NBS CIRCULAR 539
VOLUME 6

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

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ERRATA

Vol. 1. Page 24, last sentence should read, . . . a body centered lattice with four atoms in the unit cell.
Page 35, table 17, column 1, line 13, the *hkl* 620 sbould read 600. The following *hkl*'s should be delcted: 533, 622, and 444.
Page 41, table 20, the Clark Pattern, Mo 0.7093 A, should read Co 1.7889 A.

Vol. 2. Page 20, the spaee group under "lattice constant$^0_{3d}$" listed as D–R3c, should read $D^6_{3d}R\bar{3}c$.
Page 47, the space group under "lattice constants" should read D^{16}_{2h}-Pnma.

Vol. 5. Page 11, the *hkl* 400 should be 440.
Page 24, the data given for Copper(II) Fluoride, CuF_2 (cubic) should be deleted.
Page 25, the three strongest lines tabulated for the NBS pattern sbould read 222, 400, and 440.
Page 25, the missing *hkl* in the GeI_4 table for *d*-value 1.5047 is 800.
Page 30, the *d*-value 1.1448 for tbe NBS pattern should read 1.4448.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. 6—Data for 44 Inorganic Substances

Howard E. Swanson, Nancy T. Gilfrich,[1] and Marlene I. Cook [1]

Forty-four standard X-ray diffraction powder patterns are presented. Twenty-three are to replace thirty-three patterns already represented in the ASTM card file, and twenty-one are for substances not previously represented. The ASTM card file is a compilation of diffraction patterns from all sources and is used for the identification of unknown crystalline materials by matching spacing and intensity measurements. In this Circular, comparison is made of all powder diffraction data available for each of the substances reported. The patterns were made with a Geiger counter X-ray diffractometer, using samples of high purity. The *d*-values were assigned Miller indices determined by comparison with calculated interplanar spacings and from space group considerations. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible.

Included are X-ray data for the following forty-four substances: $NH_4Al(SO_4)_2 \cdot 12H_2O$, $(NH_4)_2PdCl_4$, $NH_4Cr(SO_4)_2 \cdot 12H_2O$, $(NH_4)_2GeF_6$, $NH_4Ga(SO_4)_2 \cdot 12H_2O$, $NH_4Fe(SO_4)_2 \cdot 12H_2O$, $(NH_4)_2SO_4$ (mascagnite), $(NH_4)_3ZrF_7$, SbI_3, AsI_3, BaO_2, BiI_3, $CdMoO_4$, $CaWO_4$ (scheelite), $CsAl(SO_4)_2 \cdot 12H_2O$, Cs_2PtF_6, $CsFe(SO_4)_2 \cdot 12H_2O$, Cr_3Si, GaSb, $Mg(OH)_2$ (brucite), $MgSiO_3$ (enstatite), $Hg(CN)_2$, $KAl(SO_4)_2 \cdot 12H_2O$, K_2SnCl_6, $KCr(SO_4)_2 \cdot 12H_2O$, K_2PtF_6, $KClO_4$, $RbAl(SO_4)_2 \cdot 12H_2O$, Rb_2SnCl_6, $RbCr(SO_4)_2 \cdot 12H_2O$, Rb_2PtF_6, Rb_2SiF_6, $NaNO_3$ (soda-niter), SrO_2, $TlAl(SO_4)_2 \cdot 12H_2O$, Tl_2SnCl_6, $TlCr(SO_4)_2 \cdot 12H_2O$, Tl_2SiF_6, $TlGa(SO_4)_2 \cdot 12H_2O$, $TlNO_3$, Tl_2SO_4, and ZnF_2.

INTRODUCTION

The National Bureau of Standards in its program [2] for the revision and evaluation of published X-ray data for the American Society for Testing Materials card file presents in this paper, the sixth of this series,[3] data for 44 inorganic compounds. Twenty-three of these patterns are recommended to replace 33 cards now in the file. The patterns for 21 compounds not represented in the file have been added. These compounds are ammonium chloropalladite, ammonium fluogermanate, ammonium gallium sulfate dodecahydrate, cadmium molybdate, calcium molybdate, cesium fluoplatinate, cesium iron sulfate dodecahydrate, chromium silicide, gallium antimonide, potassium chlorostannate, potassium fluoplatinate, rubidium chlorostannate, rubidium fluoplatinate, rubidium fluosilicate, thallium aluminum sulfate dodecahydrate, thallium chlorostannate, thallium chromium sulfate dodecahydrate, and thallium(I) nitrate.

The experimental procedure and general plan of these reports have not changed from that of the previous volumes of this NBS Circular. The basic technique is included and discussed in the same order that is followed in presenting the data for each compound in the body of this volume.

ASTM cards. Each section of this Circular contains a table listing the file card numbers, the ASTM index lines in order of decreasing intensity, the radiation used, and the literature references for each card. The card numbers are as revised in the second edition. This volume of Circular 539 includes the sixth set of ASTM cards.

Additional published patterns. Literature references and radiation data for patterns that had not been published as ASTM cards are listed, and the patterns are included in the tables of *d*-values and intensities.

NBS sample. Many of the samples used to make the NBS patterns are special preparations (of exceptionally high purity) obtained or prepared only in small quantities. The purity of each sample was determined by spectroscopic or chemical analysis. The limit of detection for the alkali elements is 0.05 percent for the NBS spectrographic analysis. Unless otherwise noted, the spectrographic analysis was done at the NBS. A phase-purity check was made of the nonopaque materials during the refractive index determination. Another excellent check of phase-purity was provided by the indexing of the X-ray pattern. Treating the sample by appropriate annealing, recrystallizing, or heating in a hydrothermal bomb improved the quality of most of the patterns.

At least two intensity patterns were prepared to check reproducibility of measured values. Samples that gave satisfactory intensity patterns showed a particle size average well within the range of 5 to 10 microns as was suggested by Alexander, Klug, and Kummer [1].[4] A special cell with one open end is used for making intensity measurements. An intensity sample was prepared by clamping a flat piece of glass temporarily over the surface of this holder, and, while it was held in a perpendicular position, the sample was drifted in

[1] Fellow at the National Bureau of Standards sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods.

[2] This project is sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods. This committee is composed of members from the American Society for Testing Materials, the American Crystallographic Association, and the British Institute of Physics. Financial support is also provided by the National Bureau of Standards.

[3] Other volumes were published as follows: Vol. 1 and vol. 2, June 1953; vol. 3, June 1954; vol. 4, March 1955; and vol. 5, October 1955.

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

from the open end. The glass was then carefully removed so that the surface of the sample could be exposed to the X-ray beam. For a few powder samples that did not flow readily or were prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensity values of each pattern are measured as peak height above background and are expressed as percentages of the strongest line.

Additional patterns are obtained for *d*-value measurements. These specimens were prepared by packing, into a shallow holder, a sample containing approximately 5 weight percent of tungsten powder that served as an internal standard. The lattice constant of tungsten at 25° C is 3.1648 A, as determined by Jette and Foote [2]. All of the NBS patterns are made by using filtered copper radiation ($K_{\alpha 1}$), having a wavelength of 1.5405 A.

Interplanar spacings and intensity measurements. Interplanar spacing data presented in the tables were converted to angstrom units as internationally defined in 1946 [3]. The conversions were from Bragg angle data, from *d*-values in kX units, using factor 1.00202, or from *d*-values based on wavelengths given in other than kX units. In each case the type of conversion made is indicated. The wavelengths in the tables of *d*-values and intensities are given in angstrom units. The values listed under the first section of each report are the original values taken from the literature. The table of patterns contains data based on the original work rather than that data reported on the ASTM cards.

Intensities, when not numerically evaluated, are given the following abbreviations: strong, s; medium, m; weak, w; diffuse, D; doublet, db; and very, v.

In indexing cubic patterns, the number of possible combinations of *hkl*'s for a specific value of the expression $(h^2+k^2+l^2)$ can be very great, particularly when the value becomes large. It has been customary in this Circular to make $h>k>l$ and to choose the *hkl* with the largest *h* if not limited by the space group. Also, in the case of indexing tetragonal patterns, when there were planes which could be indexed by two *hkl* values, the *hkl* having the larger *h* was chosen. Noncubic patterns were indexed by comparing *d*-values of the NBS pattern with those calculated for all possible Miller indices by the SEAC, the NBS electronic computer. The unit cells used in calculating *d*-values were obtained by partial indexing of the NBS pattern based on the cell values from literature. The noncubic indexing includes all probable indices for any given *d*-value allowed by the space group of that structure. An attempt was made to reconcile these values with published single crystal work when it was available. However, errors inherent in the indexing of powder data undoubtedly are present in some patterns.

A table comparing the three most intense lines of each pattern is included with the discussion of interplanar spacing and intensity measurements. The strongest lines are listed by Miller indices rather than *d*-values because of the variation in spacing values. The intensities measured for these three lines are of particular importance since the use of the ASTM card-file system for identification of materials is based upon the ability to sort cards by the first, second, and third strongest lines.

Structural data. The NBS lattice constants of cubic materials were calculated for all *d*-values, and the average of the last five values was assumed to be the best because of greater accuracy of measurement in the large-angle part of the pattern. The unit-cell values for each noncubic substance were determined from the *d*-values of its pattern by means of a least-squares calculation made by the SEAC. The number of significant figures reported in the NBS pattern is limited by the quality of each sample and by the crystal symmetry.

The conversion of published unit-cell data to angstrom units is presented in the same manner as that used for *d*-values. The unit-cell values were corrected for temperature for comparison with the NBS values if the temperature of measurement and the thermal expansion of the substance is known. The coefficient of linear thermal expansion as used is defined as the change in length per unit length per unit degree Celsius in the room-temperature range, unless otherwise indicated. Thermal expansion data have been given whenever the data were readily available, even though no temperature conversions were made in the unit-cell data table. The limits of errors generally published with unit-cell data are not included in the table because the number of determinations, and their accuracy and variations are such that a statistical evaluation would be unjustified.

The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter and are based upon atomic weights reported by E. Wichers [4] in 1954. The refractive index measurements are made in white light by grain immersion methods, using oils standardized in sodium light.

References

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

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

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

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Ammonium Aluminum Sulfate Dodecahydrate, $NH_4Al(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards

Card numbers	Index lines	Radiation	Source
2–0490	3. 25 1. 92 4. 30	Chromium and iron.	Quilico [1] 1928.
1–0695	3. 26 4. 30 5. 4	Molybdenum.	Hanawalt, Rinn, and Frevel [2] 1938.

The *d*-values of the Quilico pattern reported on ASTM card 2–0490 are the average values of two patterns, one made by using chromium and the other by using iron radiation.

Additional published patterns

Source	Radiation	Wavelength
Cork [3] 1927	------	--------
Vegard and Esp [4] 1928	Chromium.	Kα

NBS Sample. The sample of ammonium aluminum sulfate dodecahydrate was obtained from the J. T. Baker Chemical Co., Phillipsburg, N. J. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of iron, magnesium, silicon, and tin; and 0.0001 to 0.001 percent of calcium.

The sample is colorless. The index of refraction is 1.458.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the *d*-values of Cork, Vegard and Esp, and Quilico were calculated from Bragg angle data. The pattern of Vegard and Esp did not include intensity values.

The three strongest lines of each of the patterns are as follows:

Pattern	1	2	3
Cork	220	111	400
Quilico (chromium)	321	621	220
Quilico (iron)	321	10·2.0	230
Hanawalt, Rinn, and Frevel	321	220	210
Swanson, Gilfrich, and Cook	220	221	321

Structural data. Wyckoff [5] in 1923 determined that ammonium aluminum sulfate dodecahydrate is an alpha alum having the space group T_h–Pa3 and $4[NH_4Al(SO_4)_2 \cdot 12H_2O]$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1917	Vegard and Schjelderup [6]	12.02
1927	Cork [3]	12.21
1928	Vegard and Esp [4]	12.13
1928	Quilico [1]	12.19
1940	Klug and Alexander [7]	12.240
1955	Menary [8]	12.241 at 24° C
1956	Swanson, Gilfrich, and Cook.	12.240 at 25° C

The density of ammonium aluminum sulfate dodecahydrate calculated from the NBS lattice constant is 1.642 at 25° C.

References

[1] A. Quilico, Sugli allumi di basi organiche. I. Allums di metilammina, Gazz. chim. ital. **58,** 682–690 (1928).

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

[3] J. M. Cork, The crystal structure of some of the alums, Phil. Mag. **4,** 688–698 (1927).

[4] L. Vegard and E. Esp, The crystal structure of the alums, Ann. Physik **85,** 1152–1164 (1928).

[5] R. W. G. Wyckoff, The crystal structure of some of the alums, Am. J. Sci. **5,** 209–217 (1923).

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[7] H. P. Klug and L. Alexander, Crystal-chemical studies of the alums. III. further solid solution studies, J. Am. Chem. Soc. **62,** 2993–2995 (1940).

[8] J. W. Menary, Some lattice constants, Acta Cryst. **8,** 840 (1955).

Ammonium Aluminum Sulfate Dodecahydrate, $NH_4Al(SO_4)_2 \cdot 12H_2O$ (cubic)

hkl	1928 Quilico Cr, 2.2909 A			1928 Quilico Fe, 1.9373 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1927 Cork Mo, 0.7107 A			1928 Vegard and Esp Cr, 2.2909 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	-----	----	-----	-----	----	-----	7.0	30	12.1	7.20	92	12.5	6.94	----	12.0	7.07	56	12.2
200	5.94	w	11.9	5.86	w	11.7	----	----	----	6.14	18	12.3	6.00	----	12.0	6.13	12	12.3
210	5.33	mw	11.9	5.25	m	11.8	5.4	60	12.1	-----	----	-----	5.38	----	12.0	5.48	53	12.3
211	4.86	w	11.92	-----	----	-----	4.97	30	12.17	-----	----	-----	4.90	----	11.99	4.998	35	12.24
220	4.24	ms	12.00	4.17	ms	11.81	4.30	80	12.16	4.32	100	12.21	4.26	----	12.04	4.327	100	12.24
221	4.00	mw	12.00	3.94	ms	11.83	4.07	60	12.21	-----	----	-----	4.01	----	12.03	4.079	78	12.24
311	3.62	w	12.01	3.74	m	12.39	3.67	40	12.17	3.56	----	11.82	3.65	----	12.11	3.691	37	12.24
230	-----	----	-----	3.62	s	12.00	----	----	----	-----	----	-----	-----	----	-----	3.395	5	12.24
321	3.22	vs	12.07	3.20	vs	11.97	3.26	100	12.20	-----	----	-----	3.24	----	12.12	3.273	77	12.25
400	3.02	mw	12.10	-----	----	-----	3.05	30	12.20	3.06	83	12.24	3.04	----	12.15	3.060	28	12.24
410	2.94	mw	12.13	2.99	ms	12.32	2.95	8	12.16	-----	----	-----	2.94	----	12.14	2.967	22	12.23
411	2.85	w	12.09	2.81	w	11.93	----	----	----	-----	----	-----	2.86	----	12.13	2.883	14	12.33
331	2.78	m	12.12	-----	----	-----	2.79	12	12.16	-----	----	-----	2.79	----	12.15	2.810	33	12.25
420	2.71	mw	12.12	2.75	mw	12.30	----	----	----	-----	----	-----	2.72	----	12.16	2.738	18	12.24
421	2.64	w	12.10	2.68	mw	12.26	----	----	----	-----	----	-----	2.65	----	12.15	2.672	14	12.24
332	2.55	w	11.97	2.56	mw	12.01	2.60	12	12.20	-----	----	-----	2.59	----	12.13	2.608	11	12.23
422	2.48	vw	12.12	2.45	w	12.02	----	----	----	-----	----	-----	2.48	----	12.16	2.499	10	12.24
431	2.37	w	12.06	-----	----	-----	----	----	----	2.38	48	12.15	2.38	----	12.11	2.402	7	12.25
511	2.33	w	12.11	2.36	mw	12.26	2.34	8	12.16	-----	----	-----	2.34	----	12.15	2.358	12	12.25
432	2.25	mw	12.12	-----	----	-----	----	----	----	-----	----	-----	2.26	----	12.18	2.275	7	12.25
521	2.21	mw	12.12	2.24	m	12.23	2.25	8	12.32	-----	----	-----	2.22	----	12.16	2.237	11	12.25
-----	-----	----	-----	2.19	mw	-----	----	----	----	-----	----	-----	-----	----	-----	-----	----	-----
522	-----	----	-----	-----	----	-----	2.12	8	12.18	2.16	1	12.41	2.12	----	12.16	2.130	8	12.23
433	2.11	m	12.30	2.09	w	12.19	----	----	----	-----	----	-----	-----	----	-----	2.098	4	12.24
531	2.05	mw	12.13	2.08	m	12.32	----	----	----	-----	----	-----	2.06	----	12.18	2.068	8	12.24
600	2.02	w	12.13	-----	----	-----	2.02	8	12.12	-----	----	-----	2.03	----	12.17	2.039	10	12.23
610	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	1.997	----	12.15	2.012	10	12.24
611	1.993	mw	12.29	-----	----	-----	----	----	----	-----	----	-----	1.973	----	12.16	1.985	10	12.24
620	1.969	m	12.45	-----	----	-----	1.93	35	12.21	-----	----	-----	1.927	----	12.19	1.935	15	12.24
621	1.920	s	12.29	1.911	s	12.24	----	----	----	-----	----	-----	-----	----	-----	1.910	2	12.23
541	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	1.873	----	12.14	1.888	3	12.24
533	1.869	m	12.26	1.861	w	12.20	1.86	4	12.20	1.861	51	12.20	1.856	----	12.17	1.866	7	12.23
622	1.846	m	12.24	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1.846	6	12.24
630	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	1.813	----	12.16	1.825	6	12.24
631	1.809	w	12.26	1.800	m	12.21	1.81	16	12.28	1.793	2	12.16	1.794	----	12.17	1.805	2	12.24

