69
2.974	100	-3 1 4	30.02
2.842	2	2 0 4	31.45
2.819	55	4 0 0	31.71
2.819	18	-2 0 6	31.72
2.801	5	-4 0 4	31.93
2.775	13	-2 2 1	32.23
2.727	27	3 1 2	32.82
2.675	6	0 0 6	33.47
2.626	1	2 2 1	34.11
2.619	12	-2 2 3	34.21
2.578	10	-1 1 6	34.77
2.468	9	2 2 2	36.37
2.459	2	-2 2 4	36.51
2.440	8	-3 1 6	36.81
2.414	3	4 0 2	37.21
2.391	5	-4 0 6	37.58
2.278	2	-2 2 5	39.54
2.260	1	1 1 6	39.86
2.241	5	0 2 5	40.21
2.237	12	-5 1 2	40.29
2.197	1	-3 1 7	41.05
2.149	9	2 0 6	42.01
2.148	17	-4 2 1	42.02
2.135	20	-2 0 8	42.30
2.104	1	2 2 4	42.95
2.095	13	4 2 0	43.15
2.095	4	-2 2 6	43.15
2.051	2	-1 3 1	44.11
2.034	2	0 2 6	44.52
2.021	1	5 1 1	44.82
2.020	1	1 3 1	44.84
2.012	1	4 2 1	45.01
2.006	10	4 0 4	45.15
2.006	3	0 0 8	45.16

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.000	2	1 1 7	45.31
1.994	6	-1 1 8	45.46
1.987	2	-6 0 2	45.62
1.987	3	-4 0 8	45.62
1.984	1	-3 1 8	45.69
1.982	5	-6 0 4	45.74
1.959	3	1 3 2	46.31
1.957	4	-1 3 3	46.36
1.922	16	-2 2 7	47.26
1.912	3	4 2 2	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
1.772	5	2 2 6	51.55
1.769	1	-5 1 8	51.61
1.764	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	-2 0 10	53.72
1.690	6	-6 0 8	54.23
1.689	1	4 2 4	54.26
1.689	1	0 2 8	54.26
1.685	4	-6 2 3	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	-1 1 10	57.00
1.605	1	0 0 10	57.36
1.604	4	-6 2 6	57.42
1.569	1	-4 2 9	58.81
1.560	2	7 1 0	59.17

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

Sodium Azide, alpha, NaN_3, at −90 to −100° C (monoclinic)

Structure
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-NaN_3, exists at room temperature.

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

Scale factor
(integrated intensities) 0.1648 × 10^4

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)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.07	2	0 0 3	17.48
3.09	11	1 0 1	28.86
2.915	100	0 1 2	30.64
2.535	1	0 0 6	35.38
2.429	14	1 0 4	36.98
2.191	10	0 1 5	41.16
1.823	17	1 1 0	49.98
1.791	5	1 0 7	50.96
1.629	1	0 1 8	56.44
1.546	5	2 0 2	59.78
1.480	1	1 1 6	62.72
1.458	1	0 2 4	63.78
1.402	1	2 0 5	66.68
1.371	1	1 0 10	68.38
1.179	2	1 2 2	81.58
1.041	1	1 1 12	95.46

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.07	2	0 0 3	17.47
3.09	10	1 0 1	28.85
2.916	100	0 1 2	30.63
2.536	1	0 0 6	35.37
2.429	15	1 0 4	36.97
2.191	11	0 1 5	41.17
1.823	21	1 1 0	49.99
1.790	6	1 0 7	50.97
1.716	1	1 1 3	53.36
1.629	1	0 1 8	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	68.39
1.277	1	0 2 7	74.18
1.268	1	0 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	2	1 1 12	95.47
1.028	1	0 1 14	97.12
.804	1	1 2 14	146.93

Structure

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

Lattice parameters

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

Density

(calculated) 1.849 g/cm^3

Thermal parameters

Isotropic [ibid.]

Scattering factors

Na^0 [3.3.1A]
$N^{-0.8}$ and $N^{+0.6}$ calculated from N^{-1} and N^0 [3.3.1A]

Scale factor

(integrated intensities) 0.4484 x 10^4

Polymorphism

A monoclinic polymorph, α-NaN_3, exists at -90 to -100 °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)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.05	2	0 0 1	17.56
3.11	7	1 1 0	28.70
2.99	6	-2 0 1	29.86
2.95	35	2 0 0	30.32
2.87	100	-1 1 1	31.16
2.53	2	0 0 2	35.52
2.47	12	1 1 1	36.36
2.31	11	-2 0 2	38.92
2.25	8	2 0 1	39.98
2.14	8	-1 1 2	42.14
1.829	10	3 2 0	49.82
1.817	7	1 1 2	50.16
1.798	18	-3 1 1	50.74
1.731	2	3 1 0	52.86
1.713	3	-2 0 3	53.44
1.683	1	0 0 3	54.46
1.674	1	2 0 2	54.80
1.595	1	-1 1 3	57.72
1.554	5	2 2 0	59.44
1.495	4	-4 0 2	62.04
1.434	2	-2 2 2	64.96
1.420	2	2 2 1	65.70
1.386	2	1 1 3	67.50
1.262	1	0 0 4	75.20
1.250	1	-2 2 3	76.06
1.179	2	-1 3 1	81.58
1.157	2	-4 2 2	83.46
1.098	1	-5 1 3	89.06
1.067	1	3 1 3	92.40
1.050	1	-3 3 1	94.40
1.039	1	0 2 4	95.70
1.011	1	-1 1 5	99.22

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.05	1	0 0 1	17.55
3.11	6	1 1 0	28.70
2.99	5	-2 0 1	29.87
2.95	34	2 0 0	30.31
2.87	100	-1 1 1	31.15
2.52	1	0 0 2	35.52
2.47	12	1 1 1	36.35
2.31	11	-2 0 2	38.92
2.25	8	2 0 1	39.97
2.14	8	-1 1 2	42.15
1.829	12	0 2 0	49.81
1.817	7	1 1 2	50.16
1.798	20	-3 1 1	50.74
1.730	2	3 1 0	52.86
1.713	3	-2 0 3	53.43
1.683	1	0 0 3	54.46
1.674	1	2 0 2	54.81
1.596	1	-1 1 3	57.72
1.554	6	2 2 0	59.43
1.513	1	3 1 1	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	1 1 3	67.50
1.263	2	0 0 4	75.20
1.250	1	-2 2 3	76.05
1.235	1	2 2 2	77.20
1.190	1	-3 1 4	80.69
1.179	3	-1 3 1	81.58
1.172	1	-5 1 1	82.16
1.157	3	-4 2 2	83.45
1.127	1	4 0 2	86.25
1.122	1	5 1 0	86.74
1.098	2	-5 1 3	89.06
1.067	2	3 1 3	92.41
1.050	2	-3 3 1	94.39
1.039	1	0 2 4	95.70
1.011	1	-1 1 5	99.21
1.002	1	-3 1 5	100.45
.959	1	4 2 2	106.82
.914	1	0 4 0	114.77
.909	1	2 2 4	115.95
.899	1	-6 2 2	117.95

Sodium Calcium Aluminum Fluoride Hydrate, thomsenolite, $NaCaAlF_6 \cdot H_2O$ (monoclinic)

Structure

Monoclinic, $P2_1/c$ (14), Z=4 [Cocco et al., 1967]

Lattice parameters

a= 5.583±0.004, b=5.508±0.005, c=16.127±0.006Å, β=96°26′±3′ [ibid.]

Density

(calculated) 2.974 g/cm³ [ibid.]

Thermal parameters

Isotropic [ibid.]

Polymorphism

Thomsenolite is dimorphous with pachnolite which is also monoclinic [Gerhard, 1966]

Scattering factors

Na^0, Al^0, F^0, O^0, and Ca^0 [Hanson et al., 1964]

Scale factor

(integrated intensities) 1.498×10^4

Additional patterns

1. PDF 5-343 [Ferguson, 1946]

References

Cocco, G., P.C. Castiglione, and G. Vagliasindi (1967). The crystal structure of thomsenolite, Acta Cryst. 23, 162-166.

Ferguson, R.B. (1946). Trans.Roy. Soc. Can. 40, Sec.IV, 11-25.

Gerhard, F.B.Jr. (1966). The crystal structure of the mineral pachnolite, Acta Cryst. 21, Moscow abstracts, A 54.

Hanson, H.P., F. Herman, J.D. Lea, and S. Skillman (1964). HFS atomic scattering factors, Acta Cryst. 17, 1040-1044.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
8.01	26	0	0	2		11.04
5.55	1	1	0	0		15.96
5.21	2	0	1	1		17.02
4.54	1	0	1	2		19.54
4.34	4	1	0	2		20.46
4.005	43	0	0	4		22.18
3.907	100	1	1	0		22.74
3.867	16	-1	1	1		22.98
3.834	5	0	1	3		23.18
3.627	1	-1	1	2		24.52
3.435	7	-1	0	4		25.92
3.409	20	1	1	2		26.12
3.281	15	-1	1	3		27.16
3.241	11	0	1	4		27.50
3.087	4	1	0	4		28.90
3.042	11	1	1	3		29.34
2.915	48	-1	1	4		30.64
2.774	25	2	0	0	+	32.24
2.754	8	0	2	0		32.48
2.714	16	0	2	1		32.98
2.693	14	1	1	4		33.24
2.580	2	-1	1	5		34.74
2.535	3	2	0	2		35.38
2.486	7	-2	1	1		36.10
2.478	5	2	1	0		36.22
2.466	6	1	2	0		36.40
2.460	4	-1	2	1		36.50
2.436	5	-2	1	2		36.86
2.420	8	1	2	1		37.12
2.412	9	2	1	1	+	37.24
2.391	2	-1	2	2		37.58
2.339	2	-2	1	3		38.46
2.308	5	1	0	6		39.00
2.283	11	-1	2	3		39.44
2.270	8	0	2	4		39.68
2.208	2	-2	1	4		40.84
2.198	2	1	2	3		41.02
2.169	18	2	0	4	+	41.60
2.148	4	-1	2	4		42.02
2.128	5	1	1	6		42.44
2.114	1	0	1	7		42.74
2.089	17	0	2	5		43.28
2.062	2	-2	1	5		43.86
2.055	8	1	2	4		44.02
2.042	3	-2	0	6		44.32
2.019	4	2	1	4		44.86
2.004	38	0	0	8	+	45.22
1.958	40	-2	2	1		46.32
1.955	56	2	2	0	+	46.42
1.934	4	-2	2	2		46.94