Ammonium Aluminum Sulfate Dodecahydrate, $NH_4Al(SO_4)_2 \cdot 12H_2O$ (cubic)—Continued

hkl	1928 Quilico Cr, 2.2909 A			1928 Quilico Fe, 1.9373 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1927 Cork Mo, 0.7107 A			1928 Vegard and Esp Cr, 2.2909 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A 25°, C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A	A		A	A		A
444	1.789	w	12.52	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1.768	<1	12.25
632	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1.749	2	12.24
543	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1.731	10	12.24
711	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	1.707	----	12.19	1.714	3	12.24
640	1.701	m	12.27	1.695	m	12.22	1.70	12	12.26	-----	----	-----	-----	----	-----	1.698	2	12.24
641	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1.681	7	12.24
721	1.649	w	12.12	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1.666	9	12.24
642	1.624	m	12.15	-----	----	-----	----	----	----	-----	----	-----	1.631	----	12.21	1.635	7	12.24
722	1.610	m	12.16	1.619	ms	12.22	1.62	12	12.23	-----	----	-----	1.614	----	12.19	1.620	7	12.24
731	1.589	mw	12.21	1.604	ms	12.32	1.58	2	12.14	-----	----	-----	1.590	----	12.22	1.593	7	12.24
650	-----	----	-----	1.588	mw	12.50	----	----	----	-----	----	-----	-----	----	-----	1.568	<1	12.25
732	1.550	m	12.20	-----	----	-----	1.54	2	12.13	1.533	1	12.07	1.552	----	12.22	1.554	2	12.23
810	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	1.503	----	12.12	1.5183	4	12.241
811	1.505	w	12.23	1.503	w	12.21	----	----	----	-----	----	-----	-----	----	-----	1.5065	4	12.239
733	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	1.480	----	12.12	1.4955	10	12.241
820	1.480	mw	12.20	-----	----	-----	1.48	12	12.20	-----	----	-----	-----	----	-----	1.4850	3	12.246
821	-----	----	-----	1.474	mw	12.24	----	----	----	-----	----	-----	-----	----	-----	1.4737	2	12.242
822	1.445	m	12.26	-----	----	-----	----	----	----	1.440	15	12.22	1.440	----	12.22	1.4423	5	12.238
831	-----	----	-----	-----	----	-----	----	----	----	1.431	1	12.32	1.423	----	12.24	1.4225	7	12.237
751	1.407	mw	12.18	1.417	mw	12.27	----	----	----	-----	----	-----	1.411	----	12.22	1.4127	<1	12.234
832	1.402	m	12.30	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1.3942	<1	12.234
840	1.370	mw	12.25	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1,3689	2	12.244
841	1.356	m	12.20	1.357	ms	12.21	----	----	----	-----	----	-----	-----	----	-----	1.3602	12	12.242
902	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1.3278	5	12.242
921	-----	----	-----	1.317	m	12.21	----	----	----	-----	----	-----	-----	----	-----	1.3198	2	12.239
922	-----	----	-----	-----	----	-----	----	----	----	1.308	5	12.34	-----	----	-----	1.2971	5	12.237
851	1.285	mw	12.19	1.289	ms	12.23	----	----	----	-----	----	-----	-----	----	-----	1.2902	3	12.240
932	-----	----	-----	1.262	w	12.24	----	----	----	-----	----	-----	-----	----	-----	1.2631	<1	12.246
844	-----	----	-----	1.251	w	12.26	----	----	----	-----	----	-----	-----	----	-----	1.2494	<1	12.241
933	-----	----	-----	1.221	m	12.15	----	----	----	-----	----	-----	-----	----	-----	1.2299	3	12.237
10·1·0	-----	----	-----	-----	----	-----	----	----	----	-----	----	-----	-----	----	-----	1.2176	3	12.237
10·2·0	-----	----	-----	1.195 [a]	vs	12.19	----	----	----	1.193 [b]	13	12.17	-----	----	-----	1.2000	4	12.238
Average of last five lines			12.20			12.21			12.19			12.21			12.18			12.240

[a] Seven additional lines were omitted.

[b] Ten additional lines were omitted.

Ammonium Chloropalladite, $(NH_4)_2PdCl_4$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
3–1226	[a]	[a]	Dickinson [1] 1946.

[a] No powder data.

Additional published patterns. None.

NBS sample. The sample of ammonium chloropalladite was obtained from Johnson, Matthey & Co., Ltd. Their spectrographic analysis showed the following impurities: 0.001 to 0.01 percent of calcium; and 0.0001 to 0.001 percent of potassium.

The sample has a yellow-brown color and is optically negative. The refractive indices are $N_o=1.712$ and $N_e=1.549$.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	100	101	001

Structural data. Dickinson [1] in 1922 determined that ammonium chloropalladite has potassium chloropalladite-type structure, the space group D^1_{4h}–P4/mmm, and $1[(NH_4)_2PdCl_4]$ per unit cell.

The unit-cell measurements of Dickinson were converted fron kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1922	Dickinson [1]	7. 22	4. 27
1956	Swanson, Gilfrich, and Cook.	7. 218	4.270 at 25° C

The density of ammonium chloropalladite calculated from the NBS lattice constants is 2.124 at 25° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*
	A	
100	7. 21	100
110	5. 10	18
001	4. 26	46
101	3. 67	51
111	3. 27	42
210	3. 22	15
201	2. 756	6
211	2. 574	19
220	2. 550	31
300	2. 404	3
310	2. 280	5
221	2. 191	21
002	2. 136	8
301	2. 098	2
102	2. 046	6
311	2. 011	15
320	2. 002	13
112	1. 970	4
321	1. 813	16
400	1. 804	14
212	1. 782	6
330	1. 701	4
401	1. 662	7
222	1. 637	8
411	1. 620	6
331	1. 580	7
312	1. 559	4
322	1. 460	5
500	1. 444	4
003	1. 422	2
510	1. 4154	3
402	1. 3785	3
113	1. 3716	3
501	1. 3679	4
412	1. 3542	3
511	1. 3438	5
440	1. 2770	<1
441	1. 2232	<1
502	1. 1961	4
512	1. 1804	<1
323	1. 1605	<1
611	1. 1434	3
620	1. 1411	3
540	1. 1276	2
621	1. 1025	3
442	1. 0955	<1
541	1. 0901	2
630	1. 0763	<1
104	1. 0550	<1
114	1. 0436	1
631		
710	1. 0206	1
503	1. 0137	1
622	1. 0064	2
640	1. 0008	1
711	0. 9928	1
224	. 9850	<1
721	. 9658	2
730	. 9481	<1
731	. 9253	1
712	. 9211	1

References

[1] R. G. Dickinson, The crystal structures of potassium chloroplatinite and of potassium and ammonium chloropalladites, J. Am. Chem. Soc. **44**, 2404–2411 (1922).

Ammonium Chromium Sulfate Dodecahydrate, $NH_4Cr(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0364	4. 35 3. 29 7. 1	Molyb-denum.	Hanawalt, Rinn, and Frevel [1] 1938.

The data on ASTM card 1–0370 is for $NH_4Cr(SO_4)_2 < 12H_2O$, which is very similar to that for the dodecahydrate.

Additional published patterns. None.

NBS sample. The sample of ammonium chromium sulfate dodecahydrate was prepared at the NBS from ammonium sulfate and chromium sulfate. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of nickel; 0.001 to 0.01 percent each of aluminum, barium, cobalt, copper, magnesium, and silicon; and 0.0001 to 0.001 percent each of silver, calcium, iron, manganese, and lead.

The sample has a pale lavender color. The index of refraction is 1.482.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	220	321	111
Swanson, Gilfrich, and Cook	220	321	111

Structural data. Klug and Alexander [2] in 1940 found ammonium chromium sulfate dodecahydrate to be an alpha alum having the space group T_h^6–Pa3 and $4[NH_4Cr(SO_4)_2 \cdot 12H_2O]$ per unit cell. The structure of the alpha alums was determined by Wyckoff [3] in 1923.

The unit-cell measurement reported by Klug and Alexander has been converted from kX to angstrom units.

Lattice constants

		A
1940	Klug and Alexander [2]	12.276 at 25° C
1956	Swanson, Gilfrich, and Cook.	12.274 at 25° C

The density of ammonium chromium sulfate dodecahydrate calculated from the NBS lattice constant is 1.718 at 25° C.

References

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

[2] H. P. Klug and L. Alexander, Crystal-chemical studies of the alums. II. The purple chrome alums, J. Am. Chem. Soc. **62,** 2992–2993 (1940).

[3] R. W. G. Wyckoff, The crystal structure of the alums, Am. J. Sci. **5,** 209–217 (1923).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1956 Swanson, Gilfrich, and Cook Cu, 1,5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
111	7. 1	64	12. 3	7. 08	68	12. 3
210	5. 5	32	12. 3	5. 49	41	12. 3
211	5. 0	14	12. 2	5. 02	22	12. 3
220	4. 36	100	12. 3	4. 341	100	12. 28
221	4. 12	40	12. 4	4. 090	50	12. 27
311	3. 72	64	12. 3	3. 699	63	12. 27
222	3. 56	2	12. 3	3. 543	1	12. 28
321	3. 30	80	12. 4	3. 283	70	12. 28
400	3. 09	40	12. 4	3. 072	32	12. 29
410	2. 99	5	12. 33	2. 978	18	12. 28
411	2. 91	3	12. 35	2. 894	10	12. 28
331	2. 83	3	12. 34	2. 820	16	12. 29
420	2. 76	13	12. 34	2. 748	26	12. 29
421	2. 68	3	12. 28	2. 677	12	12. 27
332	2. 62	3	12. 29	2. 617	11	12. 27
422	2. 52	10	12. 34	2. 505	8	12. 27
431	2. 42	3	12. 34	2. 410	5	12. 29
511	2. 37	13	12. 31	2. 363	13	12. 28
432	2. 28	3	12. 28	2. 283	<1	12. 29
521	2. 25	3	12. 32	2. 244	6	12. 29
440	2. 18	2	12. 33	2. 172	6	12. 29
522	2. 14	2	12. 29	2. 137	8	12. 28
433	----	---	-----	2. 104	5	12. 27
531	2. 06	16	-----	2. 076	16	12. 28
600	----	---	-----	2. 047	12	12. 28
610	----	---	-----	2. 019	7	12. 28
611	1. 99	3	12. 27	1. 992	8	12. 28
620	1. 94	32	12. 27	1. 942	19	12. 28
---	1. 89	2	-----	------	---	------
622	----	---	-----	1. 8510	<1	12. 28
631	1. 81	3	12. 28	1. 8104	1	12. 28
444	----	---	-----	1. 7720	2	12. 28
543	----	---	-----	1. 7357	1	12. 27
711	1. 72	16	12. 28	1. 7202	9	12. 28
640	----	---	-----	1. 7019	6	12. 27
641	----	---	-----	1. 6851	<1	12. 27
642	1. 64	14	12. 27	1. 6404	6	12. 28
722	----	---	-----	1. 6258	5	12. 27
731	1. 60	10	12. 29	1. 6004	6	12. 29
732	----	---	-----	1. 5596	5	12. 280
811	----	---	-----	1. 5114	1	12. 279
820	1. 49	8	12. 29	1. 4886	5	12. 275
821	----	---	-----	1. 4773	4	12. 271
822	1. 45	6	12. 30	1. 4465	3	12. 274
831	----	---	-----	1. 4275	2	12. 280
751	----	---	-----	1. 4175	1	12. 276
662	----	---	-----	1. 4078	1	12. 273
832	----	---	-----	1. 3989	<1	12. 275
840	1. 37	6	12. 25	1. 3723	<1	12. 274
921	----	---	-----	1. 3236	<1	12. 275
664	----	---	-----	1. 3082	<1	12. 272
Average of last five lines	-----		12. 28	------	---	12. 274

Ammonium Fluogermanate, $(NH_4)_2GeF_6$ (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium fluogermanate was prepared at the NBS from ammonium chloride, germanium oxide, and hydrofluoric acid. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent of silicon; and 0.0001 to 0.001 percent each of aluminum, calcium, iron, and magnesium.

The sample is colorless and optically negative. The indices of refraction are $N_o=1.425$ and $N_e=1.419$.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	100	101	201

Structural data. Hoard and Vincent [1] in 1939 determined that ammonium fluogermanate has cadmium iodide-type structure, the space group D^3_{3d}–$P\bar{3}m1$, and $1[(NH_4)_2GeF_6]$ per unit hexagonal cell, or $3[(NH_4)_2GeF_6]$ per unit rhombohedral cell.

The unit-cell measurements reported by Hoard and Vincent were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1939	Hoard and Vincent [1]	5. 85	4.785
1956	Swanson, Gilfrich, and Cook.	5. 862	4.817 at 26° C.

The density of ammonium fluogermanate calculated from the NBS lattice constants is 2.579 at 26° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 26° C	
	d	*I*
	A	
100	5. 07	100
001	4. 81	37
101	3. 49	82
110	2. 932	20
111	2. 503	13
002	2. 407	2
201	2. 246	47
102	2. 176	10
210	1. 919	4
112	1. 862	12
211	1. 783	17
202	1. 748	19
300	1. 692	2
003	1. 605	1
301	1. 597	5
103	1. 5314	2
212	1. 5014	13
220	1. 4658	9
310, 113	1. 4084	10
302	1. 3848	4
203	1. 3570	7
311	1. 3520	3
213	1. 2314	4
401	1. 2279	3
312	1. 2154	3
004	1. 2041	1
104	1. 1717	3
320, 303	1. 1648	6
321	1. 1319	3
402	1. 1229	2
114	1. 1139	1
204	1. 0880	1
223	1. 0826	<1
411	1. 0795	2
313	1. 0589	1
322	1. 0486	<1
214	1. 0202	1
412	1. 0063	1
403	0. 9961	1
304	. 9814	1
005	. 9632	1
105	. 9465	2
421	. 9411	1
502	. 9357	1
224	. 9306	1
314, 115	. 9153	1
510, 413	. 9122	2
205	. 9008	1
511	. 8961	1
422	. 8913	2
404	. 8737	<1
215	. 8610	1
512	. 8528	<1
324	. 8373	2
601	. 8334	<1
423	. 8235	<1
431	. 8224	<1
414	. 8153	<1
225	. 8050	<1
006	. 8028	1
315	. 7951	1
513, 106	. 7929	2
432	. 7885	<1

References

[1] J. L. Hoard and W. B. Vincent, Structure of complex fluorides. Potassium hexafluogermanate and ammonia hexafluogermanate, J. Am. Chem. Soc. **61**, 2849–2852 (1939).

Ammonium Gallium Sulfate Dodecahydrate, $NH_4Ga(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium gallium sulfate dodecahydrate was prepared at the NBS from gallium dissolved in sulfuric acid and neutralized with ammonia. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, magnesium, molybdenum, and silicon; and 0.0001 to 0.001 percent each of barium, chromium, and iron.

The sample is colorless. The index of refraction is 1.468.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	220	111	311

Structural data. Klug and Kieffer [1] in 1943 found ammonium gallium sulfate dodecahydrate to be an alpha alum having the space group T_h^6–Pa3 and $4[NH_4Ga(SO_4)_2 \cdot 12H_2O]$ per unit cell. The structure of the alpha alums was determined by Wyckoff [2] in 1923.

The unit-cell measurement reported by Klug and Kieffer has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1943	Klug and Kieffer [1]	12.268
1956	Swanson, Gilfrich, and Cook.	12.267 at 25° C

The density of ammonium gallium sulfate dodecahydrate calculated from the NBS lattice constant is 1.785 at 25° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	7.08	82	12.3
210	5.48	34	12.3
211	5.02	18	12.3
220	4.337	100	12.27
221	4.092	44	12.28
311	3.700	70	12.27
222	3.539	1	12.26
321	3.280	59	12.27
400	3.067	43	12.27
410	2.975	15	12.27
411	2.893	10	12.27
331	2.814	7	12.27
420	2.744	23	12.27
421	2.678	10	12.27
332	2.616	10	12.27
422	2.505	12	12.27
431	2.406	2	12.27
511	2.362	13	12.27
432	2.278	6	12.27
521	2.241	4	12.27
440	2.171	5	12.28
522	2.136	7	12.27
433	2.103	3	12.26
531	2.074	20	12.27
600	2.044	13	12.27
610	2.018	5	12.27
611	1.990	6	12.27
620	1.941	21	12.28
621	1.918	1	12.28
622	1.8496	2	12.269
630	1.8287	2	12.267
631	1.8094	1	12.272
444	1.7704	<1	12.266
543	1.7344	2	12.264
711	1,7178	15	12.268
640	1.7007	7	12.264
702	1.6851	2	12.268
642	1.6401	12	12.273
722	1.6250	4	12.268
731	1.5970	10	12.267
650	1.5700	<1	12.262
732	1.5580	1	12.268
810	1.5214	<1	12.266
811	1.5105	2	12.271
733	1.4994	2	12.273
820	1.4880	8	12.270
821	1.4764	2	12.264
822	1.4461	5	12.271
831	1.4257	3	12.264
751	1.4163	6	12.266
840	1.3714	<1	12.267
841	1.3630	<1	12.267
Average of last five lines			12.267

References

[1] H. P. Klug and G. L. Kieffer, Crystal-chemical studies of the alums. V. The gallium alums, J. Am. Chem. Soc. **65**, 2071–2073 (1943).

[2] R. W. G. Wyckoff, The crystal structure of the alums, Am. J. Sci. **5**, 209–217 (1923).

Ammonium Iron Sulfate Dodecahydrate, $NH_4Fe(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0361	4. 37 7. 1 3. 73	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Vegard and Esp [2] 1928	Chromium.	K_α

NBS sample. The sample of ammonium iron sulfate dodecahydrate was obtained from the J. T. Baker Co., Phillipsburgh, New Jersey. It was recrystallized at the NBS from a water solution, and ground in petrolatum to prevent exposure to the air. Spectrographic analysis of the sample showed the following impurities: 0.001 to 0.01 percent each of aluminum, magnesium, nickel, and silicon; and 0.0001 to 0.001 percent each of calcium and chromium.

The sample is colorless. The index of refraction is 1.488.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn and Frevel pattern were converted from kX to angstrom units and the *d*-values of the Vegard and Esp pattern were calculated from Bragg angle data.

The intensity measurements of the NBS sample are the average values obtained from a number of patterns made with $NH_4Fe(SO_4)_2 \cdot 12H_2O$ in petrolatum, but minor orientation effects may be present. The sample was unstable and decomposed in a few minutes when not protected from the atmosphere. The data of Vegard and Esp did not include intensity measurements.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	220	111	311
Swanson, Gilfrich, and Cook	220	321	221

Structural data. Vegard and Esp [2] in 1928 found ammonium iron sulfate dodecahydrate to be an alpha alum having the space group T_h^6–Pa3 and $4[NH_4Fe(SO_4)_2 \cdot 12H_2O]$ per unit cell. The structure of the alpha alums was determined by Wyckoff [3] in 1923.

Several unit-cell measurements have been converted fom kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1917	Vegard and Schjelderup [4].	12.02
1928	Vegard and Esp [2]	12.190
1935	Lipson and Beevers [5]	12.318
1955	Menary [6]	12.324 at 24°C
1956	Swanson, Gilfrich, and Cook.	12.318 at 25°C

The density of ammonium iron sulfate dodecahydrate calculated from the NBS lattice constant is 1.713 at 25° C.

References

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

[2] L. Vegard and E. Esp, The crystal structure of the alums, Ann. Physik. **85,** 1152–1164 (1928).

[3] R. W. G. Wyckoff, The crystal structure of the alums, Am. J. Sci. **5,** 209–217 (1923).

[4] L. Vegard and H. Schjelderup, Crystal structure of the alums and the role of water of crystallization, Ann. Physik. **54,** 146–164 (1917).

[5] H. Lipson and C. A. Beevers, The crystal structure of the alums, Proc. Roy. Soc. London **148** [A], 664–680 (1935).

[6] J. W. Menary, Some lattice constants, Acta Cryst. **8,** 840 (1955).

Ammonium Iron Sulfate Dodecahydrate, $NH_4Fe(SO_4)_2 \cdot 12H_2O$ (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1928 Vegard and Esp Cr, 2.2909 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	7.1	80	12.3	6.9	--	12	7.10	54	12.3
------	--------	--	--------	6.0	--	-------	--------	--	--------
210	5.5	50	12.3	5.4	--	12	5.51	31	12.3
211	5.0	25	12.2	4.9	--	12	5.02	19	12.3
220	4.38	100	12.4	4.27	--	12.1	4.34	100	12.3
221	4.13	60	12.4	4.04	--	12.1	4.096	57	12.29
311	3.74	80	12.4	3.67	--	12.17	3.708	51	12.30
321	3.31	80	12.4	3.25	--	12.16	3.286	72	12.30
400	3.10	40	12.4	3.04	--	12.16	3.078	39	12.31
410	--------	--	--------	2.96	--	12.20	2.985	18	12.31
411	--------	--	--------	2.87	--	12.18	2.900	13	12.30
331	--------	--	--------	2.80	--	12.20	2.822	14	12.30
420	2.76	14	12.3	2.73	--	12.21	2.755	21	12.32
421	--------	--	--------	2.66	--	12.19	2.685	13	12.30
332	2.63	6	12.3	2.59	--	12.15	2.623	18	12.30
422	2.53	14	12.4	2.48	--	12.15	2.514	17	12.31
431	--------	--	--------	2.39	--	12.19	2.415	8	12.31
511	2.37	16	12.3	2.34	--	12.16	2.369	13	12.31
432	--------	--	--------	2.27	--	12.22	2.288	10	12.32
521	2.26	6	12.4	2.23	--	12.21	2.249	12	12.32
440	--------	--	--------	-------	--	-------	2.161	6	12.31
522	2.15	4	12.35	2.13	--	12.24	2.144	8	12.31
433	--------	--	--------	-------	--	-------	2.111	5	12.31
531	--------	--	--------	2.07	--	12.25	2.082	28	12.32
600	2.06	20	12.36	2.04	--	12.24	2.053	13	12.32
610	--------	--	--------	2.01	--	12.23	2.024	5	12.31
611	2.00	4	12.33	1.98	--	12.21	1.998	20	12.32
620	1.95	35	12.33	1.94	--	12.27	1.947	29	12.32
541	--------	--	--------	1.88	--	12.20	1.899	1	12.31
622	--------	--	--------	-------	--	-------	1.856	1	12.31
630	--------	--	--------	-------	--	-------	1.836	2	12.31
631	1.82	4	12.34	1.80	--	12.21	1.815	4	12.31
632	--------	--	--------	-------	--	-------	1.768	1	12.30
543	--------	--	--------	-------	--	-------	1.7412	4	12.312
711	1.72	20	--------	1.72	--	12.28	1.7244	16	12.315
640				------	--	------	1.7080	14	12.317
641	--------	--	--------	------	--	------	1.6917	2	12.316
642	1.65	18	12.35	1.64	--	12.27	1.6450	14	12.310
722	--------	--	--------	1.62	--	12.23	1.6313	1	12.316
731	1.61	12	12.37	1.598	--	12.27	1.6037	13	12.318
-------	--------	--	--------	1.563	--	-------	--------	--	--------
820	1.500	12	12.37	1.490	--	12.29	1.4931	16	12.312
822	1.458	8	12.37	1.451	--	12.31	1.4521	7	12.320
751	1.428	10	12.37	-------	--	-------	1.4223	12	12.318
841	1.380	8	12.42	-------	--	-------	1.3686	8	12.317
921	1.340	2	12.43	-------	--	-------	1.3284	1	12.319
664	1.313	4	12.32	-------	--	-------	1.3131	6	12.318
Average of last five lines-------			12.39	-------	--	12.28	--------	--	12.318

Ammonium Sulfate (mascagnite), $(NH_4)_2SO_4$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0363	4. 36 3. 12 3. 03	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Wavelength	Radiation
Jansen [2] 1929	Iron	K_α
Taylor and Boyer [3] 1938.	Molybdenum	K_α

Winchell and Benoit [4] reported two powder patterns for naturally occurring mascagnite, but they were not included because they were in very poor agreement with the other patterns.

NBS sample. The sample of ammonium sulfate was obtained from Johnson, Matthey, & Co., Ltd. Their spectrographic analysis showed faint traces of the following elements: boron, calcium, copper, iron, magnesium, sodium, and silicon.

The sample is colorless and optically positive. The indices of refraction are $\alpha=1.520$, $\beta=1.523$, and $\gamma=1.532$. $2V\simeq 50°$.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the *d*-values of the Taylor and Boyer pattern were calculated from Bragg angle data. The data of Jansen did not include intensity values.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel.	021, 111	022	130
Taylor and Boyer	200	002	021, 111
Swanson, Gilfrich, and Cook.	111	021	130

Structural data. Ogg [5] in 1928 determined that ammonium sulfate has potassium sulfate-type structure, the space group D_{16}^{2h}–Pmcn, and $4[(NH_4)_2SO_4]$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice Constants

		a	*b*	*c*
		A	*A*	*A*
1916	Ogg and Hopwood [6].	5. 963	10. 581	7.745
1930	Ogg [5]	5. 98	10. 62	7.78
1956	Swanson, Gilfrich, and Cook.	5. 994	10. 64	7.782 at 25° C

The density of ammonium sulfate calculated from the NBS lattice constants is 1.768 at 25° C.

References

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

[2] E. Jansen, Lattice changes in orthorhombic mixed crystals, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1929,** No. 13 (1929).

[3] W. Taylor and T. Boyer, An investigation into the structure of caesium and ammonium sulphates, Mem. Proc. Manchester Lit. and Phil. Soc. **72,** 125–137 (1928).

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

[5] A. Ogg, The crystal strueture of the isomorphous sulfates of potassium, ammonium, rubidium, and cesium, Phil. Mag. **5,** 354–367 (1928).

[6] A. Ogg and F. L. Hopwood, A critical test of the crystallographic law of valency volumes; erystalline structures of the alkali sulfates, Phil. Mag. **32,** 518–525 (1916).

Ammonium Sulfate (mascagnite), $(NH_4)_2SO_4$ (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1929 Jansen Fe, 1.937 A		1930 Taylor and Boyer Mo, 0.7107 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A	
020	------	----	------	----	5. 31	15	5. 31	14
110	5. 2	20	------	----	5. 22	32	5. 22	27
021	4. 37	100	------	----	4. 38	61	4. 39	63
111							4. 33	100
002	3. 92	20	------	----	3. 90	80	3. 890	35
022	3. 13	40	3. 13	----	3. 15	39	3. 139	30
112	------	----	------	----	------	----	3. 122	22
130	3. 04	40	3. 05	----	------	----	3. 055	54
200	------	----	------	----	2. 99	100	2. 998	23
122	------	----	------	----	------	----	2. 782	3
211	------	----	------	----	------	----	2. 704	5
040	2. 68	7	------	----	2. 66	43	2. 655	13
220	------	----	------	----	2. 61	17	2. 611	6
013	2. 52	7	2. 52	----	------	----	2. 521	9
221	------	----	------	----	------	----	2. 476	2
132	------	----	------	----	------	----	2. 401	3
202	------	----	------	----	------	----	2. 374	2
113	2. 32	20	2. 32	----	------	----	2. 322	17
212	------	----	------	----	------	----	2. 317	18
231	2. 18	20	2. 17	----	2. 194	18	2. 196	8
042								
222	------	----	------	----	2. 100	14	2. 168	14
033	------	----	------	----	------	----	2. 093	4
142	2. 05	1	------	----	------	----	2. 062	<1
150	------	----	------	----	------	----	2. 005	<1
232	1. 97	4	------	----	------	----	1. 973	4
004	------	----	------	----	1. 946	20	1. 945	4
151	1. 93	2	------	----	------	----	1. 942	5
014	------	----	------	----	------	----	1. 914	3
052	------	----	------	----	------	----	1. 867	1
024	------	----	------	----	------	----	1. 827	<1
060	1. 77	2	------	----	1. 772	8	1. 773	3
330	------	----	------	----	1. 738	9	1. 7400	<1
061	1. 73	2	------	----	------	----	1. 7293	1
331	1. 70	2	------	----	------	----	1. 6989	2
134	------	----	------	----	------	----	1. 6404	4
204	1. 63	5	------	----	------	----	1. 6324	4
062	------	----	------	----	------	----	1. 6130	2
214								
341	1. 56	2	------	----	------	----	1. 5647	1
015	------	----	------	----	------	----	1. 5398	<1
260	1. 52	2	------	----	------	----	1. 5260	4
400	1. 493	5	1. 50	----	1. 495	26	1. 4973	5
261								
025	------	----	------	----	------	----	1. 4938	5
342	------	----	------	----	------	----	1. 4782	1
170	------	----	------	----	------	----	1. 4734	3
					[a]			

[a] Eight additional lines were omitted.

Ammonium Zirconium Fluoride $(NH_4)_3ZrF_7$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
3–0111	5. 4 4. 71 3. 32	Molybdenum.	Dow Chemical Co.

Additional published patterns

Source	Radiation	Wavelength
Hampson and Pauling [1] 1938.	Copper---	--------

NBS sample. The sample of ammonium zirconium fluoride was prepared at the NBS from ammonium chloride, zirconium dioxide, and hydrofluoric acid. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of hafnium; 0.01 to 0.1 percent each of aluminum, calcium, potassium, and silicon; and 0.001 to 0.01 percent each of iron and magnesium.

The sample is colorless. It was too fine-grained for the determination of the indices of refraction by the conventional liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values of the Dow Chemical Co.'s pattern were converted from kX to angstrom units and the *d*-values of the Hampson and Pauling pattern were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Dow Chemical Co.	111	200	220
Hampson and Pauling	111	220	200
Swanson, Gilfrich, and Cook	111	200	220

Structural data. The structure of ammonium zirconium fluoride has not been determined but, according to Hampson and Pauling [1], the X-ray data satisfy the requirements of space group O_h^5–Fm3m. There are $4[(NH_4)_3ZrF_7]$ per unit cell.

Two unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1924	Hassel and Mark [2]	9.37
1938	Hampson and Pauling [1]	9.385
1956	Swanson, Gilfrich, and Cook.	9.417 at 24° C

The density of ammonium zirconium fluoride calculated from the NBS lattice constant is 2.213 at 24° C.

References

[1] G. C. Hampson and L. Pauling, The structure of ammonium heptafluozirconate and potassium heptafluozirconate and the configuration of the heptafluozirconate group, J. Am. Chem. Soc. **60,** 2705–2707 (1938).

[2] O. Hassel and H. Mark, Über die Struktur der isomorphen Verbindungen $(NH_4)_3ZrF_2$ und $(NH_4)_3HfF_7$, Z. Physik. **27,** 89–101 (1924).

Ammonium Zirconium Fluoride, $(NH_4)_3ZrF_7$ (cubic)

hkl	---- Dow Chemical Co. Mo, 0.7107 A			1938 Hampson and Pauling Cu, ------			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 24° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	5. 4	100	9. 4	5. 45	vvs	9. 44	5. 44	100	9. 42
200	4. 72	75	9. 44	4. 69	s	9. 38	4. 71	61	9. 42
220	3. 33	63	9. 42	3. 32	vs	9. 39	3. 33	51	9. 42
311	2. 84	18	9. 42	2. 82	w–m	9. 35	2. 84	17	9. 42
400	2. 34	38	9. 36	2. 34	m–s	9. 36	2. 356	24	9. 423
331	2. 16	8	9. 42	2. 15	vw	9. 37	2. 160	6	9. 414
420	2. 09	18	9. 35	2. 10	m	9. 41	2. 106	15	9. 417
422	1. 92	25	9. 41	1. 91	ms	9. 37	1. 921	17	9. 412
511	1. 81	31	9. 41	1. 81	m	9. 40	1. 812	19	9. 415
440	1. 66	13	9. 39	1. 66	w–m	9. 38	1. 665	2	9. 418
531	1. 59	18	9. 41	1. 59	m	9. 39	1. 592	8	9. 417
600	1. 57	13	9. 42	1. 57	w–m	9. 40	1. 569	11	9. 415
620	1. 49	18	9. 42	1. 48	w–m	9. 37	1. 4895	8	9. 420
533	1. 43	10	9. 38	1. 43	vw	9. 39	1. 4351	3	9. 417
622	------	----	------	1. 41	vw	9. 35	1. 4198	2	9. 418
444	1. 36	3	9. 42	1. 35	vvw	9. 37	1. 3592	2	9. 417
711	1. 32	8	9. 43	1. 31	w	9. 38	1. 3148	4	9. 415
640	------	----	------	1. 30	vw	9. 37	1. 3057	1	9. 416
642	1. 26	13	9. 43	1. 25	w–m	9. 38	1. 2580	4	9. 414
731	1. 22	10	9. 37	1. 22	w	9. 39	1. 2258	4	9. 416
733	------	----	------	------	----	------	1. 1507	<1	9. 418
820	------	----	------	1. 14	vw	9. 40	1. 1420	2	9. 417
822	------	----	------	1. 11	vw	9. 42	1. 1096	2	9. 415
751	------	----	------	1. 08	vvw	9. 35	1. 0870	2	9. 414
662	------	----	------	------	----	------	1. 0800	1	9. 415
840	------	----	------	1. 053	vvw	9. 42	1. 0530	<1	9. 418
911	------	----	------	1. 030	vw	9. 38	1. 0335	4	9. 416
842	------	----	------	1. 023	vw	9. 38	1. 0275	1	9. 417
664	------	----	------	0. 997	vvw	9. 35	1. 0037	2	9. 416
931	------	----	------	. 983	vvw	9. 38	0. 9872	2	9. 417
844	------	----	------	. 956	vvw	9. 37	. 9613	<1	9. 419
933	------	----	------	. 941	vw	9. 36	. 9465	2	9. 418
10·0·0	------	----	------	. 938	vvw	9. 38	. 9418	<1	9. 418
10·2·0	------	----	------	. 920	w	9. 39	. 9234	3	9. 417
951	------	----	------	. 907	vw	9. 38	. 9104	4	9. 417
10·2·2	------	----	------	------	----	------	. 9062	3	9. 418
953	------	----	------	------	----	------	. 8782	5	9. 418
10·4·0	------	----	------	------	----	------	. 8742	1	9. 415
10·4·2	------	----	------	------	----	------	. 8596	<1	9. 416
11·1·0	------	----	------	------	----	------	. 8490	2	9. 416
Average of last five lines			9. 41			9. 38			9. 417

Antimony(III) Iodide, SbI_3 (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0673	3. 30 2. 54 2. 14	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of antimony triiodide was obtained from the Fisher Scientific Company. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of bismuth; 0.001 to 0.01 percent of aluminum; and 0.0001 to 0.001 percent each of calcium and magnesium.

The sample has a red orange color and is opaque.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	113	116	300
Swanson, Gilfrich, and Cook	113	116	300

Structural data. Braekken [2] in 1930 determined that antimony triiodide has arsenic triiodide-type structure, the space group C_{3i}^2—$R\bar{3}$, and $2(SbI_3)$ per unit rhombohedral cell, or $6(SbI_3)$ per unit hexagonal cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1930	Braekken [2]	7. 46	20. 89
1947	Backer and Vegard [3]	7. 48	20. 89
1956	Swanson, Gilfrich, and Cook.	7. 485	20.93 at 25° C.

The density of antimony triiodide calculated from the NBS lattice constants is 4.929 at 25° C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
003	------	----	6. 98	7
101	6. 2	3	6. 19	4
012	5. 5	13	5. 51	11
------	3. 98	1	-------	----
110	3. 71	3	3. 74	4
015	------	----	3. 52	4
006	3. 46	4	3. 489	13
113	3. 31	100	3. 300	100
116	2. 55	40	2. 552	37
018	2. 42	1	2. 428	3
122	------	----	2. 385	3
009	------	----	2. 325	3
300	2. 14	40	2. 161	27
125	------	----	2. 114	2
303	------	----	2. 065	2
208	------	----	2. 034	1
119	1. 97	20	1. 976	17
306	------	----	1. 837	9
223	1. 80	17	1. 807	14
0·0·12	1. 73	1	1. 743	4
226	1. 64	10	1. 648	7
1·1·12	1. 57	1	1. 581	2
229	1. 453	7	1. 458	3
413	1. 383	10	1. 3858	6
2·0·14 3·0·12	1. 353	8	1. 3573	8
416	1. 303	10	1. 3107	6
0·0·16	------	----	1. 3076	6
1·2·14 2·2·12	------	----	1. 2769	1
330	------	----	1. 2476	3
419	1. 202	5	1. 2089	4
425 336	------	----	1. 1751	3
339	------	----	1. 0990	1
600	------	----	1. 0805	2
342	------	----	1. 0606	<1
606	------	----	1. 0318	1
523	------	----	1. 0266	2
3·0·18	------	----	1. 0240	1
3·3·12	------	----	1. 0148	1
526	------	----	0. 9949	1

References

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

[2] H. Braekken, Kristallstruktur der Trijodide von Arsen, Antimon und Wismut, Z. Krist. **74,** 67–72 (1930).

[3] J. Backer and L. Vegard, Investigations into the structure and properties of solid matter with the help of X-rays. The structure of AsI_3, SbI_3 and BiI_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1947,** No. 2 (1947).

Arsenic(III) Iodide, AsI_3 (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
4–0472	3. 53 2. 06 3. 16	Copper----	Institute of Physics, University College, Cardiff.
3–0493 [a]	3. 21 3. 62 2. 07	Molybdenum.	Heyworth [1] 1931.
1–0733 [a]	3. 21 3. 59 2. 53	Molybdenum.	Hanawalt, Rinn, and Frevel [2] 1938.

[a] Deleted in the 1955 index.

The data on ASTM card 4–0472 contains an entirely different pattern or phase and was not included in the table of *d*-values for comparison.

Additional published patterns. None.

NBS sample. The sample of arsenic triiodide was obtained from the City Chemical Co., New York, N. Y. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of bismuth and antimony; and 0.0001 to 0.001 percent each of iron and silicon.