Sodium Calcium Aluminum Fluoride Hydrate, thomsenolite, $NaCaAlF_6 \cdot H_2O$ (monoclinic) – continued

Calculated Pattern *(Peak heights)*						
d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
1.922	10	2	2	1		47.26
1.917	9	0	2	6		47.38
1.915	8	-2	1	6		47.44
1.910	5	1	2	5		47.58
1.883	11	0	1	8		48.30
1.872	4	2	1	5		48.60
1.865	3	2	2	2		48.78
1.848	3	-3	0	2		49.28
1.843	3	-1	1	8		49.42
1.825	6	2	0	6	+	49.94
1.820	6	1	0	8		50.08
1.814	3	-2	2	4		50.24
1.791	5	2	2	3		50.96
1.760	9	0	2	7	+	51.90
1.756	7	-3	0	4		52.04
1.752	6	-3	1	2	+	52.16
1.743	4	1	3	0		52.46
1.739	10	-1	3	1		52.58
1.731	2	-2	2	5		52.86
1.721	6	-3	1	3		53.18
1.718	8	-2	0	8		53.28
1.704	1	2	2	4		53.74
1.694	1	0	1	9		54.08
1.691	2	1	3	2		54.20
1.675	11	3	1	2	+	54.74
1.672	8	-3	1	4		54.86
1.640	14	1	3	3	+	56.02
1.638	10	1	2	7		56.10
1.615	2	3	1	3		56.96
1.612	3	-3	1	5	+	57.10
1.607	2	-3	0	6		57.28
1.603	3	0	0	10	+	57.44
1.593	1	0	3	5		57.82
1.554	1	-1	3	5		59.42
1.547	2	3	1	4	+	59.72
1.542	3	-3	1	6	+	59.92
1.539	3	0	1	10		60.08
1.519	4	1	2	8		60.96
1.515	3	3	2	1		61.12
1.496	1	0	2	9	+	62.00
1.483	2	3	2	2		62.60
1.479	2	-1	2	9		62.76
1.458	3	-2	2	8		63.80
1.448	1	2	3	3		64.26
1.440	2	3	2	3		64.66
1.432	1	2	2	7		65.10
1.416	1	-2	3	5		65.92
1.408	1	0	1	11		66.32
1.393	2	-4	0	2		67.14
1.387	1	4	0	0		67.48

Calculated Pattern *(Integrated)*					2θ(°) λ = 1.54056 Å
d (Å)	*I*	*hkl*			
8.01	21	0	0	2	11.03
5.55	1	1	0	0	15.96
5.21	2	0	1	1	17.01
4.54	1	0	1	2	19.54
4.34	4	1	0	2	20.45
4.006	43	0	0	4	22.17
3.909	100	1	1	0	22.73
3.868	13	-1	1	1	22.97
3.835	3	0	1	3	23.18
3.628	1	-1	1	2	24.52
3.436	7	-1	0	4	25.91
3.409	20	1	1	2	26.12
3.280	15	-1	1	3	27.16
3.240	12	0	1	4	27.51
3.088	5	1	0	4	28.89
3.042	11	1	1	3	29.33
2.915	52	-1	1	4	30.64
2.774	27	2	0	0	32.24
2.770	2	0	1	5	32.29
2.754	7	0	2	0	32.48
2.714	17	0	2	1	32.97
2.694	15	1	1	4	33.23
2.580	2	-1	1	5	34.74
2.535	3	2	0	2	35.38
2.486	8	-2	1	1	36.10
2.477	2	2	1	0	36.23
2.467	7	1	2	0	36.39
2.457	2	-1	2	1	36.55
2.437	5	-2	1	2	36.86
2.420	8	1	2	1	37.12
2.412	5	2	1	1	37.24
2.411	4	-2	0	4	37.27
2.391	2	-1	2	2	37.58
2.339	2	-2	1	3	38.46
2.308	5	1	0	6	39.00
2.291	1	-1	1	6	39.29
2.283	12	-1	2	3	39.43
2.270	9	0	2	4	39.68
2.208	2	-2	1	4	40.83
2.198	2	1	2	3	41.02
2.170	20	2	0	4	41.59
2.166	9	2	1	3	41.66
2.149	4	-1	2	4	42.01
2.128	6	1	1	6	42.44
2.114	1	0	1	7	42.74
2.089	20	0	2	5	43.28
2.063	2	-2	1	5	43.86
2.055	9	1	2	4	44.02
2.042	3	-2	0	6	44.33
2.019	5	2	1	4	44.86

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.004	19	-1 2 5	45.22
2.003	29	0 0 8	45.23
1.959	40	-2 2 1	46.32
1.955	27	-1 0 8	46.40
1.954	28	2 2 0	46.42
1.934	4	-2 2 2	46.94
1.922	12	2 2 1	47.26
1.917	3	0 2 6	47.38
1.914	7	-2 1 6	47.45
1.909	1	1 2 5	47.58
1.883	13	0 1 8	48.31
1.872	5	2 1 5	48.61
1.865	3	2 2 2	48.79
1.848	4	-3 0 2	49.27
1.843	2	-1 1 8	49.42
1.825	6	2 0 6	49.94
1.824	1	0 3 1	49.96
1.820	3	1 0 8	50.07
1.814	2	-2 2 4	50.26
1.790	6	2 2 3	50.97
1.763	2	-3 1 1	51.81
1.760	9	0 2 7	51.89
1.759	2	3 0 2	51.93
1.756	2	-3 0 4	52.05
1.753	3	3 1 0	52.13
1.752	4	-3 1 2	52.17
1.743	3	1 3 0	52.45
1.739	11	-1 3 1	52.57
1.730	1	-2 2 5	52.86
1.721	6	-3 1 3	53.19
1.718	8	-2 0 8	53.28
1.704	1	2 2 4	53.74
1.694	1	0 1 9	54.08
1.691	2	1 3 2	54.20
1.676	11	3 1 2	54.73
1.675	6	-1 3 3	54.77
1.673	5	-3 1 4	54.84
1.640	12	1 3 3	56.02
1.640	6	-2 1 8	56.03
1.638	7	1 2 7	56.11
1.616	2	3 1 3	56.95
1.613	1	2 2 5	57.05
1.612	3	-3 1 5	57.10
1.607	1	-3 0 6	57.28
1.603	2	2 1 7	57.43
1.603	2	0 0 10	57.46
1.593	1	0 3 5	57.83
1.554	2	-1 3 5	59.41
1.548	1	-2 2 7	59.68
1.547	1	3 1 4	59.73

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.543	2	-3 1 6	59.91
1.542	2	-3 2 1	59.94
1.539	1	0 1 10	60.08
1.521	1	2 2 6	60.85
1.518	5	1 2 8	60.97
1.515	1	3 2 1	61.12
1.496	1	1 0 10	62.00
1.495	1	0 2 9	62.01
1.483	2	3 2 2	62.61
1.479	2	-1 2 9	62.77
1.458	4	-2 2 8	63.80
1.448	2	2 3 3	64.26
1.440	2	3 2 3	64.66
1.432	1	2 2 7	65.10
1.416	1	-2 3 5	65.91
1.408	1	0 1 11	66.31
1.393	3	-4 0 2	67.13
1.387	2	4 0 0	67.47
1.377	1	0 4 0	68.03
1.372	6	0 4 1	68.31
1.371	2	-2 2 9	68.35
1.364	1	1 3 7	68.77
1.347	2	2 2 8	69.77
1.342	1	4 0 2	70.08
1.336	2	1 4 0	70.39
1.334	1	-3 2 7	70.55
1.333	1	0 4 3	70.57
1.333	3	-1 0 12	70.61
1.321	1	-3 1 9	71.31
1.314	1	1 2 10	71.76
1.307	1	-3 3 1	72.22
1.303	1	4 1 2	72.45
1.298	2	0 1 12	72.81
1.295	1	-1 1 12	72.97
1.290	1	3 3 1	73.30
1.288	3	2 1 10	73.45
1.277	2	-3 2 8	74.18
1.267	2	2 2 9	74.86
1.258	1	1 4 4	75.54
1.246	1	-1 4 5	76.41
1.245	2	-4 2 1	76.47
1.242	1	-3 3 5	76.68
1.238	1	2 3 7	76.97
1.235	1	4 1 4	77.16
1.234	3	-2 4 1	77.21
1.233	1	2 4 0	77.29
1.228	3	1 2 11	77.70
1.224	2	3 2 7	78.03
1.222	1	1 4 5	78.16
1.220	1	-3 2 9	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, $I\bar{4}$ (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
1. 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)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
7.202	5	0	1	1		12.28
5.254	2	0	2	0		16.86
4.940	3	0	0	2		17.94
4.247	13	2	1	1	+	20.90
4.115	3	1	1	2		21.58
3.601	37	0	2	2		24.70
3.326	2	3	1	0	+	26.78
3.144	2	0	1	3		28.36
2.970	39	2	2	2		30.06
2.798	4	2	3	1	+	31.96
2.759	100	1	3	2	+	32.42
2.699	4	2	1	3	+	33.16
2.629	7	0	4	0		34.08
2.471	3	0	0	4	+	36.32
2.401	1	0	3	3		37.42
2.352	18	4	2	0	+	38.24
2.346	20	1	1	4		38.34
2.321	20	0	4	2		38.76
2.237	5	0	2	4		40.28
2.216	15	3	3	2		40.68
2.184	1	2	3	3		41.30
2.123	3	2	4	2	+	42.54
2.057	1	0	5	1	+	43.98
2.017	1	1	4	3	+	44.90
1.984	21	3	1	4	+	45.70
1.9156	1	5	2	1		47.42
1.9035	2	1	5	2	+	47.74
1.8589	8	4	4	0		48.96
1.8226	1	2	1	5	+	50.00
1.8031	7	3	5	0	+	50.58
1.8011	6	0	4	4		50.64
1.7730	1	0	5	3		51.50
1.7528	8	0	6	0		52.14
1.7397	2	4	4	2		52.56
1.7037	24	4	2	4	+	53.76
1.6944	7	3	5	2	+	54.08
1.6800	1	5	2	3	+	54.58
1.6626	7	2	6	0	+	55.20
1.6521	6	0	6	2		55.58
1.6478	5	0	0	6		55.74
1.6364	1	2	3	5	+	56.16
1.5834	2	5	1	4	+	58.22
1.5759	1	6	2	2	+	58.52
1.5725	2	0	2	6		58.66
1.5065	1	2	2	6		61.50
1.4763	6	1	3	6	+	62.90
1.4700	1	4	5	3		63.20
1.4568	1	3	5	4	+	63.84
1.4297	1	0	6	4		65.20
1.3986	2	6	4	2	+	66.84