The sample has a bright orange color and is optically negative. The indices of refraction were too high for one to determine them by the conventional liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units, and the *d*-values of the Heyworth pattern were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Heyworth	113	006	030
Hanawalt, Rinn, and Frevel	113	006	015
Swanson, Gilfrich, and Cook	113	006	030

Structural data. Braekken [3] in 1930 determined that arsenic triiodide has the space group C_{3i}^2–$R\bar{3}$ and 2(AsI_3) per unit rhombohedral cell, or 6(AsI_3) per unit hexagonal cell. Arsenic triiodide is used as a structure-type.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values and the rhombohedral cell measurements reported by Heyworth have been referred to hexagonal axes.

Lattice constants

		a	*c*
		A	*A*
1930	Braekken [3]	7. 20	21. 43
1931	Heyworth [1]	7. 16	21. 49
1947	Backer and Vegard [4]	7. 20	21. 40
1956	Swanson, Gilfrich, and Cook.	7. 208	21. 45 at 25° C

The density of arsenic triiodide calculated from the NBS lattice constants is 4.703 at 25° C.

hkl	1931 Heyworth Mo, 0.7107 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
003	-----	--	-----	--	7. 15	1
------	-----	--	5. 9	7	-------	--
012	-----	--	5. 4	7	5. 40	12
006	3. 63	80	3. 60	33	3. 578	49
015	-----	--	3. 54	23	3. 536	2
113	3. 22	100	3. 22	100	3. 220	100
116	2. 54	65	-----	--	2. 538	20
030	2. 07	75	2. 08	23	2. 0800	31
119	1. 97	55	1. 97	17	1. 9880	15
306	1. 79	60	1. 79	13	1. 7984	16
0·0·12	-----	--	-----	--	1. 7880	2
223	1. 71	50	1. 74	11	1. 7477	10
226	1. 60	20	1. 60	8	1. 6096	6
1·1·12					1. 6014	5
404	-----	--	-----	--	1. 4986	1
229	1. 44	10	1. 43	4	1. 4375	4
3·0·12	-----	--	1. 35	1	1. 3558	5
143	1. 33	25	1. 33	4	1. 3376	6
2·2·12	1. 27	5	1. 27	3	1. 2687	4
3·2·10	-----	--	1. 19	1	1. 1914	<1
------	-----	--	1. 14	1	-------	--
------	-----	--	1. 08	1	-------	--
------	-----	--	1. 04	1	-------	--

References

[1] D. Heyworth, The crystal structure of arsenic triiodide, AsI_3, Phys. Rev. **38**, 351–359 (1931).

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

[3] H. Braekken, Kristallstruktur der Trijodide von Arsen, Antimon und Wismut, Z. Krist. **74**, 67–72 (1930).

[4] J. Backer and L. Vegard, Investigations into the structure and properties of solid matter with the help of X-rays. The structure of AsI_3, SbI_3 and BiI_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1947**, No. 2 (1947).

Barium Peroxide, BaO_2 (tetragonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
3–1130[a]	1. 64 1. 35 1. 13	Copper----	Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward [1] 1935.
1–0642[a]	3. 37 2. 68 2. 11	Molybdenum.	Hanawalt, Rinn, and Frevel [2] 1938.

[a] Deleted in the 1955 index.

Additional published patterns

Source	Radiation	Wavelength
Abrahams and Kalnajs [3] 1954.	Copper---	1. 5418

NBS sample. The sample of barium peroxide was precipitated from a barium chloride solution by hydrogen peroxide. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of strontium; 0.001 to 0.01 percent each of aluminum, calcium, magnesium, silicon, tin, and vanadium; and 0.0001 to 0.001 percent each of copper, iron, and manganese.

The sample is colorless. The particle size was too small for determination of the indices of refraction by the conventional liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel, and the Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward patterns were converted from kX to angstrom units.

The Abrahams and Kalnajs pattern did not include intensity measurements.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward.	222, 311	113	006, 242
Hanawalt, Rinn, and Frevel.	002, 111	200	222, 131
Swanson, Gilfrich, and Cook.	111	200	002

Structural data. Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward [1] in 1935 determined that barium peroxide has calcium carbide-type structure, the space group D_{4h}^{17}–F4/mmm, and $4(BaO_2)$ per unit cell.

Several unit-cell measurements have been compared with the NBS values. The measurements reported by Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward have been converted from kX to angstrom units. The values reported by Abrahams and Kalnajs were already expressed in angstrom units.

Lattice constants

		a	*c*
		A	*A*
1935	Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward [1].	5. 35	6. 78
1954	Abrahams and Kalnajs [3].	5. 384	6. 841
1956	Swanson, Gilfrich, and Cook.	5. 3958	6. 8513 at 25° C

The density of barium peroxide calculated from the NBS lattice constants is 5.637 at 25° C.

References

[1] J. D. Bernal, E. Djatlowa, I. Kasarnowsky, S. Reichstein, and A. G. Ward, The structure of strontium and barium peroxides SrO_2 and BaO_2, Z. Krist. **92**, 344–354 (1935).

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

[3] S. C. Abrahams and J. Kalnajs, The crystal structure of barium peroxide, Acta Cryst. **7**, 838–842 (1954).

Barium Peroxide, BaO_2 (tetragonal)

hkl	1935 Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward Cu, 1.5418 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1954 Abrahams and Kalnajs Cu, 1.5418 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
002	3.37	vw	3.38	100	3.43	----	3.42	59
111	3.27	m			3.34	----	3.33	100
200	2.67	s	2.69	80	2.701	----	2.696	68
202	2.08	s	2.11	50	2.118	----	2.120	50
113	1.93	s	1.95	50	1.958	----	1.959	46
220	1.89	m	1.89	30	1.908	----	1.9079	21
004	------	----	------	----	1.712	----	1.7131	6
222	1.643	vvs	1.65	80	1.663	----	1.6664	22
131					1.654	----	1.6556	29
204	1.435	w	1.446	8	1.446	----	1.4463	9
133	1.356	vs	1.363	40	1.366	----	1.3672	22
400	1.341	w			1.349	----	1.3493	6
115	1.279	m	1.285	16	1.288	----	1.2900	14
224	1.267	w			1.274	----	1.2749	7
402	1.243	s	1.253	16	1.255	----	1.2553	8
331					1.250	----	1.2504	7
240	1.197	m	1.202	10	1.206	----	1.2063	6
006	1.129	vs	1.139	16	1.138	----	1.1418	2
242					1.135	----	1.1379	10
333	1.101	----	1.110	6	1.111	----	1.1110	5
135	1.060	----	1.065	16	1.068	----	1.0683	12
404					1.056	----	1.0597	4
206	------	----	------	----	1.050	----	1.0514	5
151	1.039	----	1.047	8	1.045	----	1.0457	5
244	0.974	----	0.982	4	0.986	----	0.9863	5
226					.979	----	.9798	4
153	.955	----	.960	6	.959	----	.9602	7
440	------	----	------	----	.953	----	.9540	1
117	.942	----	------	----	.947	----	.9480	4
335	------	----	.932	2	.932	----	.9322	4
442	------	----	.917	4	.918	----	9188	4
351	.912	----			.916	----	.9169	6
600	------	----	.881	2	.898	----	.8994	1
406	------	----			.870	----	.8716	2
602	------	----	------	----	.869	----	.8699	2
353	------	----	------	----	.857	----	.8576	4
008	------	----	------	----			.8564	3
260	------	----	------	----	.852	----	.8532	4
137	------	----	------	----	.849	----	.8490	9
155	------	----	------	----	.836	----	.8376	10
444	------	----	------	----	.833	----	.8334	3
246	------	----	.830	2	.829	----	.8293	7
262	------	----	------	----	.827	----	.8278	7
208	------	----	------	----	.815	----	.8163	10
604	------	----	------	----	.795	----	.7962	3
228	------	----	------	----	.780	----	.7813	9

Bismuth(III) Iodide, BiI_3 (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
2–0658	3. 00 2. 15 1. 87	Copper---	Caglioti [1] 1930.

Additional published patterns. None.

NBS sample. The sample of bismuth triiodide was obtained from the Fisher Scientific Co. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent of aluminum; and 0.0001 to 0.001 percent each of calcium, copper, magnesium, and silicon.

The sample is a black opaque powder.

Interplanar spacings and intensity measurements. The *d*-values of the Caglioti pattern were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Caglioti	-	300	-
Swanson, Gilfrich, and Cook	113	116	300

Structural data. Braekken [2] in 1930 determined that bismuth triiodide has arsenic triiodide-type structure, the space group C_{3i}^2–$R\bar{3}$, and $2(BiI_3)$ per unit rhombohedral cell, or $6(BiI_3)$ per unit hexagonal cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1930	Braekken [2]	7. 513	20. 718
1947	Backer and Vegard [3]	7. 52	20. 69
1956	Swanson, Gilfrich, and Cook.	7. 522	20. 73 at 25° C.

The density of bismuth triiodide calculated from the NBS lattice constants is 5.783 at 25° C.

hkl	1930 Caglioti Cu, 1.5418 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
003	---	---	6. 92	27
101	---	---	6. 22	8
012	---	---	5. 51	5
006	---	---	3. 46	8
113	3. 26	m	3. 302	100
---	3. 00	s	---	---
116	2. 53	m	2. 544	43
---	2. 49	w	---	---
009	2. 28	m	2. 302	5
300	2. 16	s	2. 171	31
303	2. 07	ms	2. 071	5
119	1. 96	ms	1. 964	1
---	1. 91	m	---	---
---	1. 87	s	---	---
306	---	---	1. 838	5
223	1. 81	s	1. 814	11
0·0·12	1. 72	mw	1. 728	6
226	---	---	1. 652	8
309	1. 58	mw	1. 580	4
---	1. 50	mw	---	---
229	1. 44	mw	1. 456	3
413	---	---	1. 392	7
3·0·12	---	---	1. 3518	7
416	1. 31	mw	1. 3142	4
238	1. 29	m	1. 2954	4
330	1. 255	m	1. 2534	1
419	1. 209	mw	1. 2096	2
2·2·15	---	---	1. 1104	<1
1·1·18	1. 106	m	1. 1011	<1
600	1. 089	m	1. 0855	2
---	1. 048	w	---	---
523	1. 034	m	1. 0316	<1
3·3·12	1. 016	m	1. 0145	<1

References

[1] V. Caglioti, Sulla nonesistenza dei sottoiduri di bismuto, Gazz. chim. Ital. **60,** 933–935 (1930).

[2] H. Braekken, Kristallstruktur der Trijodide von Arsen, Antimon und Wismut, Z. Krist. **74,** 67–72 (1930).

[3] J. Backer and L. Vegard, Investigations into the structure and properties of solid matter with the help of X-rays. The structure of AsI_3, SbI_3 and BiI_3, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1947** No. 2 (1947).

Cadmium Molybdate, $CdMoO_4$ (tetragonal)

ASTM cards. None.

Additional published patterns.

Source	Radiation	Wavelength
Broch [1] 1930	Copper	K_α

NBS sample. The sample of cadmium molybdate was precipitated from cadmium chloride and sodium molybdate solutions and annealed at 400° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium; 0.001 to 0.01 percent each of aluminum, barium, magnesium, and silicon; and 0.0001 to 0.001 percent each of silver, calcium, chromium, copper, iron, lead, and tin.

The sample is colorless. The indices of refraction could not be determined by the conventional liquid grain immersion method because the sample was too fine-grained.

Interplanar spacings and intensity measurements. The *d*-values of the Broch pattern were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Broch	312	316	112
Swanson, Gilfrich, and Cook	112	204	312

Structural data. Broch [1] in 1930 determined that cadmium molybdate has calcium tungstate-type structure, the space group C_{4h}^6–$I4_1/a$, and $4(CdMoO_4)$ per unit cell.

The unit-cell measurements reported by Broch have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	A
1930	Broch [1]	5. 148	11. 19
1956	Swanson, Gilfrich, and Cook.	5. 1554	11. 194 at 25° C

The density of cadmium molybdate calculated from the NBS lattice constants is 6.079 at 25° C.

hkl	1930 Broch Cu, 1.5418 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		A	
112	3. 06	vs	3. 054	100
004	2. 81	s	2. 798	16
200	2. 58	s	2. 576	21
211	------	----	2. 259	4
114	------	----	2. 220	4
204	1. 895	vs	1. 896	30
220	1. 821	m	1. 823	14
116	1. 658	vs	1. 661	18
312	1. 563	vvs	1. 565	25
224	1. 526	s	1. 528	11
008	------	----	1. 400	3
400	1. 288	w	1. 289	4
208	------	----	1. 230	10
316	1. 226	vvs	1. 228	14
332	1. 187	m	1. 188	7
404	1. 170	m	1. 171	5
307				
420	1. 151	m	1. 153	6
228	1. 110	m	1. 111	4
1·1·10	1. 070	w	1. 0703	4
424	1. 064	vs	1. 0659	7
327				
336	1. 017	s	1. 0183	3
512	0. 993	w	0. 9950	7
------	. 984	m	-------	----
408	. 946	m	. 9480	3
0·0·12	------	----	. 9328	2
3·1·10	. 921	s	. 9229	6
440	------	----	. 9113	2
428	. 888	vs	. 8896	7
516			. 8891	7
2·0·12	------	----	. 8771	4
532	------	----	. 8733	7
507	------	----	. 8664	3
444				
600	------	----	. 8592	3
2·2·12	------	----	. 8304	3
3·3·10	------	----	. 8233	4
604	------	----	. 8214	5
527				
620	------	----	. 8151	4
536	------	----	. 7988	7
624	------	----	. 7825	8

References

[1] E. K. Broch, Untersuchungen über Kristallstrukturen des Wolframittypus und des Scheelittypus, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1929,** No. 8 (1930).

Calcium Molybdate (powellite), $CaMoO_4$ (tetragonal)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wavelength
Vegard [1] 1925	Copper	Kα
Zambonini and Levi [2] 1925.	Copper	Kα

NBS sample. The sample of calcium molybdate was precipitated from calcium chloride and sodium molybdate solutions and annealed at 800° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, iron, potassium, silicon, sodium, and strontium; and 0.001 to 0.01 percent each of barium, cobalt, chromium, lithium, magnesium, nickel, and vanadium.

The sample is colorless. The indices of refraction could not be determined because the particle size was too small.

Interplanar spacings and intensity measurements. The *d*-values of the Vegard and the Zambonini and Levi patterns were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Vegard	112	208, 316	312
Zambonini and Levi	112	312	208, 316
Swanson, Gilfrich, and Cook.	112	204	101

Structural data. Vegard [1] in 1925 determined that calcium molybdate has calcium tungstate-type structure, the space group C_{4h}^6–$I4_1/a$, and $4(CaMoO_4)$ per unit cell.

The "*a*" measurement reported by Zambonini and Levi (3.68 A) was multiplied by $2/\sqrt{2}$, the "*a*" measurement reported by Vegard (7.42 A) was multiplied by $\sqrt{2}/2$, and the "*c*" measurement reported by Zambonini and Levi was doubled for comparison with the NBS values. All of the measurements were converted from kX to angstrom units.

Lattice constants

		a	*c*
		A	A
1925	Vegard [1]	5. 24	11. 46
1925	Zambonini and Levi [3]	5. 20	11. 40
1943	Sillén and Nylander [4]	5. 224	11. 449
1956	Swanson, Gilfrich, and Cook.	5. 226	11. 43 at 25° C.

The density of calcium molybdate calculated from the NBS lattice constants is 4.255 at 25° C.

hkl	1925 Vegard Cu, 1.542 A		1925 Zambonini and Levi Cu, 1.542 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A 25° C.	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
101	-------	--	-------	-----	4. 76	28
112	3. 12	100	2. 97	vs	3. 10	100
004	2. 86	10	2. 73	mw	2. 86	13
200	2. 61	30	2. 51	w	2. 61	16
202	-------	--	-------	-----	2. 38	3
211	2. 32	15	2. 19	m	2. 290	10
114	-------	--	-------	-----	2. 262	6
213	-------	--	-------	-----	1. 993	5
204	1. 932	60	1. 88	m	1. 929	30
220	1. 855	30	1. 81	m	1. 848	13
116	1. 700	40	1. 66	s	1. 694	14
215	-------	--	1. 60	m	1. 635	5
312	1. 590	70	1. 55	vs	1. 588	22
224	1. 557	20	1. 52	ms	1. 552	9
321	1. 439	10	1. 41	w	1. 438	3
008	-------	--	-------	-----	1. 429	2
305	1. 389	10	-------	-----	1. 386	3
323	1. 345	10	1. 34	vvw	1. 355	4
217	-------	--	-------	-----	1. 339	3
400	1. 295	10	-------	-----	1. 307	4
411	-------	--	-------	-----	1. 260	2
208	1. 254	90	1. 24	vs	1. 254	7
316					1. 249	12
332	1. 207	30	1. 21	vw	1. 204	5
404	-------	--	1. 19	mw	1. 188	5
420	1. 172	20	1. 18	w	1. 169	4
---	-------	--	1. 16	vw	------	--
228	1. 136	10	1. 12	w	1. 130	3
1·1·10	-------	--	-------	-----	1. 092	3
327	-------	--	-------	-----	1. 084	<1
424	1. 088	60	1. 08	mw	1. 082	4
318						
501	-------	--	1. 07	w	1. 041	2
336	1. 039	30	1. 03	w	1. 0344	3
512	1. 012	50	1. 004	ms	1. 0087	5
521	0. 9695	10	0. 961	vw	0. 9670	3
514	------	--	-------	-----	. 9643	3
408						
329	. 9549	10	-------	-----	. 9555	1
0·0·12	-------	--	-------	-----	. 9527	2
505	-------	--	. 950	w	. 9504	3
523	. 9427	30	. 938	s	. 9402	4
3·1·10						
440	. 9286	5	. 924	vw	. 9238	1
428	. 9075	80	. 904	s	. 9047	3
516					. 9026	5
419	-------	--	. 896	w	. 8973	1
2·0·12	-------	--	-------	-----	. 8951	1
532	. 8880	50	. 8857	ms	. 8855	4
507	-------	--	-------	-----	. 8802	3
444	-------	--	. 8792	m	. 8790	3
600	-------	--	-------	-----	. 8710	1
2·2·12	. 8499	20	. 8485	ms	. 8467	2
613	. 8389	20	. 8400	mw	. 8380	2
3·3·10						
604	------	--	-------	-----	. 8331	2
518						

Calcium Molybdate (powellite), $CaMoO_4$ (tetragonal)—Continued

hkl	1925 Vegard Cu, 1.542 A		1925 Zambonini and Levi Cu, 1.542 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A 25° C.	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
620	-------	--	.8283	w	.8263	2
536	.8145	60	.8131	s	.8110	1
543	.7978	30	.7990	m	.7974	2
624	-------	--	.7945	w	.7938	4

References

[1] L. Vegard, Results of crystal analysis; space lattices and atomic dimensions, Skrifter Norske Videnskaps-Akad. Oslo I. Mat.-Naturv. Kl. **1925**, No. 11 (1925).

[2] F. Zambonini and G. R. Levi, Ricerche sull'isomorfismo dei molibdati metalli delle terre rare quelli del calcio, dello stronzio, del bario e del piombo. II. Struttura dei molbdati di Ca, Sr, Ba, Pb, Rend. accad. Lincei **2**, 225-230 (1925).

[3] F. Zambonini and G. R. Levi, Ricerche sull'isomorfismo dei molibdati metalli delle terre rare quelli del calcio, dello stronzio, del bario e del piombo. III. De dezioni dall'analisi röntgenografica dei molibdati di Ca, Sr, Ba, Pb, Rend. accad. Lincei **2**, 303-305 (1925).

[4] L. G. Sillen and A. Nylander, On the oxygen positions in tungstates and molybdates with the scheelite structure, Arkiv. Kemi., Mineral. Geol. **17**, No. 4 (1943-44).

Calcium Tungstate (scheelite), $CaWO_4$ (tetragonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–0806	3.09 4.76 1.92	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
2–0619	3.04 1.24 1.90	Copper----	British Museum.

Additional published patterns

Source	Radiation	Wavelength
Vegard [2] 1926----------	Copper---	1.54
Barth [3] 1926----------	Copper---	1.539

NBS sample. The sample of calcium tungstate furnished by the U. S. Natural Museum is from the Greenhorn Mountains near Kernville, Calif. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of molybdenum; 0.01 to 0.1 percent of sodium; 0.001 to 0.01 percent each of aluminum, silicon, and strontium; and 0.0001 to 0.001 percent each of silver, chromium, copper, magnesium, and manganese. A pattern of synthetic scheelite showed no appreciable change in *d*-values.

The sample is colorless and optically positive. The refractive indices are $N_0=1.918$ and $N_e=1.935$.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel, and the British Museum patterns were converted from kX to angstrom units and the *d*-values of the Vegard and Barth patterns were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel--	112, 103	101	204
British Museum----------	112, 103	316	204
Vegard----------	112, 103	312	204
Barth----------	112, 103	204	116
Swanson, Gilfrich and Cook--	112	101	103

Structural data. Vegard [2] in 1926 determined that calcium tungstate has the space group C_{4h}^6–$I4_1/a$ and $4(CaWO_4)$ per unit cell. Calcium tungstate is used as a structure-type.

The "*a*" measurements reported by Vegard [3] and by Aanerud [4] have been multiplied by 2/2 for comparison with the NBS values. All unit-cell measurements have been converted from kX to angstrom units.

Lattice constants

		a	*c*
		A	*A*
1926	Vegard [2]----------	5.27	11.37
1926	Barth [3]----------	5.27	11.37
1931	Aanerud [4]----------	5.255	11.372
1943	Sillén and Nylander [5]---	5.241	11.371
1956	Swanson, Gilfrich and Cook.	5.242	11.372 at 25°C

The density of calcium tungstate calculated from the NBS lattice constants is 6.120 at 25°C.

Calcium Tungstate (scheelite), $CaWO_4$ (tetragonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		---- British Museum Cu, 1.5405 A		1926 Vegard Cu, 1.5418 A		1926 Barth Cu, 1.5418 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A	
101	4.78	31	4.63	70	------	----	------	----	4.76	53
112	3.10	100	3.05	100	3.11	100	3.10	s	3.10	100
103									3.072	31
004	2.84	8	2.80	50	2.88	10	2.86	w	2.844	14
200	2.62	13	2.60	50	2.623	35	2.64	w	2.622	23
211	2.28	10	2.26	50	2.316	25	2.25	w	2.296	19
114			2.11	20					2.256	3
105	1.98	5	2.05	20	2.013	10	2.10	w	2.0864	5
213			2.02	20			2.00	w	1.9951	13
-----	------	----	1.97	50	------	----	------	----	------	----
204	1.92	23	1.90	90	1.929	50	1.93	s	1.9278	28
220	1.85	8	1.83	50	1.855	30	1.86	m	1.8538	12
-----	------	----	1.79	20	------	----	------	----	------	----
-----	------	----	1.75	20	------	----	------	----	------	----
301	------	----	1.71	20	------	----	1.73	w	1.7278	5
116	1.67	10	1.67	70	1.685	35	1.69	s	1.6882	16
215	1.62	5	1.62	50	1.642	10	1.64	s	1.6332	10
312	1.58	20	1.58	90	1.592	60	1.60	s	1.5921	30
224	1.54	10	1.54	70	1.557	30	1.56	m	1.5532	14
321	------	----	1.43	50	1.443	15	1.45	w	1.4427	6
008	------	----	1.41	20	------	----	1.43	w	1.4219	2
305	------	----	1.38	50	1.387	15	1.39	w	1.3859	3
323	------	----	1.35	50	1.361	10	1.36	w	1.3577	4
217	------	----	1.33	50	1.337	10	1.34	w	1.3358	3
400	------	----	1.30	20	1.313	10	1.32	w	1.3106	3
411	------	----	------	----	------	----	------	----	1.2638	2
316	1.243	10	1.24	100	1.241	55	1.25	s	1.2488	13
109	------	----	1.22	20	------	----	1.23	m	1.2284	2
332	1.200	3	1.20	70	1.211	25	1.21	w	1.2074	5
413									1.2054	5
404										
307	------	----	1.18	70	1.193	15	1.20	w	1.1901	4
420	1.165	3	1.17	60	1.171	15	1.18	w	1.1728	1
228	------	----	1.12	50	1.126	20	1.14	w	1.1280	5
415	------	----	1.11	20	1.111	10	1.12	m	1.1096	2
1·1·10										
424	1.080	5	1.08	90	1.088	50	1.10	s	1.0870	5
327									1.0838	8
501	------	----	------	----	1.039	15	------	----	1.0439	3
2·0·10										
336	------	----	------	----	------	----	------	----	1.0351	2
1·0·11	1.010	3	------	----	1.014	40	------	----	1.0140	6
512									1.0116	4
521									0.9699	1
2·2·10	------	----	------	----	0.9682	10	------	----		
408	------	----	------	----					.9636	4
329	------	----	------	----	.9541	15	------	----	.9537	3
505	------	----	------	----					.9522	3
0·0·12	------	----	------	----	------	----	------	----	.9476	3
523	------	----	------	----	------	----	------	----	.9427	<1
3·1·10	------	----	------	----	.9390	20	------	----	.9378	5
440	------	----	------	----	.9275	5	------	----	.9268	<1
428	------	----	------	----	.9060	50	------	----	.9042	23
516										
419	------	----	------	----	------	----	------	----	.8962	2

Calcium Tungstate (scheelite), $CaWO_4$ (tetragonal)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		---- British Museum Cu, 1.5405 A		1926 Vegard Cu, 1.5418 A		1926 Barth Cu, 1.5418 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
525	------	----	------	----	0. 8913	30	------	----	0. 8949	3
2·0·12	------	----	------	----	------	----	------	----	. 8912	3
532	------	----	------	----	------	----	------	----	. 8879	3
444 / 507	------	----	------	----	. 8808	25	------	----	. 8809	4
600	------	----	------	----	------	----	------	----	. 8736	2
2·2·12	------	----	------	----	. 8461	25	------	----	. 8439	2
3·2·11	------	----	------	----	------	----	------	----	. 8426	1
3·3·10	------	----	------	----	------	----	------	----	. 8368	2
604 / 527	------	----	------	----	. 8386	30	------	----	. 8352	4
620	------	----	------	----	. 8324	10	------	----	. 8289	2
622	------	----	------	----	------	----	------	----	. 8197	1
536	------	----	------	----	. 8159	30	------	----	. 8124	4
509	------	----	------	----	------	----	------	----	. 8070	2
615	------	----	------	----	------	----	------	----	. 8059	1
4·1·11	------	----	------	----	------	----	------	----	. 8022	2
543	------	----	------	----	------	----	------	----	. 8003	2
624	------	----	------	----	. 7981	40	------	----	. 7958	8
606	------	----	------	----	------	----	------	----	. 7937	5

References

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

[2] L. Vegard, Results of crystal analysis, Phil. Mag. **1**, 1151–1193 (1926).

[3] T. Barth, The structure of synthetic, metamict, and recrystallized fergusonite, Norske Geol. Tidsskr. **9**, 24–36 (1926).

[4] K. Aanerud, Mischkristallbildung der Scheelitgruppe durch fällung von Lösungen, Avhandl. Norske Videnskaps-Akad. Oslo. I. Mat.-Naturv. Kl. **1931**, No. 13 (1931).

[5] L. G. Sillén and A. Nylander, On the oxygen positions in tungstates and molybdates with the scheelite structure, Arkiv. Kemi. Mineral. Geol. **17**, No. 4 (1943–44).

Cesium Aluminum Sulfate Dodecahydrate, $CsAl(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0367	4. 35 2. 83 5. 5	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of cesium aluminum sulfate dodecahydrate was prepared at the NBS from cesium chloride, aluminum sulfate and sulfuric acid. Spectographic analysis showed the following impurities: 0.01 to 0.1 percent of rubidium; 0.001 to 0.01 percent each of potassium, magnesium, and silicon; and 0.0001 to 0.001 percent each of barium, calcium, chromium, copper, iron, lithium, sodium, and lead.

The sample is colorless. The index of refraction is 1.455.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	220	331	210
Swanson, Gilfrich, and Cook	220	331	420

Structural data. Lipson [2] in 1935 determined that cesium aluminum sulfate dodecahydrate has the beta alum-type structure, having the space group T_h^6–Pa3 and 4[$CsAl(SO_4)_2 \cdot 12H_2O$] per unit cell.

Two unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1927	Cork [3]	12. 33
1935	Lipson and Beevers [4]	12. 358
1956	Swanson, Gilfrich, and Cook.	12.358 at 25° C.

The density of cesium aluminum sulfate dodecahydrate calculated from the NBS lattice constant is 1.999 at 25° C.

Cesium Aluminum Sulfate Dodecahydrate, $CsAl(SO_4)_2 \cdot 12H_2O$ (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	7. 1	18	12. 3	7. 1	20	12. 3
200	6. 1	23	12. 2	6. 19	32	12. 4
210	5. 5	38	12. 3	5. 53	35	12. 4
211	5. 0	3	12. 2	5. 04	8	12. 4
220	4. 35	100	12. 3	4. 371	100	12. 36
221	4. 11	15	12. 33	4. 116	21	12. 35
311	----	---	----	3. 724	13	12. 35
222	3. 57	15	12. 37	3. 566	22	12. 35
302	----	---	----	3. 427	6	12. 36
321	3. 30	18	12. 35	3. 302	19	12. 35
400	3. 09	18	12. 36	3. 090	34	12. 36
410	----	---	----	2. 998	14	12. 36
331	2. 84	75	12. 38	2. 835	67	12. 36
420	2. 76	25	12. 34	2. 763	40	12. 36
421	----	---	----	2. 695	8	12. 35
422	2. 52	20	12. 34	2. 522	24	12. 36
511	2. 37	20	12. 31	2. 378	22	12. 36
432	----	---	----	2. 294	3	12. 35
521	----	---	----	2. 256	4	12. 36
440	2. 17	5	----	2. 184	10	12. 36
522				2. 152	<1	12. 36
531	----	---	----	2. 089	8	12. 36
600	2. 06	8	12. 36	2. 060	12	12. 36
611	----	---	----	2. 004	5	12. 36
620	1. 95	25	12. 33	1. 954	24	12. 36
621	----	---	----	1. 9309	1	12. 363

Cesium Aluminum Sulfate Dodecahydrate, $CsAl(SO_4)_2 \cdot 12H_2O$ (cubic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
533	1. 88	10	12. 33	1. 8845	13	12. 358
622	----	---	----	1. 8642	6	12. 366
630	----	---	----	1. 8419	3	12. 356
631	----	---	----	1. 8226	1	12. 362
444	----	---	----	1. 7842	2	12. 361
711	----	---	----	1. 7302	5	12. 356
640	1. 71	8	12. 33	1. 7140	11	12. 360
641	----	---	----	1. 6978	1	12. 360
721	----	---	----	1. 6814	2	12. 356
642	1. 65	20	12. 35	1. 6512	16	12. 356
722	----	---	----	1. 6366	2	12. 356
731	1. 60	5	12. 29	1. 6091	6	12. 360
732	----	---	----	1. 5692	1	12. 356
810	----	---	----	1. 5328	2	12. 358
811	----	---	----	1. 5206	1	12. 353
733	----	---	----	1. 5100	3	12. 360
820	1. 498	10	12. 35	1. 4986	10	12. 358
653	----	---	----	1. 4784	<1	12. 369
822	----	---	----	1. 4568	9	12. 361
830	----	---	----	1. 4467	1	12. 361
751	----	---	----	1. 4269	1	12. 357
662	----	---	----	1. 4182	3	12. 364
832	----	---	----	1. 4082	2	12. 357
840	----	---	----	1. 3821	5	12. 362
911	----	---	----	1. 3566	5	12. 359
842	----	---	----	1. 3484	2	12. 358
664	----	---	----	1. 3172	4	12. 356
851	----	---	----	1. 3023	1	12. 355
931	----	---	----	1. 2950	5	12. 354
844	----	---	----	1. 2614	3	12. 359
10·0·0	----	---	----	1. 2356	<1	12. 356
10·2·0	----	---	----	1. 2120	6	12. 360
10·2·2	----	---	----	1. 1890	3	12. 356
953	----	---	----	1. 1525	4	12. 359
10·4·0	----	---	----	1. 1476	2	12. 360
Average of last five lines	----	---	12. 33	------	---	12. 358

References

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

[2] H. Lipson, Existence of three alum structures, Nature **135**, 912 (1935).

[3] J. M. Cork, The crystal structure of some of the alums, Phil. Mag. **4**, 688–698 (1923).

[4] H. Lipson and C. A. Beevers, The crystal structure of the alums, Proc. Roy. Soc. London **148** [A], 664–680 (1935).

Cesium Fluoplatinate, Cs_2PtF_6 (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium fluoplatinate used for the NBS pattern was prepared by T. P. Perros, George Washington University, Washington, D. C. The cesium content of this sample was found by flame spectrometer analysis at George Washington University to be 46.2 percent. The computed theoretical value is 46.23 percent.

The sample has a yellow color and is optically negative. The indices of refraction are $N_o = 1.568$ and $N_e = 1.542$.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	101	110	201

Structural data. Mellor and Stephenson [1] in 1951 determined that cesium fluoplatinate has potassium fluogermanate-type structure, the space group D^3_{3d}–$P\bar{3}m1$, and $1(Cs_2PtF_6)$ per unit hexagonal cell or $3(Cs_2PtF_6)$ per unit rhombohedral cell.

The unit-cell measurements reported by Sharpe [2] were given in angstrom units.

Lattice constants

		a	*c*
		A	*A*
1953	Sharpe [2]	6. 22	5. 01
1956	Swanson, Gilfrich, and Cook.	6. 225	5. 018 at 25° C

The density of cesium fluoplatinate calculated from the NBS lattice constants is 5.669 at 25° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*
	A	
100	5. 40	13
001	5. 02	9
101	3. 67	100
110	3. 114	58
111	2. 647	5
002	2. 510	2
201	2. 374	39
102	2. 276	20
210	2. 036	2
211	1. 8878	20
202	1. 8363	12
300	1. 7967	9
003	1. 6732	2
103	1. 5978	3
212	1. 5818	11
220	1. 5565	8
113	1. 4733	7
311	1. 4326	7
203	1. 4213	2
401	1. 3014	3
312	1. 2840	4
004	1. 2545	2
303	1. 2245	4
104	1. 2218	3
321	1. 2005	2
402	1. 1870	3
410	1. 1764	2
114	1. 1633	2
223	1. 1388	3
322	1. 1090	1
214	1. 0686	1

References

[1] D. P. Mellor and N. C. Stephenson, The crystal structure of potassium hexafluoroplatinate, Aust. J. Sci. Research. A4, 406–11 (1951).

[2] A. G. Sharpe, The chemistry of platinum metals. Part II. Fluoropalladates and fluoroplatinates, J. Chem. Soc. **1953**, 197–199.

Cesium Iron Sulfate Dodecahydrate, $CsFe(SO_4)_2 \cdot 12HO_2$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium iron sulfate dodecahydrate was prepared at the NBS from cesium bromide and iron sulfate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, magnesium, and rubidium; 0.001 to 0.01 percent each of copper, potassium, manganese, nickel, silicon, and titanium; and 0.0001 to 0.001 percent each of barium, calcium, and chromium.

The sample is light tan. The index of refraction is 1.484.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	220	331	420

Structural data. Cesium iron sulfate dodecahydrate appears to be a beta alum since the intensities of the NBS pattern agree closely with those of the other beta alums. Lipson [1] in 1935 determined the structure of the beta alums having the space group T_h^6–Pa3 and $4[CsFe(SO_4)_2 \cdot 12H_2O]$ per unit cell.

The NBS unit-cell measurement is as follows:

Lattice constant

		A
1956	Swanson, Gilfrich, and Cook.	12.434 at 25° C

The density of cesium iron sulfate dodecahydrate calculated from the NBS lattice constant is 2.063 at 25°C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	7.2	6	12.4
200	6.21	43	12.42
210	5.56	33	12.42
211	5.07	8	12.42
220	4.392	100	12.42
221	4.139	24	12.42
311	3.746	1	12.42
222	3.584	28	12.42
230	3.445	6	12.42
321	3.318	20	12.41
400	3.106	35	12.42
410	3.012	12	12.42
331	2.849	54	12.42
420	2.778	50	12.42
421	2.710	8	12.42
422	2.536	34	12.42
511	2.392	12	12.43
432	2.307	4	12.42
521	2.268	5	12.42
440	2.197	12	12.42
600	2.072	22	12.43
611	2.016	3	12.43
620	1.966	28	12.43
621	1.942	<1	12.43
533	1.895	7	12.43
622	1.874	7	12.43
444	1.794	<1	12.43
711	1.740	5	12.42
640	1.724	10	12.43
721	1.691	1	12.43
642	1.6609	21	12.429
731	1.6187	5	12.434
810	1.5419	3	12.431
733	1.5179	5	12.424
820	1.5076	11	12.432
821	1.4975	6	12.439
822	1.4654	9	12.434
662	1.4259	6	12.431
840	1.3904	6	12.436
911	1.3646	2	12.432
842	1.3566	4	12.435
Average of last five lines			12.434

References

[1] H. Lipson, Existence of three alum structures, Nature **135,** 912 (1935).

Chromium Silicide, Cr_3Si (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
6–0692	2. 04 1. 22 1. 86	Chromi-um.	Borén [1] 1933.

Additional published patterns. None.

NBS sample. The sample of chromium silicide was prepared at the NBS by Raymond F. Walker and Sylvanus F. Holley. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of vanadium; 0.001 to 0.01 percent each of aluminum, calcium, iron, manganese, lead, tin, and titanium; and 0.0001 to 0.001 percent each of copper and magnesium.