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

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(^\circ)$ $\lambda = 1.54056$ Å
1.3963	4	0 4 6	66.96
1.3796	2	6 2 4 +	67.88
1.3722	1	3 3 6	68.30
1.3493	2	2 4 6 +	69.62
1.3300	7	7 3 2 +	70.78
1.3146	4	0 8 0	71.74
1.2874	1	1 5 6 +	73.50
1.2743	1	8 2 0 +	74.38
1.2705	1	0 8 2	74.64
1.2559	1	4 6 4 +	75.66
1.2393	3	6 6 0	76.86
1.2360	2	0 0 8	77.10
1.2330	1	4 4 6	77.32
1.2164	4	3 5 6 +	78.58
1.2054	2	3 7 4 +	79.44
1.2006	2	0 6 6	79.82
1.1868	1	5 7 2 +	80.94
1.1606	1	0 8 4	83.16
1.1584	1	1 3 8	83.36
1.1439	2	8 4 2 +	84.66
1.1333	1	6 2 4 +	85.64
1.1305	2	1 9 2 +	85.90
1.1184	1	0 4 8	87.06
1.1079	2	6 6 4	88.10
1.1059	1	3 3 8	88.30
1.1041	1	7 1 6 +	88.48
1.0957	1	7 5 4 +	89.34
1.0939	2	2 4 8 +	89.52
1.0920	2	6 4 6 +	89.72
1.0584	1	3 7 6 +	93.40
1.0512	1	1 9 4 +	94.24
1.0094	1	2 10 2 +	99.48
.9764	2	4 10 0 +	104.16

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(^\circ)$ $\lambda = 1.54056$ Å
7.203	8	0 1 1	12.28
5.258	4	0 2 0	16.85
4.943	5	0 0 2	17.93
4.247	19	2 1 1	20.90
4.247	3	1 2 1	20.90
4.117	5	1 1 2	21.57
3.602	66	0 2 2	24.70
3.325	2	3 1 0	26.79
3.325	1	1 3 0	26.79
3.304	1	0 3 1	26.96
3.145	4	0 1 3	28.36
2.971	79	2 2 2	30.05
2.797	3	3 2 1	31.97
2.797	4	2 3 1	31.97
2.759	96	3 1 2	32.42
2.759	100	1 3 2	32.42
2.699	5	2 1 3	33.17
2.699	4	1 2 3	33.17
2.629	14	0 4 0	34.07
2.472	4	0 0 4	36.32
2.470	2	1 4 1	36.35
2.401	2	0 3 3	37.42
2.351	18	4 2 0	38.24
2.351	16	2 4 0	38.24
2.346	21	1 1 4	38.34
2.321	41	0 4 2	38.76
2.237	11	0 2 4	40.28
2.216	33	3 3 2	40.69
2.184	2	2 3 3	41.30
2.123	3	4 2 2	42.54
2.123	4	2 4 2	42.54
2.058	1	2 2 4	43.95
2.057	1	0 5 1	43.98
2.017	1	4 1 3	44.90
2.017	1	1 4 3	44.90
1.984	23	1 3 4	45.70
1.984	25	3 1 4	45.70
1.9158	3	5 2 1	47.42
1.9034	2	5 1 2	47.74
1.9034	3	1 5 2	47.74
1.8590	19	4 4 0	48.96
1.8228	1	1 2 5	49.99
1.8228	1	2 1 5	49.99
1.8035	7	5 3 0	50.57
1.8035	8	3 5 0	50.57
1.8008	7	0 4 4	50.65
1.7729	1	0 5 3	51.50
1.7527	18	0 6 0	52.14
1.7400	5	4 4 2	52.55
1.7037	30	4 2 4	53.76

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

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.7037	27	2 4 4	53.76
1.7030	2	1 6 1	53.78
1.6943	7	5 3 2	54.08
1.6943	7	3 5 2	54.08
1.6800	2	5 2 3	54.58
1.6800	1	2 5 3	54.58
1.6627	8	6 2 0	55.20
1.6627	8	2 6 0	55.20
1.6519	15	0 6 2	55.59
1.6478	4	0 0 6	55.74
1.6367	1	3 2 5	56.15
1.6367	1	2 3 5	56.15
1.6201	1	4 5 1	56.78
1.6088	2	1 1 6	57.21
1.5835	2	5 1 4	58.21
1.5835	2	1 5 4	58.21
1.5760	1	6 2 2	58.52
1.5760	1	2 6 2	58.52
1.5724	4	0 2 6	58.66
1.5310	1	1 6 3	60.42
1.5065	4	2 2 6	61.50
1.4765	8	3 1 6	62.89
1.4765	8	1 3 6	62.89
1.4699	1	4 5 3	63.21
1.4569	1	5 3 4	63.84
1.4569	2	3 5 4	63.84
1.4297	2	0 6 4	65.20
1.3987	3	6 4 2	66.83
1.3987	3	4 6 2	66.83
1.3962	9	0 4 6	66.97
1.3894	1	5 2 5	67.34
1.3808	1	7 3 0	67.81
1.3796	2	2 6 4	67.88
1.3796	2	6 2 4	67.88
1.3723	3	3 3 6	68.29
1.3495	3	2 4 6	69.61
1.3495	3	4 2 6	69.61
1.3299	11	7 3 2	70.79
1.3299	10	3 7 2	70.79
1.3145	10	0 8 0	71.75
1.2874	1	5 1 6	73.50
1.2874	2	1 5 6	73.50
1.2753	1	8 2 0	74.32
1.2753	1	2 8 0	74.32
1.2743	1	7 1 4	74.38
1.2743	1	1 7 4	74.38
1.2704	3	0 8 2	74.65
1.2560	1	6 4 4	75.65
1.2560	1	4 6 4	75.65
1.2393	8	6 6 0	76.86

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.2359	3	0 0 8	77.11
1.2331	3	4 4 6	77.31
1.2165	5	5 3 6	78.57
1.2165	6	3 5 6	78.57
1.2055	3	7 3 4	79.43
1.2055	4	3 7 4	79.43
1.2006	5	0 6 6	79.82
1.1867	2	7 5 2	80.95
1.1867	2	5 7 2	80.95
1.1606	2	0 8 4	83.17
1.1585	1	1 3 8	83.35
1.1438	3	8 4 2	84.66
1.1438	3	4 8 2	84.66
1.1333	2	8 2 4	85.64
1.1333	2	2 8 4	85.64
1.1305	2	9 1 2	85.90
1.1305	2	1 9 2	85.90
1.1185	2	0 4 8	87.05
1.1079	5	6 6 4	88.10
1.1060	2	3 3 8	88.29
1.1040	1	1 7 6	88.48
1.1040	2	7 1 6	88.48
1.0958	1	7 5 4	89.33
1.0958	1	5 7 4	89.33
1.0940	4	2 4 8	89.52
1.0940	3	4 2 8	89.52
1.0921	3	6 4 6	89.71
1.0921	3	4 6 6	89.71
1.0584	2	7 3 6	93.41
1.0584	2	3 7 6	93.41
1.0511	1	9 1 4	94.25
1.0511	1	1 9 4	94.25
1.0195	1	3 5 8	98.15
1.0195	1	5 3 8	98.15
1.0100	1	0 6 8	99.39
1.0095	1	10 2 2	99.47
1.0095	1	2 10 2	99.47
1.0003	1	9 5 2	100.72
1.0003	1	5 9 2	100.72
.9919	1	2 6 8	101.90
.9919	1	6 2 8	101.90
.9764	3	10 4 0	104.17
.9764	4	4 10 0	104.17
.9717	2	0 2 10	104.88
.9677	1	0 10 4	105.50

Sodium Calcium Beryllium Fluorosilicate, leucophanite, $NaCaBeFSi_2O_6$ (orthorhombic)

Structure
Orthorhombic, $P2_12_12_1$ (19), Z=4 [Cannillo et al., 1967]

Lattice parameters
a=7.401±0.008, b= 7.420±0.008, c= 9.939± 0.005Å [ibid.]

Density
(calculated) 2.961 g/cm^3 [ibid.]

Thermal parameters
Isotropic [ibid.]

Scattering factors
Be^{+1}, $F^{-\frac{1}{2}}$, $Na^{+\frac{1}{2}}$, Si^{+2}, O^{-1} [3.3.1A]
Ca^{+1} [3.3.1B]

Scale factor
(integrated intensities) 2.059 x 10^4

Additional patterns
1. PDF 18-711 [Neumann and Bergstal, Min. Geol. Museum, Oslo, Norway]

Reference
Cannillo, E., G. Giuseppetti,and V.Tazzoli (1967). The crystal structure of leucophanite, Acta Cryst. 23, 255-259.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
5.94	20	0	1	1	+	14.90
4.97	14	0	0	2		17.84
4.63	5	1	1	1		19.14
4.13	?	1	0	2	+	21.52
3.604	40	1	1	?		24.68
3.469	13	?	0	1	+	25.66
3.312	3	1	?	0	+	26.90
3.144	5	1	?	1	+	28.36
3.023	11	0	1	3	+	29.52
2.972	30	0	?	?		30.04
2.968	33	?	0	?		30.08
2.756	100	?	1	?	+	32.46
2.620	9	?	?	0		34.20
2.534	1	?	?	1		35.40
2.485	?	0	0	4		36.12
2.471	1	0	?	3		36.32
2.400	2	0	3	1		37.44
2.355	10	1	0	4	+	38.18
2.346	14	1	3	0	+	38.34
2.341	17	3	1	0	+	38.42
2.318	28	?	?	?		38.82
2.283	3	1	3	1		39.44
2.278	4	3	1	1		39.52
2.245	5	1	1	4		40.14
2.214	12	0	3	2		40.72
2.210	16	3	0	?		40.80
2.118	3	3	1	?		42.66
2.055	?	?	?	3		44.02
1.988	19	?	1	4	+	45.60
1.899	?	3	?	?	+	47.86
1.855	5	0	4	0		49.08
1.850	7	4	0	0		49.20
1.803	4	?	?	4		50.58
1.799	4	1	4	0		50.70
1.795	4	4	1	0		50.82
1.770	?	1	4	1		51.58
1.767	?	4	1	1		51.70
1.751	4	0	?	5	+	52.18
1.747	11	3	3	0	+	52.34
1.734	1	4	0	?		52.76
1.720	1	3	3	1		53.20
1.705	18	1	3	4		53.70
1.704	17	3	1	4		53.74
1.692	4	1	4	?		54.16
1.688	4	4	1	?		54.30
1.656	7	4	?	0	+	55.44
1.648	5	3	3	2		55.74
1.616	1	0	1	6		56.92
1.583	3	3	?	4	+	58.22
1.579	5	1	1	6	+	58.38

Sodium Calcium Beryllium Fluorosilicate, leucophanite, $NaCaBeFSi_2O_6$ (orthorhombic) – continued

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.575	3	2 4 2	58.56
1.571	1	4 2 2	58.72
1.545	1	3 3 3	59.80
1.515	2	3 1 5 +	61.10
1.512	2	0 2 6 +	61.24
1.482	5	2 1 6 +	62.64
1.466	1	3 4 1	63.38
1.440	1	1 5 1	64.70
1.400	4	2 2 6	66.76
1.397	3	1 5 2	66.94
1.393	2	5 1 2	67.12
1.377	2	4 2 4 +	68.00
1.375	2	0 3 6 +	68.14
1.352	3	3 1 6 +	69.44
1.332	1	1 5 3	70.64
1.327	4	2 5 2	70.94
1.325	5	5 2 2	71.10
1.310	3	4 4 0	72.04
1.306	2	1 2 7	72.26
1.299	1	4 4 1	72.76
1.290	1	3 2 6 +	73.36
1.272	1	3 5 0 +	74.56
1.267	2	4 4 2	74.90
1.260	1	5 3 1	75.38
1.253	1	5 1 4	75.84
1.242	1	0 0 8	76.64
1.237	2	0 6 0 +	77.06
1.234	3	6 0 0 +	77.28
1.219	2	1 4 6	78.40
1.217	2	4 1 6	78.50
1.205	1	2 5 4	79.50
1.202	2	3 3 6 +	79.72
1.182	1	6 1 2	81.34
1.174	1	1 5 5	82.00
1.172	1	2 4 6	82.20
1.168	1	2 3 7	82.50
1.141	1	2 6 2	84.88
1.139	1	6 2 2	85.08
1.132	1	3 5 4	85.76
1.127	1	5 4 2 +	86.24
1.123	1	2 2 8	86.66
1.110	1	0 3 8 +	87.88
1.107	1	0 6 4	88.18
1.105	2	3 4 6 +	88.42
1.097	3	3 1 8 +	89.16
1.095	2	1 6 4	89.42
1.093	2	1 5 6 +	89.62
1.092	2	5 1 6	89.74
1.010	1	2 6 5	99.38

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
5.95	21	0 1 1	14.89
5.94	7	1 0 1	14.91
4.97	19	0 0 2	17.83
4.64	8	1 1 1	19.13
4.13	1	0 1 2	21.50
4.13	2	1 0 2	21.52
3.606	62	1 1 2	24.67
3.476	10	0 2 1	25.61
3.468	13	2 0 1	25.67
3.317	3	1 2 0	26.86
3.312	3	2 1 0	26.90
3.146	6	1 2 1	28.34
3.142	3	2 1 1	28.38
3.025	10	0 1 3	29.50
3.024	8	1 0 3	29.52
2.973	36	0 2 2	30.03
2.968	31	2 0 2	30.08
2.759	94	1 2 2	32.43
2.756	100	2 1 2	32.46
2.620	15	2 2 0	34.20
2.533	2	2 2 1	35.40
2.485	3	0 0 4	36.12
2.471	1	0 2 3	36.32
2.400	3	0 3 1	37.44
2.356	7	0 1 4	38.16
2.356	8	1 0 4	38.17
2.346	16	1 3 0	38.34
2.344	4	1 2 3	38.37
2.342	4	2 1 3	38.40
2.341	14	3 1 0	38.42
2.318	47	2 2 2	38.82
2.283	4	1 3 1	39.44
2.279	5	3 1 1	39.52
2.245	8	1 1 4	40.13
2.214	18	0 3 2	40.71
2.210	18	3 0 2	40.80
2.121	2	1 3 2	42.58
2.118	4	3 1 2	42.66
2.055	4	2 2 3	44.03
2.014	1	2 3 1	44.98
1.989	18	1 2 4	45.58
1.987	20	2 1 4	45.61
1.900	2	2 3 2	47.83
1.898	2	3 2 2	47.87
1.859	2	1 1 5	48.97
1.855	7	0 4 0	49.07
1.850	10	4 0 0	49.20
1.824	1	0 4 1	49.97
1.803	7	2 2 4	50.59
1.799	4	1 4 0	50.69

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.795	4	4 1 0	50.82
1.771	3	1 4 1	51.58
1.767	3	4 1 1	51.70
1.752	3	0 2 5	52.16
1.751	3	2 0 5	52.19
1.747	2	2 3 3	52.32
1.747	16	3 3 0	52.34
1.746	2	3 2 3	52.36
1.738	1	0 4 2	52.62
1.734	2	4 0 2	52.75
1.720	2	3 3 1	53.20
1.706	27	1 3 4	53.69
1.704	22	3 1 4	53.75
1.692	7	1 4 2	54.17
1.688	4	4 1 2	54.28
1.658	7	2 4 0	55.36
1.656	4	0 0 6	55.42
1.656	9	4 2 0	55.45
1.648	8	3 3 2	55.74
1.636	1	2 4 1	56.19
1.633	1	4 2 1	56.28
1.617	1	0 1 6	56.91
1.584	2	2 3 4	58.19
1.584	2	2 2 5	58.21
1.583	3	3 2 4	58.22
1.581	2	1 4 3	58.31
1.579	5	1 1 6	58.38
1.578	4	4 1 3	58.42
1.573	1	2 4 2	58.64
1.571	1	4 2 2	58.73
1.545	1	3 3 3	59.81
1.517	2	1 3 5	61.05
1.515	3	3 1 5	61.11
1.513	1	0 2 6	61.23
1.512	1	2 0 6	61.26
1.482	5	1 2 6	62.63
1.481	6	2 1 6	62.66
1.466	2	3 4 1	63.37
1.455	1	4 1 4	63.92
1.440	2	1 5 1	64.69
1.429	1	3 3 4	65.24
1.400	9	2 2 6	66.75
1.396	2	1 5 2	66.96
1.395	1	0 1 7	67.06
1.393	2	5 1 2	67.12
1.379	2	2 4 4	67.90
1.378	3	4 2 4	67.98
1.377	1	2 5 0	68.01
1.376	2	0 3 6	68.06
1.375	2	3 0 6	68.13

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.375	2	5 2 0	68.15
1.364	1	2 5 1	68.75
1.362	1	5 2 1	68.89
1.354	1	0 5 3	69.33
1.353	1	3 4 3	69.39
1.353	3	1 3 6	69.40
1.352	1	4 3 3	69.43
1.352	3	3 1 6	69.45
1.351	1	5 0 3	69.50
1.332	2	1 5 3	70.65
1.327	9	2 5 2	70.95
1.325	9	5 2 2	71.09
1.312	1	3 3 5	71.90
1.310	8	4 4 0	72.03
1.305	1	1 2 7	72.33
1.299	2	4 4 1	72.75
1.290	1	2 3 6	73.33
1.289	1	3 2 6	73.36
1.273	1	4 3 4	74.50
1.272	1	4 2 5	74.52
1.272	1	3 5 0	74.56
1.267	3	4 4 2	74.90
1.260	2	5 3 1	75.38
1.253	1	5 1 4	75.84
1.242	3	0 0 8	76.63
1.237	4	0 6 0	77.05
1.236	1	0 4 6	77.13
1.234	1	4 0 6	77.24
1.234	3	6 0 0	77.29
1.224	1	6 0 1	77.99
1.219	5	1 4 6	78.40
1.217	4	4 1 6	78.50
1.205	2	2 5 4	79.50
1.203	2	5 2 4	79.63
1.202	3	3 3 6	79.71
1.185	1	1 6 2	81.12
1.182	2	6 1 2	81.35
1.174	2	1 5 5	82.00
1.172	1	2 4 6	82.18
1.168	1	2 3 7	82.49
1.165	1	2 6 1	82.80
1.159	1	4 4 4	83.32
1.142	2	2 6 2	84.87
1.139	2	6 2 2	85.08
1.132	2	3 5 4	85.76
1.131	1	5 3 4	85.86
1.127	2	4 5 2	86.19
1.127	2	5 4 2	86.25
1.123	2	2 2 8	86.66
1.114	1	4 1 7	87.52

Sodium Silicate, alpha (III), $Na_2Si_2O_5$ (orthorhombic)

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;O(1) 1.548; O(2) 0.988; O(3) 1.190

Density
(calculated). 2.50 g/cm^3 [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
O°, Na°, Si° [3.3.1A]

Scale factor
(integrated intensities) 1.969 x 10^4

Additional patterns

1. 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-$Na_2Si_2O_5$,Acta Cryst. B24, 13-19.