The sample has a dark-grey color and is opaque.

Interplanar spacings and intensity measurements. The *d*-values of the Borén pattern were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Borén	210	321	211
Swanson, Gilfrich, and Cook	210	211	200

Structural data. Borén [1] in 1933 determined that chromium silicide has beta tungsten-type structure, the space group O_h^3–Pm3n, and 2(Cr_3Si) per unit cell. So-called beta tungsten was found to be an oxide by Hägg and Schönberg [2].

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1933	Borén [1]	4.564
1956	Swanson, Gilfrich, and Cook.	4.5578 at 25° C

The density of chromium silicide calculated from the NBS lattice constant is 6.457 at 25° C.

hkl	1933 Borén Cr, 2.2909 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
110	3. 22	m	4. 56	3. 22	13	4. 560
200	2. 29	m+	4. 58	2. 279	25	4. 559
210	2. 04	s+	4. 56	2. 039	100	4. 558
211	1. 863	s	4. 562	1. 8610	50	4. 558
---	1. 612	vw	---	----	--	----
310	1. 441	w	4. 556	1. 4415	5	4. 5584
222	1. 317	m	4. 564	1. 3156	9	4. 5574
320	1. 265	s	4. 562	1. 2641	12	4. 5578
321	1. 220	s+	4. 563	1. 2179	19	4. 5570
400	---	---	---	1. 1394	8	4. 5576
420	---	---	---	1. 0192	5	4. 5580
421	---	---	---	0. 9946	15	4. 5577
332	---	---	---	. 9717	5	4. 5578
430	---	---	---	. 9116	5	4. 5580
520	---	---	---	. 8464	12	4. 5578
521	---	---	---	. 8321	8	4. 5576
440	---	---	---	. 8057	10	4. 5577
Average of last five lines			4. 561	----	--	4. 5578

References

[1] B. Borén, Röntgenuntersuchung der Legierungen von Silicium mit Chrom, Mangan, Kobalt und Nickel, Ark. Kem. Mineral. Geol. **11a,** Nr. 10, 1–28 (1933).

[2] G. Hägg and N. Schönberg, β-Tungsten as a tungsten oxide, Acta Cryst. **7,** 351–352 (1954)

Gallium Antimonide, GaSb (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of gallium antimonide was prepared by William R. Hosler at the NBS. Spectrographic analysis of the sample showed the following impurities: 0.01 to 0.1 percent each of iron and silicon; 0.001 to 0.01 percent each of aluminum and magnesium; and 0.0001 to 0.001 percent each of barium, calcium, copper, and manganese.

The sample is a black opaque powder.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	111	220	311

Structural data. Goldschmidt [1] in 1926 determined that gallium antimonide has zinc sulfide-type structure, the space group T_d^2–$F\bar{4}3m$, and 4(GaSb) per unit cell.

The unit-cell measurement reported by Goldschmidt has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1926	Goldschmidt [1]	6.105
1956	Swanson, Gilfrich, and Cook.	6.095 at 25° C

The density of gallium antimonide calculated from the NBS lattice constant is 5.616 at 25° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	3. 520	100	6. 097
200	3. 048	11	6. 095
220	2. 156	67	6. 099
311	1. 838	44	6. 097
222	1. 759	3	6. 094
400	1. 524	11	6. 095
331	1. 399	17	6. 097
420	1. 363	3	6. 096
422	1. 244	20	6. 096
511	1. 1738	10	6. 099
440	1. 0776	5	6. 096
531	1. 0304	9	6. 096
600	1. 0158	1	6. 095
620	0. 9638	4	6. 096
533	. 9294	5	6. 094
622	. 9188	1	6. 095
444	. 8796	2	6. 094
711	. 8534	5	6. 095
640	. 8452	1	6. 095
642	. 8144	7	6. 094
731	. 7936	7	6. 095
Average of last five lines			6. 095

References

[1] V. M. Goldschmidt, Geochemische Verteilungsgesetze der Elemente. VIII. Untersuchungen über Bau und Eigenschaften von Krystallen, **1926**, No. 8, (1926).

Magnesium Hydroxide (brucite), $Mg(OH)_2$ (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–1169	2. 35 4. 75 1. 79	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.
2–1092	2. 37 4. 76 1. 79	Molybdenum.	United Steel Companies, England.

A third ASTM card, 2–1395, reporting the data of Hansen and Brownmiller, is for magnesium oxide, and not for magnesium hydroxide as indicated on the card. This card is listed in the card file index under magnesium oxide hydrate. Previous to 1950 the original card was labeled MgO (see NBS Circular 539, vol. 1, p. 37).

Additional published patterns

Source	Radiation	Wavelength
		A
Aminoff [2] 1921	Iron	1. 93
Levi and Ferrari [3] 1921	Copper	Kα
Natta and Passerini [4] 1928	Cobalt	
Bury, Davis, and Grime [5] 1932.	Copper	Kα

NBS sample. The sample of magnesium hydrox-

ide was prepared at the NBS by G. F. Rynders by heating magnesium oxide and water in a hydrothermal bomb at 20,000 psi and 600° C for 3 days. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of calcium; 0.001 to 0.01 percent each of silver, aluminum, boron, iron, silicon, strontium, and titanium; and 0.0001 to 0.001 percent each of barium, chromium, and copper.

The sample is colorless and optically positive. The indices of refraction are $N_o = 1.561$ and $N_e = 1.581$.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel, the United Steel Companies, and the Bury, Davis, and Grime patterns were converted from kX to angstrom units and the *d*-values of the Aminoff, the Levi and Ferrari, and the Natta and Passerini patterns were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	101	001	102
United Steel Companies	101	001	102
Aminoff	101	102	110
Levi and Ferrari	101	102	110
Natta and Passerini	101	102	110
Bury, Davis, and Grime	001	102	101
Swanson, Gilfrich, and Cook	101	001	102

Structural data. Aminoff [2] in 1921 determined that magnesium hydroxide has cadmium iodide-type structure, the space group D^3_{3d}—$P\bar{3}m1$, and $1[Mg(OH)_2]$ per unit hexagonal cell, or $3[Mg(OH)_2]$ per unit rhombohedral cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Magnesium Hydroxide (brucite), $Mg(OH)_2$ (trigonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		---- United Steel Companies Mo, 0.7107 A		1921 Aminoff Fe, 1.937 A		1921 Levi and Ferrari Cu, 1.542 A		1928 Natta and Passerini Co, 1.790 A		1932 Bury, Davis, and Grime Cu, 1.542 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		A		A	
001	4.76	53	4.77	80	4.5	33	4.59	ms	3.8	mw	4.80	vs	4.77	90
100	------	--	------	--	------	--	------	----	2.56	m	------	----	2.725	6
101	2.35	100	2.37	100	2.32	100	2.36	vs	2.32	vs	2.39	s	2.365	100
102	1.79	40	1.79	80	1.77	83	1.78	s	1.77	s	1.809	vs	1.794	56
110	1.57	33	1.57	70	1.56	83	1.55	s	1.56	s	1.582	vw	1.573	36
111	1.493	17	1.49	60	1.48	50	1.49	m	1.48	ms	1.500	vw	1.494	18
103	1.373	13	1.37	60	1.37	50	1.34	m	1.34	ms	1.375	s	1.373	16
200	------	--	------	--	------	--	------	----	------	----	------	----	1.363	2
201	1.319	9	1.31	60	1.30	50	1.28	m	1.29	ms	1.318	vw	1.310	11
004	------	--	------	--	------	--	------	----	------	----	1.197	vw	1.192	2
202	1.185	7	1.18	50	1.18	67	1.17	m	1.18	mw	1.190	vw	1.183	9
113	------	--	------	--	------	--	------	----	------	----	------	----	1.118	1
104	------	--	1.09	20	1.09	33	1.10	vw	------	----	1.093	vw	1.092	3
203	1.033	3	1.03	40	1.03	50	1.021	m	------	----	------	----	1.034	5
210	------	--	------	--	------	--	------	----	------	----	------	----	1.030	1
211	1.007	4	1.00	60	1.01	50	0.982	m	1.007	ms	------	----	1.0067	7
005	------	--	------	--	------	--	------	----	------	----	------	----	0.9543	1
114	------	--	0.95	40	------	--	------	----	------	----	------	----	.9503	5
212	0.947	4	.94	60	------	--	.941	ms	0.947	mw	------	----	.9455	8
300	------	--	.91	40	------	--	.904	w	------	----	------	----	.9085	3
105	------	--	------	--	------	--	------	----	------	----	------	----	.9001	<1
204	------	--	------	--	------	--	------	----	------	----	------	----	.8974	1
301	------	--	------	--	------	--	.888	w	------	----	------	----	.8923	2
213	.864	1	------	--	------	--	.862	ms	------	----	------	----	.8643	5
115	------	--	------	--	------	--	.808	ms	------	----	------	----	.8156	3
---	------	--	------	--	------	--	.788	ms	------	----	------	----	-------	---
220	------	--	------	--	------	--	.782	w	------	----	------	----	.7865	3

Lattice constants

		a	*c*
		A	*A*
1921	Aminoff [2]	3. 14	4. 76
1921	Levi and Ferrari [3]	3. 14	4. 76
1928	Natta and Passerini [4]	3. 12	4. 74
1932	Bury, Davis, and Grime [5].	3. 16	4. 79
1956	Swanson, Gilfrich, and Cook	3. 147	4. 769 at 26° C.

The density of magnesium hydroxide calculated from the NBS lattice constants is 2.368 at 26° C.

References

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[4] G. Natta and L. Passerini, Soluzioni solide perprecipitazione, Gazz. chim. ital. **58,** 592–618 (1928).

[5] C. R. Bury, E. R. H. Davis and G. Grime, The system magnesium oxide-magnesium chloride-water, J. Chem. Soc. **1932,** 2008–2015 (1932).

Magnesium Silicate (enstatite), $MgSiO_3$ (orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
3–1173	1. 26 1. 32 1. 23	Iron	Haraldsen [1] 1930.
1–0773 [a]	3. 16 1. 97 1. 49	Molybdenum.	Hanawalt, Rinn, and Frevel [2] 1938.
2–0546	3. 16 2. 86 2. 53	Molybdenum.	Physics Department, Newcastle-on-Tyne, England.
3–0522	3. 16 2. 86 1. 48	Cobalt	Clark [3] 1946.

[a] Deleted in 1955 index.

Additional published patterns

Source	Radiation	Wavelength
Büssem and Schusterius [4] 1938.	Copper	
Thilo and Rogge [5] 1939	Iron	
Atlas [6] 1952	Iron	

Atlas gives patterns for both synthetic and naturally occurring enstatite. The pattern included in the table is for synthetic enstatite, which contains 2 percent of lithium fluoride.

NBS sample. The sample of enstatite used for the NBS pattern is sample number 971 from the National Museum. It was a portion of the Bishopville meteorite found in Sumter County, S. C. This was felt to be the best source of enstatite available, as attempts at synthesis have yielded mixtures of enstatite and clinoenstatite. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of aluminum, calcium, and iron; 0.01 to 0.1 percent each of chromium, manganese, sodium, and titanium; and 0.001 to 0.01 percent each of silver, boron, copper, and nickel.

The NBS sample is colorless and is optically positive. The refractive indices are $\alpha=1.649$, $\beta=1.653$, and $\gamma=1.658$.

Interplanar spacings and intensity measurements. The *d*-values of the Newcastle, the Clark, and the Hanawalt, Rinn, and Frevel patterns were converted from kX to angstrom units, and the *d*-values of the Haraldsen, the Büssem and Schusterius, and the Thilo and Rogge patterns were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Haraldsen	----	--	----------
Hanawalt, Rinn, and Frevel.	240, 221	361	2·11·1, 3·10·1
Physics Department, Newcastle-on-Tyne.	240, 221	160	311
Clark	240, 221	160	2·11·1, 3·10·1
Büssem and Schusterius.	240, 221	421	2·11·1, 3·10·1
Thilo and Rogge	240, 221	160	311
Atlas	240, 221	160	022
Swanson, Gilfrich, and Cook.	240, 221	160	022

Structural data. Warren and Modell [7] in 1930 determined that enstatite has the space group D_{2h}^{15}–Pcab and 16($MgSiO_3$) per unit cell.

Two other polymorphic forms of $MgSiO_3$ are recognized. Atlas [6] gives additional powder pattern data for these forms. Clinoenstatite is obtained by heating $MgSiO_3$ in air above 1,115° C. Protoenstatite is a slightly higher temperature form. The proto form reverts to the clino with grinding.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1929	Grossner and Mussgung [8].	8. 84	18. 23	5. 20
1930	Warren and Modell [7].	8. 86	18. 20	5. 20
1932	Takané [9]	8. 84	18. 16	5. 19
1952	Atlas [6]	8. 89	18. 20	5. 20
1956	Swanson, Gilfrich, and Cook.	8. 829	18. 22	5. 192 at 26° C.

The density of enstatite calculated from the NBS lattice constants is 3.194 at 26° C.

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[1] H. Haraldsen, Beiträge zur Kenntnis der thermischen Umbildung des Talks, Neues Jahrb. Mineral. Geol. Beilage Bd. A **61,** 139–164 (1930).

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[7] B. E. Warren and D. I. Modell, The structure of enstatite $MgSiO_3$, Z. Krist. **75,** 1–14 (1930).

[8] B. Gossner and F. Mussgung, Über Enstatit und sein Verhältnis zur Pyroxen- und Amphibolgruppe, Z. Krist. **70,** 234–248 (1929).

[9] K. Takané, Crystal structure of bronzite from Chichijima in the Bonin Islands, Proc. Imp. Acad. Tokyo **8,** 308–311 (1932).

Magnesium Silicate (enstatite), $MgSiO_3$ (orthorhombic)

hkl	1930 Haraldsen Fe, 1.9373 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		Physics Dept. England Mo, 0.7107 A		1946 Clark Co, 1.7902 A		1938 Büssem and Schusterius Cu, 1.5418 A		1939 Thilo and Rogge Fe, 1.9373 A		1952 Atlas Fe, 1.973 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*		*A*		*A*	
120	--	--	--	--	--	--	--	--	--	--	--	--	6. 30	10	6. 33	1
200	--	--	--	--	4. 41	30	4. 41	vvw	--	--	4. 47	vw	4. 38	20	4. 41	14
----	3. 617	vvw	--	--	--	--	--	--	--	--	--	--	4. 02	30	--	--
----	3. 520	vw	--	--	--	--	--	--	3. 48	mw	3. 50	w	--	--	--	--
211	3. 292	w	--	--	3. 30	50	3. 29	vw	--	--	3. 31	w	3. 28	30	3. 303	35
----	--	--	--	--	--	--	--	--	3. 20	vw	3. 24	vw	--	--	--	--
240, 221	3. 175	s	3. 17	100	3. 16	100	3. 16	vs	3. 14	vs	3. 17	vs	3. 14	100	3. 167	100
----	--	--	--	--	--	--	--	--	--	--	2. 99	vvw	--	--	--	--
231	2. 998	m	2. 92	33	2. 96	50	2. 93	vw	--	--	2. 94	vw	2. 92	40	2. 941	44
160	2. 895	m			2. 87	70	2. 86	s	2. 90	s	2. 89	vs	2. 85	60	2. 872	87
151	--	--	--	--	--	--	2. 81	vvw	2. 83	vw	2. 84	vvw	2. 81	20	2. 825	23
241	2. 730	vvw	2. 73	20	2. 71	50	2. 70	vw	2. 71	m	2. 72	w	2. 69	40	2. 706	26
311	2. 551	m	2. 56	27	2. 54	60	2. 52	vw	2. 54	s	2. 54	s	2. 52	40	2. 534	43
022	2. 469	m	--	--	2. 48	60	2. 48	mw	--	--	2. 49	s	2. 48	60	2. 494	51
340, 251	--	--	--	--	--	--	2. 44	vvw	2. 46	w	2. 47	s	2. 46	30	2. 471	31
331	2. 311	vvw	--	--	--	--	--	--	--	--	--	--	2. 37	10	2. 358	7
080	--	--	2. 30	20	--	--	--	--	2. 30	ms	--	--	--	--	2. 280	5
042, 261, 171, 212	--	--	--	--	--	--	--	--	2. 24	w	--	--	2. 24	10	2. 252	7
341	--	--	--	--	--	--	--	--	2. 18	w	--	--	2. 22	10	2. 232	7
360	2. 119	vw	--	--	--	--	2. 10	vw	2. 12	vw	2. 12	w	2. 10	50	2. 114	24
351	--	--	--	--	2. 11	60	2. 08	vw	2. 07	w	2. 10	w	2. 08	40	2. 096	21
271, 152	--	--	--	--	2. 05	20	2. 04	vvw	--	--	2. 06	vw	2. 05	30	2. 058	13
280, 224	--	--	--	--	--	--	2. 01	vvw	--	--	2. 02	vw	2. 02	20	2. 019	10