Williamson,J. and F.P. Glasser (1966). The crystallization of $Na_2O \cdot 2SiO_2$-SiO_2 glasses, Phys. Chem. Glasses 7, 127-128.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(^\circ)$ λ = 1.54056 Å
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	2	1	7	1		47.38
1.869	20	3	4	0		48.68
1.846	8	1	8	0		49.32
1.829	1	3	3	1		49.80
1.773	1	0	6	2		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	3	4	0	0		57.48
1.581	1	1	0	3		58.30
1.573	4	1	1	3		58.62
1.565	2	2	8	1		58.96
1.558	1	3	6	1		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

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.448	5	2 1 3	64.28
1.444	9	2 9 1	64.48
1.431	3	3 8 0	65.14
1.429	5	2 2 3	65.24
1.407	2	1 5 3	66.36
1.399	2	2 3 3	66.80
1.364	3	3 6 2	68.76
1.360	3	4 6 0 +	68.98
1.347	3	1 6 3	69.76
1.341	2	4 0 2	70.14
1.336	1	4 1 2	70.44
1.319	1	1 11 1	71.46
1.305	3	0 10 2	72.36
1.300	1	3 7 2	72.68
1.297	1	3 0 3	72.88
1.285	2	0 12 0	73.64
1.266	1	4 4 2	74.94
1.264	1	5 2 0	75.06
1.253	1	4 7 1	75.88
1.236	2	3 8 2 +	77.12
1.232	2	4 8 0	77.38
1.224	1	0 0 4	78.00
1.220	1	0 1 4	78.28
1.209	1	2 10 2	79.18
1.196	2	3 5 3	80.22
1.188	1	4 6 2	80.80
1.171	1	1 3 4	82.30
1.161	2	2 8 3	83.14
1.150	6	5 5 1	84.06
1.143	1	2 0 4	84.70
1.138	3	4 9 1 +	85.20
1.135	3	1 13 1	85.48
1.111	1	4 10 0	87.78
1.109	3	2 9 3	88.00
1.106	1	0 6 4	88.30
1.101	1	4 8 2 +	88.76
1.086	1	1 14 0 +	90.40
1.041	1	6 1 1	95.42
1.040	1	3 3 4	95.56
1.024	1	3 4 4	97.58
1.023	1	6 3 1	97.72
1.012	1	4 10 2	99.16
1.009	1	2 11 3	99.48
1.005	1	5 9 1	100.12
.9941	1	1 15 1	101.58
.9926	1	1 14 2	101.80
.9791	1	3 14 0 +	103.76
.9767	1	6 1 2	104.12
.9582	1	5 5 3	107.00
.9566	1	3 7 4 +	107.26

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
4.929	55	1 2 0	17.98
3.891	7	1 0 1	22.84
3.856	43	0 4 0	23.05
3.772	95	1 1 1	23.56
3.474	4	1 2 1	25.62
3.304	100	1 4 0	26.96
3.204	19	2 0 0	27.82
3.102	5	1 3 1	28.75
2.959	1	2 2 0	30.18
2.739	5	1 4 1	32.67
2.642	32	2 1 1	33.91
2.533	18	2 2 1	35.41
2.464	1	2 4 0	36.43
2.448	60	0 0 2	36.68
2.417	14	1 5 1	37.17
2.386	14	1 6 0	37.67
2.377	4	2 3 1	37.81
2.333	2	0 2 2	38.55
2.262	1	1 1 2	39.82
2.201	3	2 4 1	40.96
2.145	5	1 6 1	42.10
2.067	2	0 4 2	43.77
2.005	9	2 6 0	45.18
1.967	18	1 4 2	46.11
1.958	3	3 0 1	46.33
1.945	13	2 0 2	46.65
1.942	4	3 1 1	46.73
1.930	2	2 1 2	47.04
1.928	3	0 8 0	47.10
1.917	2	1 7 1	47.38
1.869	24	3 4 0	48.69
1.846	10	1 8 0	49.32
1.830	1	3 3 1	49.79
1.773	2	0 6 2	51.51
1.746	2	3 4 1	52.36
1.709	3	1 6 2	53.59
1.653	5	3 5 1	55.54
1.652	1	2 8 0	55.59
1.645	2	2 5 2	55.83
1.643	4	3 6 0	55.92
1.602	3	4 0 0	57.47
1.582	1	1 0 3	58.29
1.573	5	1 1 3	58.63
1.565	3	2 8 1	58.96
1.558	1	3 6 1	59.28
1.551	2	2 6 2	59.55
1.549	1	1 2 3	59.63
1.542	9	0 10 0	59.93
1.536	3	3 3 2	60.19
1.515	2	4 1 1	61.10

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
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	4 7 1	75.89
1.242	1	2 11 1	76.63
1.236	1	5 1 1	77.10
1.236	3	3 8 2	77.13
1.232	1	4 8 0	77.38
1.224	1	0 0 4	78.00
1.220	1	0 1 4	78.29
1.209	1	2 10 2	79.19
1.196	4	3 5 3	80.23
1.189	1	4 6 2	80.78
1.171	1	1 3 4	82.29
1.161	2	2 8 3	83.13
1.151	11	5 5 1	84.06
1.143	1	2 0 4	84.70
1.138	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	0 6 4	88.38
1.102	1	0 14 0	88.73
1.101	1	4 8 2	88.83
1.086	1	1 14 0	90.38
1.085	1	2 13 1	90.47

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.072	1	2 12 2	91.83
1.055	1	1 7 4	93.75
1.049	1	1 11 3	94.48
1.041	2	6 1 1	95.42
1.040	2	3 3 4	95.57
1.024	3	3 4 4	97.58
1.023	1	6 3 1	97.73
1.012	2	4 10 2	99.16
1.009	1	2 11 3	99.48
1.005	1	5 9 1	100.13
.9941	2	1 15 1	101.59
.9925	1	1 14 2	101.81
.9816	1	3 6 4	103.40
.9791	1	3 14 0	103.76
.9790	1	6 0 2	103.77
.9771	1	6 1 2	104.07
.9707	1	4 1 4	105.03
.9631	1	2 12 3	106.23
.9582	2	5 5 3	107.01
.9567	1	3 7 4	107.25
.9490	1	1 13 3	108.51
.9385	1	5 6 3	110.33
.9296	1	2 2 5	111.91
.9221	1	0 11 4	113.31
.9193	1	2 13 3	113.84
.9091	2	3 14 2	115.84
.9059	1	1 6 5	116.49

Structure

Hexagonal, $R\bar{3}$ (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]
Zr^{4+} 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 × 10^4

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 $Na_7Zr_6F_{31}$, 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 (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
7.41	76	1 0 1	11.94
6.60	12	1 1 0	12.62
5.05	21	0 2 1	17.56
4.78	35	0 1 2	20.24
4.07	41	1 2 -1 +	21.80
3.987	20	3 0 0	22.28
3.702	6	2 0 2	24.02
3.453	10	2 2 0	25.78
3.262	10	2 1 -2 +	27.32
3.142	38	0 0 3	28.38
3.123	100	1 3 1 +	28.58
2.850	6	4 0 1	31.36
2.712	22	1 3 -2 +	33.00
2.635	3	2 3 -1	34.00
2.609	1	4 1 0	34.34
2.488	3	3 0 3 +	36.08
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	2 4 1	41.04
2.133	1	5 0 2	42.34
2.090	5	1 2 -4	43.26
2.038	8	4 2 2 +	44.42
2.008	9	1 4 -3 +	45.12
1.9545	12	1 5 2 +	46.42
1.9209	46	1 3 4	47.28
1.9148	59	5 2 0 +	47.44
1.8625	9	0 1 5	48.86
1.8575	6	3 3 3	49.00
1.8511	2	4 0 4	49.18
1.8145	7	3 4 2 +	50.24
1.7905	6	1 6 1	50.96
1.7404	2	2 1 -5	52.54
1.7008	2	6 1 2	53.86
1.6812	3	3 5 1 +	54.54
1.6391	17	1 3 -5 +	56.06
1.6348	39	2 6 -1 +	56.22
1.6311	22	4 2 -4	56.36
1.6060	2	5 3 2	57.32
1.5873	2	1 5 -4	58.06
1.5838	2	1 7 0	58.20
1.5715	2	0 0 6	58.70
1.5643	5	2 6 2 +	59.00
1.5114	2	5 4 1 +	61.28
1.4793	1	0 8 1	62.90
1.4622	2	0 3 6	63.58
1.4564	1	5 4 -2	63.86
1.4479	3	4 2 5	64.28
1.4439	2	7 2 -1	64.48
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 5 -4 +	69.20
1.3463	1	4 1 6 +	69.80
1.2907	1	1 2 -7	73.28
1.2481	3	1 3 7	76.22
1.2453	5	2 6 5	76.42
1.2426	8	9 1 -1 +	76.62
1.2341	1	0 6 6	77.24
1.2148	3	2 5 -6 +	78.70
1.2115	3	6 5 -2 +	78.96

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.40	64	1 0 1	11.94
6.90	10	1 1 0	12.81
5.05	19	0 2 1	17.55
4.39	34	0 1 2	20.23
4.08	9	2 1 1	21.79
4.08	33	1 2 -1	21.79
3.986	19	3 0 0	22.28
3.702	6	2 0 2	24.02
3.452	10	2 2 0	25.79
3.263	5	1 2 2	27.31
3.263	6	2 1 -2	27.31
3.143	33	0 0 3	28.37
3.129	100	1 3 1	28.51
3.129	1	3 1 -1	28.51
2.850	7	4 0 1	31.36
2.713	1	3 1 2	32.99
2.713	23	1 3 -2	32.99
2.634	3	2 3 -1	34.01
2.609	1	4 1 0	34.34
2.468	2	3 0 3	36.37
2.468	1	0 3 3	36.37
2.371	1	3 2 -2	37.91
2.324	2	2 2 -3	38.71
2.318	2	0 5 1	38.81
2.313	1	1 0 4	38.91
2.198	4	2 4 1	41.04
2.133	1	5 0 2	42.34
2.094	1	1 5 -1	43.16
2.090	6	1 2 -4	43.25
2.038	6	4 2 2	44.42
2.038	4	2 4 -2	44.42
2.008	1	4 1 3	45.12
2.008	2	1 4 3	45.12
2.008	5	1 4 -3	45.12
2.008	4	4 1 -3	45.12
1.9545	11	1 5 2	46.42
1.9545	4	5 1 -2	46.42
1.9245	1	4 3 1	47.19
1.9245	4	3 4 -1	47.19
1.9214	55	1 3 4	47.27
1.9148	57	5 2 0	47.44
1.9148	3	2 5 0	47.44
1.8628	12	0 1 5	48.85
1.8568	1	3 3 3	49.02
1.8510	1	4 0 4	49.18
1.8145	5	3 4 2	50.24
1.8145	4	4 3 -2	50.24
1.7904	7	1 6 1	50.96
1.7404	2	2 1 -5	52.54
1.7006	2	6 1 2	53.86

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.6809	1	7 0 1	54.55
1.6809	3	3 5 1	54.55
1.6393	18	1 3 -5	56.05
1.6393	1	3 1 5	56.05
1.6353	17	5 2 3	56.20
1.6353	2	2 5 3	56.20
1.6353	4	2 5 -3	56.20
1.6353	17	5 2 -3	56.20
1.6332	17	2 6 -1	56.28
1.6313	1	4 2 -4	56.35
1.5061	2	5 3 2	57.32
1.5878	2	1 5 -4	58.05
1.5839	1	1 7 0	58.20
1.5715	2	0 0 6	58.70
1.5643	6	2 6 2	59.00
1.5643	1	6 2 -2	59.00
1.5113	3	5 4 1	61.29
1.5098	1	3 4 -4	61.35
1.4763	2	0 8 1	62.90
1.4620	4	0 3 6	63.59
1.4562	2	5 4 -2	63.87
1.4479	4	4 2 5	64.28
1.4437	1	7 2 -1	64.49
1.4424	2	1 6 4	64.56
1.4303	2	2 2 6	65.17
1.4249	1	8 0 2	65.45
1.4171	3	5 1 -5	65.85
1.3844	3	8 1 1	67.61
1.3832	1	3 5 4	67.68
1.3808	1	5 5 0	67.81
1.3609	1	4 3 -5	68.94
1.3574	3	6 4 -1	69.15
1.3563	12	2 6 -4	69.21
1.3462	1	4 1 6	69.80
1.3462	1	4 1 -6	69.80
1.3109	1	2 1 5	71.97
1.2937	1	7 3 -2	73.08
1.2909	1	1 2 -7	73.27
1.2661	1	5 3 5	74.95
1.2480	4	1 3 7	76.23
1.2453	5	2 6 5	76.42
1.2426	4	6 5 1	76.62
1.2426	5	9 1 -1	76.62
1.2340	1	0 6 6	77.25
1.2281	1	4 0 7	77.69
1.2148	2	2 5 -6	78.71
1.2148	1	5 2 6	78.71
1.2148	1	5 2 -6	78.71
1.2114	1	9 1 2	78.96
1.2114	2	6 5 -2	78.96

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/cm^3

Thermal parameters

Anisotropic [ibid.]

Scattering factors

Sr^{2+}, $N^{-0.8}$, $N^{+0.6}$, calculated from Sr^0 and K^0 averaged, from N^{-1} and N^0 [3.3.1A]

Scale factor

(integrated intensities) 15.021 × 10^4

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)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
4.89	61	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		33.12
2.685	39	0	2	2		33.34
2.501	60	3	3	1		35.88
2.445	8	2	2	2		36.72
2.164	21	5	1	1		41.70
2.112	18	1	5	1		42.78
2.058	6	4	4	0		43.96
1.988	13	4	2	2		45.60
1.967	28	2	4	2	+	46.10
1.909	19	5	3	1		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		55.54
1.630	4	3	3	3		56.40
1.618	8	0	6	2		56.84
1.611	3	7	1	1		57.12
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	7	3	1		61.94
1.478	4	8	0	0		62.84
1.468	3	3	7	1		63.28
1.432	6	6	4	2	+	65.08
1.426	6	2	2	4	+	65.40
1.419	3	4	6	2		65.74
1.417	6	3	5	3		65.84
1.372	2	6	6	0		68.32
1.352	3	4	0	4		69.48
1.343	3	0	4	4		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		74.14
1.275	2	9	1	1		74.36
1.267	3	2	8	2	+	74.90
1.240	1	1	3	1		76.78
1.228	1	7	3	3		77.66

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
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	6	4		82.66
1.158	1	10	2	0		83.42
1.156	2	3	1	5		83.58
1.155	2	7	7	1		83.70
1.153	2	1	3	5		83.82
1.126	1	2	10	0		86.32
1.122	2	5	7	3		86.74
1.120	2	9	5	1		86.88
1.103	1	5	9	1		88.58
1.102	1	10	0	2		88.72
1.097	1	9	1	3		89.20
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	11	1	1		93.94
1.043	2	0	8	4		95.22
1.040	2	3	9	3	+	95.52
1.037	2	3	5	5		96.00
1.028	1	10	4	2	+	97.00
1.024	1	1	11	1		97.58
1.020	1	11	3	1		98.10
1.018	2	6	6	4		98.28
1.011	1	9	7	1		99.32
1.009	1	4	10	2		99.58
.9978	1	0	2	6	+	101.06
.9936	2	8	4	4	+	101.62
.9913	2	6	10	0		101.98
.9815	1	5	9	3		103.40
.9782	1	5	5	5		103.90
.9555	1	7	3	5	+	107.44
.9460	1	11	1	3		109.02
.9455	1	4	2	6		109.12
.9431	1	2	4	6	+	109.52
.9247	1	12	2	2		112.82
.9211	1	10	2	4	+	113.50
.9048	1	2	10	4	+	116.72
.9025	2	3	11	3	+	117.18
.9011	2	2	12	2	+	117.48
.8965	1	13	1	1		118.46

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
4.89	59	1	1	1	18.12
4.12	100	2	2	0	21.57
3.177	92	3	1	1	28.06
3.122	5	1	3	1	28.57
2.868	30	0	4	0	31.16
2.703	31	2	0	2	33.11
2.686	45	0	2	2	33.33
2.501	70	3	3	1	35.88
2.445	9	2	2	2	36.72
2.164	27	5	1	1	41.71
2.112	22	1	5	1	42.78
2.058	8	4	4	0	43.96
1.988	15	4	2	2	45.60
1.968	14	1	1	3	46.09
1.967	23	2	4	2	46.11
1.909	26	5	3	1	47.59
1.885	6	3	5	1	48.24
1.863	10	6	2	0	48.84
1.819	9	2	6	0	50.11
1.780	8	3	1	3	51.27
1.770	9	1	3	3	51.58
1.653	7	6	0	2	55.54
1.630	6	3	3	3	56.39
1.618	11	0	6	2	56.85
1.611	3	7	1	1	57.13
1.589	4	5	5	1	57.99
1.589	1	6	2	2	58.01
1.568	5	1	7	1	58.84
1.561	1	2	6	2	59.14
1.525	4	5	1	3	60.68
1.520	2	0	0	4	60.90
1.505	2	1	5	3	61.50
1.497	1	7	3	1	61.93
1.478	6	8	0	0	62.84
1.468	5	3	7	1	63.29
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	6	2	65.73
1.417	8	3	5	3	65.85
1.372	3	6	6	0	68.31
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	8	0	73.33
1.289	3	7	1	3	73.39

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.278	5	5 5 3	74.14
1.276	1	9 1 1	74.28
1.267	1	1 7 3	74.89
1.267	5	2 8 2	74.91
1.240	2	1 9 1	76.77
1.226	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	4	6 2 4	81.69
1.166	4	2 6 4	82.66
1.158	2	10 2 0	83.42
1.156	3	3 1 5	83.57
1.155	1	7 7 1	83.70
1.153	2	1 3 5	83.81
1.126	2	2 10 0	86.33
1.122	3	5 7 3	86.75
1.120	2	9 5 1	86.88
1.112	1	3 3 5	87.72
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	2	11 1 1	93.95
1.043	3	0 8 4	95.21
1.041	2	3 9 3	95.51
1.041	1	5 3 5	95.51
1.037	3	3 5 5	96.00
1.029	1	8 8 0	96.94
1.028	2	10 4 2	97.01
1.024	2	1 11 1	97.59
1.020	3	11 3 1	98.11
1.018	3	6 6 4	98.29
1.011	2	9 7 1	99.33
1.009	2	4 10 2	99.57
1.005	1	10 6 0	100.02
1.003	1	7 9 1	100.31
.9983	1	2 0 6	100.93
.9979	3	0 2 6	101.05
.9949	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)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
.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
.9478	1	3 7 5	108.72
.9461	1	11 1 3	109.01
.9454	1	4 2 6	109.12
.9432	2	2 4 6	109.51
.9425	1	5 11 1	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
.9048	3	2 10 4	116.72
.9044	1	9 9 1	116.79
.9026	2	3 11 3	117.18
.9025	1	5 7 5	117.18
.9012	3	2 12 2	117.47
.9011	1	6 0 6	117.48
.8965	2	13 1 1	118.46
.8953	1	0 6 5	118.71
.8896	1	9 1 5	119.97

Titanium Sulfide, Ti_2S (orthorhombic)

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/cm^3

Thermal parameters

Isotropic [ibid.]

Scattering factors

S°, Ti° [Hanson et al., 1964]

Scale factor

(integrated intensities) 5.806×10^4

Reference

Hanson, H.P., F. Herman, J.D. Lea, and S. Skillman (1964). HFS atomic scattering factors, Acta Cryst. 17, 1040-1044.