Magnesium Silicate (enstatite), $MgSiO_3$ (orthorhombic) (Continued)

hkl	1930 Haraldsen Fe, 1.9373 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		Physics Dept. England Mo, 0.7107 A		1946 Clark Co, 1.7902 A		1938 Büssem and Schusterius Cu, 1.5418 A		1939 Thilo and Rogge Fe, 1.9373 A		1952 Atlas Fe, 1.973 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		A		A		A	
421	--	--	--	--	1. 97	20	1. 971	vvw	1. 98	vs	1. 99	w	1. 98	30	1. 984	13
361	1. 968	s	1. 97	47	1. 96	40	1. 946	vw	--	--	1. 96	w	1. 95	40	1. 958	24
431	--	--	--	--	--	--	--	--	1. 91	w	--	--	1. 92	10	1. 926	4
162																
281	--	--	--	--	--	--	1. 869	vvw	--	--	--	--	1. 88	10	1. 887	6
441	--	--	--	--	--	--	1. 831	vvw	--	--	1. 84	vvw	1. 85	10	1. 854	3
332																
262																
380	1. 807	vvw	--	--	--	--	--	--	1. 81	mw	--	--	1. 83	10	1. 800	7
172																
460	--	--	--	--	1. 78	30	--	--	--	--	1. 79	vw	1. 782	20	1. 786	10
1·10·0																
451	1. 760	vvw	--	--	--	--	1. 774	vvw	--	--	1. 77	vw	1. 770	10	1. 773	7
291	1. 713	vw	--	--	1. 73	20	1. 722	vvw	1. 75	w	1. 73	w	1. 730	20	1. 732	8
381	--	--	1. 71	10	1. 70	20	--	--	1. 71	m	1. 70	w	--	--	1. 702	9
272	--	--	--	--	--	--	--	--	1. 69	w	1. 68	w	1. 698	20	1. 698	8
182	--	--	--	--	--	--	--	--	1. 66	mw	--	--	1. 676	20	1. 679	9
412																
471	1. 640	s	1. 64	13	--	--	1. 628	vvw	1. 64	s	1. 64	vw	1. 648	10	1. 649	7
----	--	--	--	--	--	--	--	--	--	--	--	--	1. 640	10	--	--
----	--	--	--	--	--	--	--	--	--	--	--	--	1. 628	10	--	--
2·10·1	1. 605	s	--	--	1. 60	50	1. 601	vvw	1. 59	w	1. 60	vw	1. 606	30	1. 603	20
391	--	--	--	--	--	--	1. 577	vvw	1. 57	w	1. 58	vw	1. 585	20	1. 588	10
----	--	--	--	--	--	--	--	--	1. 54	w	--	--	--	--	--	--
551	1. 521	w	--	--	1. 52	40	1. 519	vvw	--	--	--	--	1. 526	10	1. 525	7
243	--	--	--	--	--	--	1. 513	vvw	1. 52	w	1. 52	w	1. 517	20	1. 520	14
2·11·1	1. 497	m	1. 493	40	1. 48	60	1. 475	m	1. 50	vs	1. 48	s	1. 484	80	1. 485	34
3·10·1																
[a]	1. 474	vw	--	--	1. 47	30	1. 463	w	1. 46	m	1. 47	s	1. 471	40	1. 470	22
	1. 457	vw	--	--	--	--	--	--	1. 45	vvw	1. 44	vvw	--	--	--	--
	--	--	--	--	1. 42	20	1. 411	vvw	--	--	1. 42	vw	1. 417	20	1. 418	6
	1. 395	vvw	--	--	1. 39	50	1. 384	w	--	--	1. 39	s	1. 395	20	1. 392	17
	--	--	--	--	--	--	--	--	--	--	--	--	1. 389	40	--	--
	1. 376	m	--	--	--	--	1. 372	vvw	--	--	1. 38	w	1. 377	20	1. 379	6
	1. 358	m	--	--	1. 36	20	1. 354	vvw	--	--	1. 35	vw	1. 359	10	1. 360	2
	1. 338	vw	--	--	1. 34	20	1. 332	vvw	--	--	1. 34	vw	[b]	--	--	--
	1. 316	vs	1. 315	27	1. 31	30	1. 300	vw	--	--	1. 30	s		--	1. 307	6
	1. 288	vvw	--	--	1. 29	30	1. 290	vvw	--	--	1. 30	w		--	--	--
	--	--	--	--	--	--	--	--	--	--	1. 28	vvw		--	--	--
	--	--	--	--	--	--	1. 274	vvw	--	--	1. 28	vvw		--	--	--
	1. 262	vvs	1. 267	13	--	--	1. 262	vvw	--	--	1. 26	s		--	1. 267	8
	--	--	--	--	--	--	1. 245	vvw	--	--	1. 25	w		--	1. 252	5
	1. 231	vs	1. 230	13	--	--	1. 222	vvw	--	--	1. 23	w		--	1. 229	3
	1. 214	vw	--	--	--	--	1. 203	vvw	--	--	--	--		--	--	--
	1. 172	vvw	--	--	--	--	--	--	--	--	--	--		--	--	--
	1. 140	vvw	1. 144	7	--	--	--	--	--	--	--	--		--	--	--
	--	--	1. 055	7	--	--	1. 044	vvw	--	--	--	--		--	--	--
	--	--	0. 994	7	--	--	--	--	--	--	--	--		--	--	--
	--	--	. 950	7	--	--	--	--	--	--	--	--		--	--	--
	--	--	. 874	7	--	--	--	--	--	--	--	--		--	--	--

[a] Indexing of the NBS powder pattern became quite difficult in the back portion of the pattern, but as these lines were distinct they were retained without indexing.

[b] Twenty-nine additional lines were omitted.

Mercury(II) Cyanide, $Hg(CN)_2$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0504	3. 72 4. 85 2. 51	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of mercuric cyanide was obtained from the Fisher Scientific Co. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of silicon; 0.001 to 0.01 percent each of aluminum and magnesium; and 0.0001 to 0.001 percent each of calcium and iron.

The sample is colorless and optically negative. The refractive indices are $N_o=1.640$ and $N_e=1.490$.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn and Frevel	112	200	312
Swanson, Gilfrich, and Cook	112	200	312

Structural data. Hassel [2] in 1926 determined that mercuric cyanide has the space group D_{2d}^{12}-$I\bar{4}2d$ and 8[$Hg(CN)_2$] per unit cell. Mercuric cyanide is used as the structure-type.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1926	Hassel [2]	9. 69	8. 94
1928	Fricke and Havestad [3]	9. 76	8. 96
1956	Swanson, Gilfrich, and Cook.	9. 693	8. 896 at 25°C

The density of mercuric cyanide calculated from the NBS lattice constants is 4.015 at 25° C.

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[2] O. Hassel, Röntgenographische Untersuchung des tetragonal kristallisierenden Quecksilberzyanids, Z. Krist. **64,** 217–223 (1926).

[3] R. Fricke and L. Havestad, Die Kristallstruktur des Quecksilbercyanids, Z. anorg. Chem. **171,** 344–350 (1928).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
101	------	----	6. 54	7
200	4. 86	83	4. 85	69
211	------	----	3. 897	13
112	3. 73	100	3. 734	100
220	3. 43	13	3. 427	21
301	3. 04	10	3. 036	19
103	2. 87	7	2. 834	4
321	2. 59	10	2. 573	<1
312	2. 52	67	2. 524	49
213	2. 42	13	2. 447	11
400	------	----	2. 422	9
411	2. 28	10	2. 272	10
004	2. 22	7	2. 224	9
303	------	----	2. 184	3
420	2. 17	13	2. 167	13
332	2. 02	33	2. 031	10
204			2. 021	13
323	------	----	1. 991	4
501	1. 90	10	1. 894	10
224	1. 86	7	1. 865	8
413	------	----	1. 842	5
521	1. 76	10	1. 764	5
512			1. 748	16
440	1. 68	7	1. 713	1
215	------	----	1. 646	<1
404	------	----	1. 638	4
503	1. 61	10	1. 622	6
611	------	----	1. 5681	4
532	1. 56	10	1. 5570	10
424	------	----	1. 5520	7
523	------	----	1. 5380	4
541	1. 49	7	1. 4921	5
325	------	----	1. 4837	<1
622	1. 46	7	1. 4489	8
514	------	----	1. 4457	<1
631	1. 43	7	1. 4257	3
206	------	----	1. 4184	2
613	1. 40	7	1. 4031	3
543	------	----	1. 3481	2
316	------	----	1. 3346	6
505	------	----	1. 3106	7
525	------	----	1. 2652	8
406				
624	------	----	1. 2620	2
336	------	----	1. 2439	1
811	------	----	1. 1915	1
516	------	----	1. 1692	5
545	------	----	1. 1530	<1
644	------	----	1. 1502	1
653	------	----	1. 1449	2
635	------	----	1. 1214	1
417	------	----	1. 1183	1
813	------	----	1. 1141	2
536	------	----	1. 1062	1
840	------	----	1. 0839	1
208				
507	------	----	1. 0628	2
228	------	----	1. 0577	<1

Potassium Aluminum Sulfate Dodecahydrate, $KAl(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0384	4. 29 4. 03 3. 24	Molybdenum.	Hanawalt, Rinn, and Frevel [1] (1938).

Additional published patterns

Source	Radiation	Wavelength
Vegard and Esp [2] 1928	Chromium.	K_α

NBS sample. The sample of potassium aluminum sulfate dodecahydrate was obtained from the General Chemical Co., New York, N. Y. Spectographic analysis showed the following impurities: 0.001 to 0.01 percent each of chromium, magnesium, rubidium, and silicon; and 0.0001 to 0.001 percent each of barium, calcium, cesium, iron, lithium, and sodium.

The sample is colorless. The index of refraction is 1.454.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the *d*-values of the Vegard and Esp pattern were calculated from Bragg angle data. The data of Vegard and Esp did not include intensity values.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	220	221	321
Swanson, Gilfrich, and Cook	220	321	221

Structural data. Wyckoff [5] in 1923 determined that potassium aluminum sulfate dodecahydrate is an alpha alum having the space group T_h^6–Pa3, and $4[KAl(SO_4)_2 \cdot 12H_2O]$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1927	Cork [4]	12.16
1928	Vegard and Esp [2]	12.11
1930	Foote, Blake, and France [5].	12.11
1935	Lipson and Beevers [6]	12.157
1940	Klug and Alexander [7]	12.158 at 25° C
1955	Menary [8]	12.164 at 24° C
1956	Swanson, Gilfrich, and Cook.	12.157 at 25° C

The density of potassium aluminum sulfate dodecahydrate calculated from the NBS lattice constant is 1.753 at 25° C.

References

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

[2] L. Vegard and E. Esp, The crystal structure of the alums, Ann. Physik. **85,** 1152–1164 (1928).

[3] R. W. G. Wyckoff, The crystal structure of the alums, Am. J. Sci. **5,** 209–217 (1923).

[4] J. M. Cork, The crystal structure of some of the alums, Phil. Mag. **4,** 688–698 (1927).

[5] F. G. Foote, F. C. Blake, and W. G. France, Adsorption at crystal-solution interfaces. V. Effect of adsorbed dye on the lattice size of potassium alum crystals, J. Phys. Chem. **34,** 2236–2240 (1930).

[6] H. Lipson and C. A. Beevers, The crystal structure of alums, Proc. Roy. Soc. London **148** [A], 664–680 (1935).

[7] H. P. Klug and L. Alexander, Crystal-chemical studies of the alums. I. Solid solutions of potassium aluminum alum and ammonium aluminum alum, J. Am. Chem. Soc. **62,** 1492–1493 (1940).

[8] J. W. Menary, Some lattice constants, Acta Cryst. **8,** 840 (1955).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1928 Vegard and Esp Cr, 2.2909 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	7. 0	4	12. 1	------	----	----	7. 02	10	12. 16
210	5. 4	20	12. 1	5. 38	----	12. 0	5. 44	39	12. 16
211	4. 97	8	12. 2	4. 89	----	12. 0	4. 96	20	12. 16
220	4. 30	100	12. 2	4. 24	----	12. 0	4. 298	100	12. 16
221	4. 04	40	12. 1	4. 00	----	12. 0	4. 053	47	12. 16
311	3. 66	4	12. 1	3. 65	----	12. 1	3. 667	11	12. 16
321	3. 25	40	12. 2	3. 23	----	12. 2	3. 250	54	12. 16
400	3. 04	16	12. 2	3. 03	----	12. 1	3. 039	27	12. 16
410	2. 94	12	12. 1	2. 94	----	12. 1	2. 950	19	12. 16
411	2. 86	10	12. 1	2. 85	----	12. 1	2. 866	15	12. 16

Potassium Aluminum Sulfate Dodecahydrate, $KAl(SO_4)_2 \cdot 12H_2O$ (cubic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1928 Vegard and Esp Cr, 2.2909 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
331	2. 79	20	12. 2	2. 78	----	12. 1	2. 789	36	12. 16
420	2. 72	6	12. 2	2. 71	----	12. 1	2. 719	16	12. 16
421	2. 65	6	12. 1	2. 64	----	12. 1	2. 654	12	12. 16
332	2. 59	6	12. 2	2. 58	----	12. 1	2. 593	10	12. 16
422	2. 47	6	12. 1	2. 47	----	12. 1	2. 482	7	12. 16
431	------	----	------	2. 37	----	12. 1	2. 385	4	12. 16
511	2. 33	8	12. 1	2. 33	----	12. 1	2. 340	9	12. 16
432	2. 25	4	12. 1	2. 25	----	12. 1	2. 259	3	12. 16
521	2. 21	6	12. 1	2. 21	----	12. 1	2. 220	7	12. 16
440	------	----	------	------	----	----	2. 150	2	12. 16
522	2. 11	6	12. 1	2. 11	----	12. 1	2. 118	8	12. 16
433	------	----	------	------	----	----	2. 085	5	12. 16
531	------	----	------	------	----	----	2. 055	2	12. 16
600	2. 02	8	12. 1	2. 02	----	12. 1	2. 027	9	12. 16
610	------	----	------	1. 99	----	12. 1	2. 000	5	12. 16
611	1. 97	6	12. 1	1. 97	----	12. 1	1. 973	5	12. 18
620	1. 92	16	12. 1	1. 92	----	12. 1	1. 924	15	12. 17
621	------	----	------	------	----	----	1. 899	3	12. 16
541	1. 86	2	12. 0	------	----	----	1. 877	3	12. 16
533	------	----	------	1. 85	----	12. 1	1. 855	3	12. 16
622	------	----	------	------	----	----	1. 833	4	12. 16
630	------	----	------	------	----	----	1. 812	2	12. 16
631	------	----	------	1. 79	----	12. 1	1. 793	3	12. 16
543	------	----	------	------	----	----	1. 719	1	12. 16
711	1. 69	4	12. 1	1. 70	----	12. 1	1. 702	4	12. 16
640	------	----	------	------	----	----	1. 686	4	12. 16
641	------	----	------	------	----	----	1. 670	3	12. 16
721	------	----	------	------	----	----	1. 654	2	12. 15
642	1. 62	8	12. 1	1. 61	----	12. 1	1. 624	7	12. 15
722	------	----	------	------	----	----	1. 610	4	12. 15
731	------	----	------	1. 59	----	12. 2	1. 582	1	12. 15
650	------	----	------	1. 55	----	12. 1	1. 5565	2	12. 157
732	------	----	------	------	----	----	1. 5440	2	12. 158
811	------	----	------	1. 50	----	12. 2	1. 4964	2	12. 157
820	------	----	------	1. 48	----	12. 2	1. 4744	7	12. 158
821	------	----	------	------	----	----	1. 4640	2	12. 161
822	------	----	------	------	----	----	1. 4328	2	12. 168
831	------	----	------	------	----	----	1. 4139	3	12. 163
751	------	----	------	------	----	----	1. 4043	1	12. 162
662	------	----	------	------	----	----	1. 3952	2	12. 166
752	------	----	------	------	----	----	1. 3853	2	12. 156
840	------	----	------	------	----	----	1. 3592	3	12. 157
841	------	----	------	------	----	----	1. 3510	4	12. 159
911	------	----	------	------	----	----	1. 3343	1	12. 156
842	------	----	------	------	----	----	1. 3267	1	12. 159
921	------	----	------	------	----	----	1. 3116	2	12. 163
922	------	----	------	------	----	----	1. 2892	2	12. 162
851	------	----	------	------	----	----	1. 2814	2	12. 156
932	------	----	------	------	----	----	1. 2542	2	12. 160
844	------	----	------	------	----	----	1. 2408	2	12. 157
941	------	----	------	------	----	----	1. 2282	2	12. 159
933	------	----	------	------	----	----	1. 2218	2	12. 157
10·0·0	------	----	------	------	----	----	1. 2158	3	12. 158
10·1·0	------	----	------	------	----	----	1. 2094	2	12. 154
Average of last five lines			12. 1	------	----	12. 2	---------	----	12. 157

Potassium Chlorostannate, K_2SnCl_6 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
3–1295	[a]	[a]	Dickinson [1] 1922.

[a] No powder data

Additional published patterns. None.

NBS sample. The sample of potassium chlorostannate was precipitated from a potassium chloride and stannic chloride solution by hydrochloric acid. Spectrographic analysis shows the following impurities: 0.01 to 0.1 percent each of aluminum, sodium, and silicon; 0.001 to 0.01 percent each of chromium and rubidium; and 0.0001 to 0.001 percent each of barium, calcium, iron, and magnesium.

The sample is colorless. The index of refraction is 1.653.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	111	400	311

Structural data. Dickinson [1] in 1922 determined that potassium chlorostannate has potassium chloroplatinate-type structure, the space group O_h^5–Fm3m, and $4(K_2SnCl_6)$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1922	Dickinson [1]	9.98
1935	Engel [2]	10.003
1956	Swanson, Gilfrich, and Cook.	10.002 at 25° C

The density of potassium chlorostannate calculated from the NBS lattice constant is 2.718 at 25° C.

References

[1] R. G. Dickinson, The crystal structures of potassium and ammonium chlorostannates, J. Am. Chem. Soc. **44,** 276–288 (1922).

[2] G. Engel, Die Kristallstrukturen einiger Hexachlorokomplexsalze, Z. Krist. **90,** 341–373 (1935).

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	5. 78	100	10. 01
200	5. 01	38	10. 01
220	3. 54	40	10. 01
311	3. 018	41	10. 01
222	2. 886	27	10. 00
400	2. 502	51	10. 01
331	2. 297	12	10. 01
420	2. 239	13	10. 01
422	2. 0429	15	10. 008
511	1. 9255	14	10. 005
440	1. 7691	25	10. 008
531	1. 6911	11	10. 005
600	1. 6673	6	10. 004
533	1. 5258	4	10. 005
622	1. 5080	1	10. 003
444	1. 4440	6	10. 004
711	1. 4011	5	10. 006
640	1. 3879	1	10. 008
642	1. 3370	5	10. 005
731	1. 3026	3	10. 006
800	1. 2506	2	10. 005
733	1. 2222	<1	10. 004
820	1. 2135	1	10. 007
822	1. 1788	1	10. 002
751	1. 1552	2	10. 004
840	1. 1186	4	10. 006
911	1. 0980	2	10. 003
842	1. 0916	1	10. 005
664	1. 0666	<1	10. 006
931	1. 0487	2	10. 004
844	1. 0211	3	10. 005
933	1. 0053	2	10. 003
10·0·0	1. 0009	<1	10. 001
10·2·0	0. 9809	2	10. 003
951	. 9671	2	10. 004
953	. 9329	1	10. 004
10·4·0	. 9289	1	10. 005
10·4·2	. 9132	1	10. 004
11·1·1	. 9018	<1	10. 001
880	. 8841	<1	10. 002
11·3·1	. 8738	2	10. 001
10·4·4	. 8706	1	10. 002
10·6·0	. 8579	1	10. 005
11·3·3	. 8484	1	10. 002
12·0·0	. 8336	2	10. 003
11·5·1	. 8247	<1	9. 999
12·2·2	. 8112	1	10. 001
11·5·3	. 8034	1	10. 002
12·4·0	. 7908	1	10. 003
12·4·2	. 7811	1	10. 003
Average of last five lines			10. 002

Potassium Chromium Sulfate Dodecahydrate, $KCr(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0376	4. 31 3. 68 3. 26	Molybde-num.	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Vegard and Esp [2] 1928--	Chromi-um.	Kα

NBS sample. The sample of potassium chromium sulfate dodecahydrate was obtained from the General Chemical Co., New York, N. Y. The sample was recrystallized at the NBS from a water solution, dried, and protected from air with petrolatum. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of iron, magnesium, sodium, lead, rubidium, silicon, and vanadium; and 0.0001 to 0.001 percent each of barium, calcium, cesium, and lithium.