Owens, J.P., B.R. Conard, and H.F. Franzen (1967). The crystal structure of Ti_2S, Acta Cryst. 23, 77-82.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 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	0 1 1	27.58
3.108	8	1 1 1	28.70
2.838	9	4 0 0	31.50
2.730	1	1 5 0	32.78
2.709	7	0 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 0	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
2.428	11	4 3 0	37.00
2.361	50	1 4 1	38.08
2.354	32	3 2 1	38.20
2.343	20	0 6 0	38.38
2.256	39	3 5 0	39.92
2.241	29	5 1 0	40.20
2.221	100	2 4 1	40.58
2.203	95	3 3 1	40.94
2.166	9	2 6 0	41.66
2.160	23	5 2 0	41.78
2.146	46	0 5 1	42.08
2.132	15	4 1 1	42.36
2.108	5	1 5 1	42.86
2.062	23	4 2 1	43.86
2.043	7	5 3 0	44.30
2.035	6	3 4 1	44.48
2.007	3	2 5 1	45.14
1.997	8	4 5 0	45.38
1.992	10	3 6 0	45.50
1.978	16	1 7 0	45.84
1.907	14	5 4 0	47.66
1.892	1	6 0 0	48.06
1.875	3	6 1 0	48.52
1.857	19	5 1 1	49.00
1.827	1	6 2 0	49.88
1.774	1	3 7 0	51.46
1.754	2	6 3 0	52.10
1.737	11	1 8 0	52.66
1.719	1	0 7 1	53.26
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	10	6 6 0 +	63.12
1.463	1	5 6 1	63.52
1.457	1	7 0 1	63.84
1.449	1	7 1 1	64.22
1.433	2	4 0 2	65.04
1.427	8	7 2 1	65.36
1.419	4	6 5 1	65.76
1.412	2	8 1 0	66.14
1.406	2	0 10 0	66.44
1.403	7	1 9 1 +	66.62
1.391	16	7 3 1 +	67.24
1.387	9	2 5 2	67.46
1.370	10	5 7 1 +	68.42
1.362	3	4 8 1	68.86
1.354	6	0 6 2	69.32
1.346	7	6 5 1	69.84
1.337	14	3 5 2	70.34

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.334	16	5 1 2	70.54
1.327	4	4 4 2	70.98
1.324	11	3 9 1	71.14
1.316	8	5 7 2 +	71.64
1.299	3	8 1 1	72.74
1.288	3	5 3 2	73.44
1.286	4	1 10 1 +	73.56
1.282	6	5 8 1	73.86
1.277	4	4 5 2	74.22
1.275	4	3 6 2	74.30
1.272	8	1 7 2	74.56
1.265	2	4 9 1	75.00
1.262	3	2 10 1	75.22
1.259	2	4 10 0	75.42
1.256	3	9 1 0	75.64
1.252	7	5 4 2	75.94
1.247	2	2 11 0	76.30
1.243	2	6 1 2	76.60
1.228	1	6 2 2	77.66
1.225	6	3 10 1	77.92
1.214	1	8 6 0	78.80
1.212	1	3 7 2	78.92
1.211	1	3 11 0	79.02
1.206	1	6 3 2	79.42
1.200	8	1 8 2 +	79.86
1.192	1	7 8 0	80.54
1.186	1	1 11 1	80.98
1.180	1	2 8 2	81.48
1.178	2	4 10 1	81.68
1.175	2	9 1 1	81.94
1.172	1	0 12 0	82.20
1.165	2	4 11 0 +	82.74
1.163	2	9 2 1	82.98
1.159	4	8 7 0	83.32
1.156	3	7 1 2	83.58
1.143	6	9 3 1	84.72
1.138	3	3 11 1	85.24
1.132	2	1 9 2 +	85.76
1.125	4	5 10 1	86.46
1.122	3	7 8 1	86.74
1.121	2	10 2 0	86.84
1.118	2	9 4 1	87.12
1.115	8	2 9 2 +	87.36
1.110	3	9 6 0	87.84
1.103	3	10 3 0	88.58
1.101	8	6 6 2	88.76
1.094	8	8 7 1	89.50
1.084	1	2 12 1	90.52
1.083	2	4 12 0	90.68
1.077	3	1 13 0	91.36

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.98	2	1 2 0	14.81
4.42	2	2 2 0	20.09
3.653	1	3 1 0	24.34
3.332	1	3 2 0	26.74
3.231	2	0 1 1	27.58
3.108	7	1 1 1	28.70
2.838	9	4 0 0	31.50
2.729	1	1 5 0	32.78
2.709	6	0 3 1	33.04
2.654	12	2 2 1	33.75
2.635	1	1 3 1	33.99
2.631	2	4 2 0	34.04
2.575	1	3 4 0	34.81
2.520	2	2 5 0	35.60
2.495	43	3 0 1	35.96
2.457	20	3 1 1	36.54
2.427	11	4 3 0	37.00
2.361	50	1 4 1	38.09
2.352	4	3 2 1	38.24
2.343	17	0 6 0	38.38
2.257	39	3 5 0	39.91
2.241	28	5 1 0	40.21
2.221	100	2 4 1	40.58
2.208	9	4 4 0	40.84
2.203	88	3 3 1	40.94
2.166	7	2 6 0	41.66
2.160	18	5 2 0	41.78
2.146	46	0 5 1	42.07
2.132	13	4 1 1	42.36
2.108	5	1 5 1	42.86
2.062	24	4 2 1	43.87
2.043	7	5 3 0	44.30
2.035	5	3 4 1	44.49
2.007	3	2 5 1	45.14
1.997	8	4 5 0	45.37
1.992	6	3 6 0	45.49
1.978	17	1 7 0	45.84
1.907	16	5 4 0	47.65
1.892	1	6 0 0	48.06
1.875	3	6 1 0	48.52
1.857	21	5 1 1	49.00
1.827	1	6 2 0	49.88
1.774	1	3 7 0	51.47
1.754	2	6 3 0	52.09
1.737	12	1 8 0	52.66
1.719	1	0 7 1	53.26
1.711	1	4 5 1	53.50
1.708	3	3 6 1	53.61
1.679	1	2 8 0	54.62
1.660	47	0 0 2	55.29

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.654	1	5 4 1	55.53
1.639	1	4 7 0	56.05
1.630	1	5 6 0	56.39
1.611	2	7 1 0	57.14
1.600	4	6 2 1	57.54
1.587	3	4 6 1	58.07
1.551	4	6 3 1	59.56
1.548	1	1 9 0	59.70
1.506	10	2 9 0	61.52
1.504	7	5 7 0	61.60
1.472	13	6 6 0	63.11
1.470	1	4 7 1	63.20
1.463	1	5 6 1	63.52
1.457	1	7 0 1	63.83
1.449	1	7 1 1	64.22
1.433	3	4 0 2	65.04
1.427	10	7 2 1	65.36
1.419	4	6 5 1	65.75
1.412	2	8 1 0	66.14
1.406	2	0 10 0	66.44
1.404	1	4 2 2	66.55
1.403	7	1 9 1	66.62
1.391	17	7 3 1	67.24
1.391	6	8 2 0	67.27
1.386	1	2 5 2	67.51
1.372	5	2 9 1	68.33
1.370	4	4 3 2	68.41
1.370	8	5 7 1	68.41
1.369	1	4 9 0	68.51
1.362	4	4 8 1	68.85
1.355	7	0 6 2	69.31
1.346	8	6 6 1	69.84
1.337	17	3 5 2	70.34
1.334	12	5 1 2	70.54
1.327	4	4 4 2	70.98
1.324	13	3 9 1	71.14
1.318	4	2 6 2	71.55
1.316	8	5 2 2	71.64
1.316	1	8 4 0	71.67
1.299	4	8 1 1	72.73
1.288	3	5 3 2	73.44
1.287	1	5 9 0	73.53
1.286	3	1 10 1	73.57
1.282	7	5 8 1	73.87
1.277	4	4 5 2	74.22
1.275	3	3 6 2	74.31
1.272	9	1 7 2	74.57
1.265	2	4 9 1	75.01
1.262	3	2 10 1	75.21
1.260	1	4 10 0	75.38

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.256	3	9 1 0	75.65
1.252	9	5 4 2	75.93
1.247	2	2 11 0	76.30
1.243	2	6 1 2	76.60
1.229	1	6 2 2	77.66
1.225	8	3 10 1	77.93
1.214	1	8 6 0	78.79
1.212	1	3 7 2	78.91
1.211	1	3 11 0	79.00
1.206	1	6 3 2	79.41
1.200	8	1 8 2	79.66
1.200	3	5 9 1	79.87
1.192	2	7 8 0	80.53
1.186	1	1 11 1	80.98
1.180	1	2 8 2	81.47
1.178	2	4 10 1	81.68
1.175	2	9 1 1	81.94
1.172	1	0 12 0	82.21
1.166	1	4 7 2	82.66
1.165	2	4 11 0	82.75
1.163	1	9 2 1	82.98
1.159	6	8 7 0	83.32
1.156	2	7 1 2	83.57
1.143	9	9 3 1	84.71
1.138	5	3 11 1	85.23
1.132	1	6 9 1	85.73
1.132	2	1 9 2	85.76
1.131	1	10 1 0	85.82
1.126	1	7 3 2	86.33
1.125	5	5 10 1	86.46
1.122	2	7 8 1	86.74
1.120	2	10 2 0	86.86
1.118	1	9 4 1	87.13
1.115	9	2 9 2	87.35
1.115	7	5 7 2	87.42
1.111	4	9 6 0	87.84
1.103	3	10 3 0	88.58
1.101	12	6 6 2	88.76
1.100	1	1 12 1	88.93
1.100	1	4 11 1	88.93
1.094	13	8 7 1	89.50
1.085	2	2 12 1	90.51
1.083	2	4 12 0	90.68
1.077	4	1 13 0	91.36
1.075	2	8 1 2	91.50
1.073	2	2 2 3	91.71
1.073	2	0 10 2	91.77
1.066	6	9 2 2	92.53
1.065	1	7 9 1	92.59
1.062	3	2 13 0	92.94

2,4,6-Trinitrophenetole, $C_2H_5OC_6H_2(NO_2)_3$ (orthorhombic)

Structure

Orthorhombic, $Pca2_1$ (29), Z=4 [Gramaccioli et al. 1968]

Lattice parameters

a = 23.7858 ±.0008Å, b = 7.3580 ±.0007Å, c=6.2645 ±.0004Å(published as a=23.7848± .0008,b=7.3577 ±.0007,c=6.2642 ±.0004Å,) [ibid.]

Thermal parameters

Anisotropic [ibid.]

Density

(calculated) 1.557 g/cm^3 [ibid.]

Scattering factors

H° [McWeeny, 1951]
C°, N°, O°, [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 6.288×10^{-4}

Reference

Cromer, D.T. and J.T. Waber (1965). Scattering factors computed from relativistic Dirac-Slater wave functions, Acta Cryst. **18**, 104-109.

Gramaccioli, C.M., R.Destro, and M. Simonetta (1968). The structure of 2,4,6-Trinitrophenetole, Acta Cryst. B24,129-136.

McWeeny,R. (1951). X-ray scattering by aggregates of bonded atoms. I. Analytical approximations in single-atom scattering Acta Cryst 4, 513-519

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
11.87	29	2 0 0	7.44
7.357	39	0 1 0	12.02
7.031	37	1 1 0	12.58
6.258	18	2 1 0	14.14
5.941	5	4 0 0	14.90
5.542	20	2 0 1	15.98
5.394	22	3 1 0	16.42
4.677	25	1 1 1	18.96
4.624	5	4 1 0	19.18
4.427	9	2 1 1	20.04

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
4.312	10	4 0 1	20.58
4.088	3	3 1 1	21.72
3.720	100	4 1 1	23.90
3.678	13	0 2 0	24.18
3.490	13	6 1 0	25.50
3.368	5	5 1 1	26.44
3.351	5	6 0 1	26.58
3.144	6	1 2 1	28.36
3.134	5	0 0 2	28.46
3.064	5	2 2 1	29.12
3.050	6	6 1 1	29.26
3.029	4	2 0 2	29.46
2.945	7	3 2 1	30.32
2.910	3	5 2 0	30.70
2.882	2	0 1 2	31.00
2.861	3	1 1 2	31.24
2.801	17	2 1 2 +	31.92
2.768	9	7 1 1 +	32.32
2.696	1	6 2 0	33.20
2.639	6	5 2 1	33.94
2.593	1	4 1 2	34.56
2.523	2	8 1 1	35.56
2.487	2	9 1 0	36.08
2.477	10	6 2 1	36.24
2.403	1	2 3 0	37.40
2.385	1	0 2 2	37.68
2.373	1	1 2 2	37.88
2.343	2	3 3 0	38.38
2.338	2	2 2 2	38.48
2.319	1	7 2 1	38.80
2.312	3	8 2 0 +	38.92
2.284	1	3 2 2	39.42
2.223	2	10 0 1	40.54
2.197	2	7 1 2 +	41.04
2.156	1	8 0 2	41.86
2.132	4	5 2 2 +	42.36
2.128	3	10 1 1	42.44
2.059	3	5 3 1 +	43.94
1.9812	3	2 1 3	45.76
1.9698	1	4 0 3	46.04
1.9521	1	7 2 2	46.48
1.9474	2	3 1 3	46.60
1.9028	1	10 2 1	47.76
1.8953	2	7 3 1	47.96
1.8901	2	12 0 1	48.10
1.8603	1	8 2 2	48.92
1.8343	1	10 1 2	49.66

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
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	2 0 1	15.98
5.393	20	3 1 0	16.42
4.677	23	1 1 1	18.96
4.625	4	4 1 0	19.17
4.427	9	2 1 1	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	5	5 1 1	26.44
3.350	5	6 0 1	26.59
3.145	6	1 2 1	28.36
3.132	3	0 0 2	28.47
3.065	5	2 2 1	29.11
3.049	6	6 1 1	29.27
3.029	4	2 0 2	29.46
2.945	8	3 2 1	30.32
2.910	3	5 2 0	30.70
2.882	2	0 1 2	31.00
2.861	3	1 1 2	31.24
2.801	17	2 1 2	31.93
2.799	3	4 2 1	31.95
2.771	5	4 0 2	32.28
2.768	7	7 1 1	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
2.477	12	6 2 1	36.24
2.465	1	5 1 2	36.42
2.402	2	2 3 0	37.41
2.385	1	0 2 2	37.69
2.373	1	1 2 2	37.88
2.343	2	3 3 0	38.38
2.338	1	2 2 2	38.47
2.319	1	7 2 1	38.80
2.312	2	8 2 0	38.91
2.312	1	9 1 1	38.93
2.284	1	3 2 2	39.42
2.224	2	10 0 1	40.53
2.198	2	7 1 2	41.03
2.195	1	3 3 1	41.10
2.156	1	8 0 2	41.86

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.132	2	5 2 2	42.36
2.132	2	4 3 1	42.36
2.129	1	10 1 1	42.43
2.059	3	5 3 1	43.94
2.0567	1	2 0 3	43.99
1.9808	3	2 1 3	45.77
1.9702	1	4 0 3	46.03
1.9521	2	7 2 2	46.48
1.9473	2	3 1 3	46.60
1.9031	1	10 2 1	47.75
1.8955	1	7 3 1	47.95
1.8898	2	12 0 1	48.11
1.8604	1	8 2 2	48.92
1.8345	1	10 1 2	49.66

Uric Acid, $C_5H_4N_4O_3$ (monoclinic)

Structure
Monoclinic, $P2_1/a$ (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:

C	H	N	O
(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^0, N^0, O^0, H^0 [3.3.1A]

Scale factor
(integrated intensities) 1.914 x 10^4

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)	I	hkl	2θ(°) λ = 1.54056 Å
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
3.864	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)	I	hkl	2θ(°) λ = 1.54056 Å
3.281	14	4 0 0	27.16
3.227	3	2 2 0	27.66
3.209	5	4 1 1	27.78
3.180	55	1 2 1	28.04
3.093	100	0 2 1	28.84
3.087	69	2 2 1	28.90
3.000	3	4 1 0	29.76
2.866	25	1 2 -1 +	31.18
2.826	1	3 2 0	31.64
2.815	2	0 0 2	31.76
2.796	9	4 0 2	31.98
2.632	2	0 1 2	34.04
2.615	1	4 1 2	34.26
2.566	15	4 2 1	34.94
2.454	3	4 2 0	36.58
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	7	6 0 2	40.14
2.240	6	0 2 2	40.22
2.186	5	6 0 0	41.26
2.166	2	1 3 -1 +	41.66
2.148	1	6 1 2	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
1.6402	1	8 0 0	56.02
1.6180	2	6 2 -1	56.86
1.6117	2	4 4 0 +	57.10
1.6045	1	8 2 2	57.38
1.5898	3	2 4 2	57.96
1.5789	1	1 4 2	58.40
1.5745	1	5 1 -2	58.58
1.5466	4	0 4 2	59.74
1.5132	1	2 0 4 +	61.20

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.56	37	2 0 0	13.49
6.45	1	1 1 0	13.72
5.63	18	0 0 1	15.72
4.91	46	2 1 0	18.05
4.76	8	1 1 1	18.64
4.48	1	0 1 1	19.79
3.864	39	1 1 -1	23.00
3.838	16	3 1 1	23.15
3.701	6	0 2 0	24.02
3.590	2	2 0 -1	24.78
3.280	14	4 0 0	27.16
3.224	2	2 2 0	27.65
3.209	4	4 1 1	27.78
3.179	55	1 2 1	28.04
3.093	100	0 2 1	28.84
3.087	7	2 2 1	28.90
2.999	3	4 1 0	29.77
2.866	24	1 2 -1	31.16
2.862	5	2 1 2	31.22
2.825	1	3 2 0	31.64
2.815	1	0 0 2	31.76
2.796	10	4 0 2	31.98
2.632	2	0 1 2	34.04
2.616	1	4 1 2	34.25
2.577	1	2 2 -1	34.78
2.566	16	4 2 1	34.94
2.455	3	4 2 0	36.57
2.425	3	4 0 -1	37.04
2.404	2	1 1 -2	37.37
2.310	5	2 3 0	38.96
2.278	3	5 2 1	39.53
2.265	2	2 0 -2	39.77
2.244	7	6 0 2	40.14
2.241	4	0 2 2	40.21
2.187	5	6 0 0	41.29

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.167	2	1 3 -1	41.64
2.166	1	2 1 -2	41.67
2.148	1	6 1 2	42.03
2.095	1	1 2 -2	43.14
2.028	2	4 2 -1	44.64
1.909	1	3 3 2	47.58
1.877	2	0 0 3	48.46
1.8076	2	6 1 3	50.45
1.8062	1	3 2 3	50.49
1.7976	3	7 2 1	50.74
1.7912	2	2 2 3	50.94
1.7839	1	8 0 1	50.98
1.7683	1	3 2 -2	51.45
1.7582	1	0 4 1	51.97
1.7480	1	6 1 -1	52.29
1.7443	1	1 2 3	52.39
1.6741	1	0 2 3	54.79
1.6648	2	6 2 3	55.12
1.6401	1	8 0 0	56.03
1.6179	2	8 2 -1	56.86
1.6118	1	4 4 0	57.09
1.6114	1	6 2 1	57.11
1.6043	1	8 2 2	57.39
1.5898	3	2 4 2	57.97
1.5789	1	1 4 2	58.40
1.5741	1	5 1 -2	58.60
1.5465	6	0 4 2	59.74
1.5133	1	2 0 4	61.20
1.5124	1	5 4 0	61.23

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 8[5]

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

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

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A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

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A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

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A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE MINERAL INDEX

*Natural mineral.

M– Monagraph 25.

CUMULATIVE MINERAL INDEX—Continued

*Natural mineral.

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