The sample has a violet color. The index of refraction is 1.482.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units, and the *d*-values of the Vegard and Esp pattern were calculated from Bragg angle data. The data of Vegard and Esp did not include intensity values.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel-----	220	311	321
Swanson, Gilfrich, and Cook-----	220	321	221

Structural data. Cork [3] in 1927 found potassium chromium sulfate dodecahydrate to be an alpha alum having space group T_h^6–Pa3, and $4[KCr(SO_4)_2 \cdot 12H_2O]$ per unit cell. The structure of the alpha alums was determined by Wyckoff [3] in 1923.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1917	Vegard and Schjelderup [5]-	11.95
1927	Cork [3]----------	12.16
1928	Vegard and Esp [2]-------	12.05
1935	Lipson and Beevers [6]----	12.196
1940	Klug and Alexander [7]----	12.200 at 25° C
1955	Menary [8]----------	12.204 at 24° C
1956	Swanson, Gilfrich, and Cook.	12.196 at 25° C

The density of potassium chromium sulfate dodecahydrate calculated from the NBS lattice constant is 1.828 at 25° C.

References

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

[2] L. Vegard and E. Esp, Über die Kristallstruktur der Alaune, Ann. Physik. **85,** 1152–1164 (1928).

[3] J. M. Cork, The crystal structure of some of the alums, Phil. Mag. **4,** 688–698 (1927).

[4] R. W. G. Wyckoff, The crystal structure of the alums, Z. Krist. **57,** 209–217 (1923).

[5] L. Vegard and H. Schjelderup, Die Kristallstruktur der Alaune und die Rolle des Kristallwasser, Ann. Physik. **54,** 146–164 (1917).

[6] H. Lipson and C. A. Beevers, The crystal structure of the alums, Proc. Roy. Soc. London **148** [A], 664–680 (1935).

[7] H. P. Klug and L. Alexander, Crystal-chemical studies of the alums. II. The purple chrome alums, J. Am. Chem. Soc. **62,** 2992–2993 (1940).

[8] J. W. Menary, Some lattice constants, Acta Cryst. **8,** 840 (1955).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1928 Vegard and Esp Cr, 2.2909 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	7. 0	12	12. 1	------	----	------	7. 0	19	12. 2
210	5. 5	16	12. 3	5. 36	----	12. 0	5. 45	28	12. 2
211	4. 99	8	12. 2	4. 90	----	12. 0	4. 973	14	12. 18
220	4. 31	100	12. 2	4. 29	----	12. 1	4. 312	100	12. 20
221	4. 09	30	12. 3	3. 99	----	12. 0	4. 060	40	12. 18
311	3. 69	60	12. 2	3. 63	----	12. 0	3. 670	32	12. 17
222	------	----	------	------	----	------	3. 516	8	12. 18
321	3. 27	35	12. 2	3. 21	----	12. 0	3. 257	46	12. 19
400	3. 05	30	12. 2	3. 01	----	12. 1	3. 046	27	12. 19
410	------	----	------	2. 92	----	12. 0	2. 956	16	12. 19

Potassium Chromium Sulfate Dodecahydrate, $KCr(SO_4)_2 \cdot 12H_2O$ (cubic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1928 Vegard and Esp Cr, 2.2909 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
411	2.88	2	12.2	2.84	----	12.1	2.872	10	12.19
331	2.82	12	12.3	2.76	----	12.0	2.796	19	12.19
420	2.73	12	12.2	2.70	----	12.0	2.725	18	12.19
421	------	----	------	2.63	----	12.1	2.667	10	12.21
332	2.60	6	12.2	2.57	----	12.0	2.598	9	12.19
422	2.49	12	12.2	2.46	----	12.0	2.488	14	12.19
------	------	----	------	2.37	----	------	--------	----	--------
511	2.34	6	12.2	2.32	----	12.1	2.347	9	12.19
432	2.25	6	12.1	2.24	----	12.1	2.2657	6	12.20
------	------	----	------	2.20	----	------	--------	----	--------
440	2.15	4	12.2	------	----	------	2.1552	5	12.192
522	------	----	------	2.10	----	12.1	2.1223	6	12.192
433	------	----	------	------	----	------	2.0910	3	12.193
531	------	----	------	------	----	------	2.0620	7	12.199
600	2.03	12	12.2	2.02	----	12.1	2.0329	12	12.197
610	------	----	------	1.99	----	12.1	2.0043	6	12.192
611	1.97	6	12.1	1.96	----	12.1	1.9786	5	12.197
620	1.93	16	12.2	1.92	----	12.1	1.9290	17	12.200
541	------	----	------	------	----	------	1.8805	1	12.187
533	1.85	4	12.1	1.84	----	12.1	1.8592	3	12.192
622	------	----	------	------	----	------	1.8370	9	12.185
630	------	----	------	------	----	------	1.8174	2	12.195
------	------	----	------	1.785	----	------	--------	----	--------
444	1.74	4	12.1	------	----	------	1.7590	1	12.187
543	------	----	------	------	----	------	1.7235	4	12.187
711	------	----	------	------	----	----	1.7072	3	12.192
640	1.69	8	12.2	1.683	----	12.14	1.6908	5	12.193
642	1.63	10	12.2	1.623	----	12.14	1.6287	9	12.188
722	------	----	------	1.609	----	12.13	1.6148	4	12.192
731	------	----	------	1.581	----	12.14	1.5873	2	12.192
732	------	----	------	1.544	----	12.16	1.5483	1	12.191
811	------	----	------	------	----	------	1.5010	2	12.194
820	------	----	------	1.473	----	12.15	1.4807	9	12.210
822	------	----	------	1.435	----	12.18	1.4361	2	12.191
751	------	----	------	------	----	------	1.4078	1	12.192
662	------	----	------	------	----	------	1.3977	<1	12.185
832	------	----	------	------	----	------	1.3892	<1	12.190
841	------	----	------	------	----	------	1.3549	<1	12.194
664	------	----	------	------	----	------	1.2996	1	12.191
922	------	----	------	------	----	------	1.2926	1	12.194
851	------	----	------	------	----	------	1.2849	1	12.190
844	------	----	------	------	----	------	1.2447	<1	12.196
933	------	----	------	------	----	------	1.2260	1	12.199
10·2·0	------	----	------	------	----	------	1.1957	1	12.194
10·2·2	------	----	------	------	----	------	1.1732	<1	12.192
962	------	----	------	------	----	------	1.1087	1	12.196
11·1·1	------	----	------	------	----	------	1.1002	1	12.202
11·2·1	------	----	------	------	----	------	1.0863	<1	12.194
10·6·0	------	----	------	------	----	------	1.0457	1	12.195
10·6·2	------	----	------	------	----	------	1.0303	1	12.191
12·1·1	------	----	------	------	----	------	1.0093	<1	12.195
11·5·1	------	----	------	------	----	------	1.0063	1	12.201
12·2·2	------	----	------	------	----	------	0.9890	<1	12.193
11·5·3	------	----	------	------	----	------	.9795	1	12.195
12·4·2	------	----	------	------	----	------	.9523	<1	12.195
10·8·2	------	----	------	------	----	------	.9408	<1	12.194
Average of last five lines	-------		12.2	------	----	12.15	--------	----	12.196

Potassium Fluogermanate, K_2GeF_6 (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium fluogermanate was prepared at the NBS from potassium chloride, germanium oxide and hydrofluoric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of sodium and silicon; 0.001 to 0.01 percent each of aluminum, barium, calcium, and rubidium; and 0.0001 to 0.001 percent each of silver, copper, iron, magnesium, and strontium.

The sample is colorless, and optically negative. The indices of refraction are too low to be determined by the conventional grain immersion method.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	101	201	100

Structural data. Hoard and Vincent [1] in 1939 determined that potassium fluogermanate has cadmium iodide-type structure, the space group D^3_d–$P\bar{3}m1$, and $1(K_2GeF_6)$ per unit hexagonal cell, or $3(K_2GeF_6)$ per unit rhombohedral cell.

The unit-cell values reported by Hoard and Vincent have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1939	Hoard and Vincent [1]	5. 63	4. 66
1956	Swanson, Gilfrich, and Cook.	5. 632	4.668 at 25° C.

The density of potassium fluogermanate calculated from the NBS lattice constants is 3.428 at 25° C.

References

[1] J. L. Hoard and W. B. Vincent, Structures of complex fluorides. Potassium hexafluogermanate and ammonia hexafluogermanate, J. Am. Chem. Soc. **61,** 2849–2852 (1939).

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*
	A	
100	4. 89	56
001	4. 667	25
101	3. 371	100
110	2. 815	40
111	2. 410	8
002	2. 333	6
201	2. 161	62
102	2. 105	19
210	1. 844	<1
112	1. 797	3
211	1. 715	15
202	1. 686	16
300	1. 6260	7
003	1. 5558	1
301	1. 5352	<1
103	1. 4826	1
212	1. 4467	11
220	1. 4084	10
113	1. 3620	9
203	1. 3118	6
311	1. 2995	4
222	1. 2060	<1
213	1. 1897	<1
401	1. 1801	4
312	1. 1705	<1
004	1. 1670	4
104	1. 1348	4
303	1. 1240	4
321	1. 0883	1
402	1. 0806	2
114	1. 0782	1
410	1. 0644	<1
204	1. 0525	<1
223	1. 0442	<1
313	1. 0214	<1
322	1. 0086	<1
214	0. 9860	1
403	. 9598	<1
304	. 9484	<1
005	. 9336	1
105	. 9170	5
421	. 9041	1
502	. 9000	<1
224	. 8983	<1
314	. 8836	<1
413	. 8784	1
205	. 8716	<1
511	. 8610	<1
422	. 8574	<1
215	. 8329	2
512	. 8203	1
600	. 8130	<1
324	. 8077	<1
333	. 8038	<1
423	. 7930	<1

Potassium Fluoplatinate, K_2PtF_6 (trigonal)

ASTM cards. None.

Additional published patterns

Source	Radiation	Wavelength
Mellor and Stephenson [1]	Copper	1. 54

NBS sample. The sample of potassium fluoplatinate used for the NBS pattern was prepared by T. P. Perros, George Washington University, Washington, D. C. The potassium content of this sample was observed by flame spectrometer analysis at George Washington University to be 20.2 percent. The computed theoretical value is 20.18.

The sample has a yellow color and is optically negative. The indices of refraction are N_o–1.528 and N_e–1.500.

Interplanar spacings and intensity measurements. The *d*-values for the Mellor and Stephenson pattern were obtained from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Mellor and Stephenson [1]	101	100	201
Swanson, Gilfrich, and Cook	101	100	110

Structural data. Mellor and Stephenson [1] in 1951 determined that potassium fluoplatinate has potassium fluogermanate-type structure, the space group D_{3d}^3—$P\bar{3}m1$, and $1(K_2PtF_6)$ per unit hexagonal cell, or $3(K_2PtF_6)$ per unit rhombohedral cell.

Two unit-cell measurements given in angstrom units are compared with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1951	Mellor and Stephenson [1].	5. 76	4. 64
1953	Sharpe [2]	5. 76	4. 64
1956	Swanson, Gilfrich, and Cook.	5. 778	4. 635 at 25° C

The density of potassium fluoplatinate calculated from the NBS lattice constants is 4.800 at 25° C.

References

[1] D. P. Mellor and N. C. Stephenson, The crystal structure of potassium hexafluoroplatinate, Aust. J. Sci. Research. **A4,** 406–11 (1951).

[2] A. G. Sharpe, The chemistry of platinum metals. Part II. Fluoropalladates and fluoroplatinates, J. Chem. Soc. **1953,** 197–9.

hkl	1951 Mellor and Stephenson Cu, 1.540 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
100	5. 03	s	5. 01	97
001	4. 65	ms	4. 62	34
101	3. 40	vs	3. 40	100
110	2. 88	ms	2. 889	47
200	------	----	2. 501	6
111	------	----	2. 450	23
201	2. 20	s	2. 201	40
102	2. 10	s	2. 102	24
210	1. 889	w	1. 890	11
112	1. 806	w	1. 807	8
211	1. 748	ms	1. 7502	23
202	1. 698	ms	1. 6995	16
300	1. 665	w	1. 6676	7
301	1. 568	w	1. 5690	5
003	1. 541	vw	1. 5449	2
103	1. 474	vw	1. 4758	4
212	1. 464	ms	1. 4652	12
220	1. 445	ms	1. 4441	8
310	1. 389	vw	1. 3879	5
221	1. 378	vw	1. 3785	6
113	1. 363	ms	1. 3623	7
302	------	----	1. 3537	2
311	------	----	1. 3293	8
203	1. 315	ms	1. 3144	3
401	1. 208	w	1. 2081	4
213	1. 197	vw	1. 1968	5
312	1. 190	w	1. 1906	5
004	------	----	1. 1591	2
303	------	----	1. 1335	4
104	------	----	1. 1291	4
321	1. 114	w+	1. 1141	5
402	1. 101	w+	1. 1007	5
410	1. 092	w+	1. 0921	4
114	------	----	1. 0757	2
411	------	----	1. 0626	1
223	------	----	1. 0551	4
204	------	----	1. 0518	2
313	------	----	1. 0327	3
322	------	----	1. 0287	4
214	0. 988	s	0. 9881	4
501	------	----	. 9783	3
304	------	----	. 9518	1
005	------	----	. 9272	4
502	. 918	vw	. 9188	2
105	------	----	. 9116	2
224	. 904	w	. 9040	2
413	------	----	. 8918	5
314 / 332	. 890	s	. 8897	6
115 / 511	. 883	vw	. 8821	4
422	------	----	. 8756	3
205	. 870	vw	. 8696	3
512	------	----	. 8381	4
215	------	----	. 8327	3
324	------	----	. 8158	1
305	------	----	. 8104	1
423	------	----	. 8067	2
520	------	----	. 8016	2
414	------	----	. 7949	2
521	------	----	. 7897	4

Potassium Perchlorate, $KClO_4$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0589	3. 48 3. 13 2. 88	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

A pattern for the cubic form of potassium perchlorate is reported on ASTM card 2–0326.

Additional published patterns. None.

NBS sample. The sample of potassium perchlorate was obtained from the City Chemical Corp., New York, N. Y. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of barium and rubidium; 0.001 to 0.01 percent each of aluminum, molybdenum, lead, and silicon; and 0.0001 to 0.001 percent each of calcium, iron, lithium, and magnesium.

The sample is colorless and optically positive with the indices of refraction $\alpha = 1{\cdot}472$, $\beta = 1{\cdot}473$, and $\gamma = 1.476$. $2V \cong 50°$.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	210	211	112
Swanson, Gilfrich, and Cook	210	211	112

Structural data. Basche and Mark [4] in 1926 determined that potassium perchlorate has barium sulfate-type structure, the space group D_{2h}^{16}–Pnma, and $4(KClO_4)$ per unit cell.

The cubic form of potassium perchlorate has been reported as being stable from 300° to 400° C by Herrmann and Ilge [2] and Braekken and Harang [3].

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
101	5. 6	8	5. 61	13
011	4. 45	29	4. 47	30
200			4. 42	9
111	4. 01	2	3. 98	<1
201	3. 79	2	3. 78	13
002	3. 63	20	3. 629	29
210	3. 49	100	3. 487	100
102	3. 35	16	3. 359	31
211	3. 14	100	3. 145	78
112	2. 89	80	2. 890	67
020	2. 82	20	2. 831	28
202			2. 809	6
301	------	----	2. 733	<1
121	2. 52	50	2. 528	14
212			2. 515	19
220	2. 38	2	2. 385	3
302	------	----	2. 290	6
221	2. 26	8	2. 267	8
400	------	----	2. 215	3
122	2. 16	50	2. 167	24
113			2. 158	22
312	------	----	2. 123	7
401	2. 11	40	2. 118	25
410	2. 05	2	2. 063	4
321	------	----	1. 967	3
402	------	----	1. 891	1
303	1. 86	8	1. 870	4
004	------	----	1. 813	1
123	------	----	1. 800	4
412	------	----	1. 792	<1
313	1. 78	6B	1. 776	6
420	1. 73	2	1. 743	2
114	1. 68	12	1. 696	6
511	1. 64	20	1. 646	7
403	------	----	1. 633	3
323	1. 55	8	1. 560	5
024	------	----	1. 528	<1
124	------	----	1. 506	2
521	------	----	1. 470	1
610	------	----	1. 428	2
423	------	----	1. 416	<1
611	------	----	1. 402	2
513	------	----	1. 386	2
324	------	----	1. 356	2
215	------	----	1. 339	<1
523	------	----	1. 275	2

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1926	Basche and Mark [4].	8. 86	5. 66	7. 24
1928	Büssem and Herrmann [5].	8. 87	5. 67	7. 25
1932	Gottfried and Schusterius [6].	8. 852	5. 661	7. 255
1940	Greenberg and Waldon [7].	8. 8552	5. 6635	7. 2547 at 23 to 29° C.
1956	Swanson, Gilfrich, and Cook.	8. 857	5. 663	7. 254 at 25° C.

The density of potassium perchlorate calculated from the NBS lattice constants is 2.529 at 25° C.

References

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

[2] K. Herrmann and W. Ilge, Röntgenographische Strukturerforschung der kubischen Modifikation der Perchlorate, Z. Krist. **75,** 41–65 (1930).

[3] H. Braekken and L. Harang, Die kubische Hochtemperaturstruktur einiger Perchlorate, Z. Krist. **75,** 538–549 (1930).

[4] W. Basche and H. Mark, Über die Struktur von Verbindungen des Typus $MeXO_4$, Z. Krist. **64,** 1–70 (1926).

[5] W. Büssem and H. Herrmann, Strukturuntersuchung des Silberpermanganats, Z. Krist. **74,** 458–568 (1930).

[6] C. Gottfried and C. Schusterius, Die Struktur von Kaliumund Ammoniumperchlorat, Z. Krist. **84,** 65–73 (1932).

[7] A. L. Greenberg and G. H. Walden, Studies of equilibrium solid solutions of ionic lattices. Systems: $KMnO_4$-$KClO_4$-H_2O and NH_4Cl-$MnCl_2$-H_2O, J. Chem. Phys. **8,** 645 (1940).

Rubidium Aluminum Sulfate Dodecahydrate, $RbAl(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0372	4. 34 2. 81 3. 28	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation	Wavelength
Cork [2] 1927	--------	---------

NBS sample. The sample of rubidium aluminum sulfate dodecahydrate was prepared at the NBS from rubidium sulfate and aluminum sulfate. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of cesium and potassium; 0.001 to 0.01 percent each of barium, magnesium, lead, and silicon; and 0.0001 to 0.001 percent each of silver, calcium, chromium, iron, lithium, manganese, and sodium.

The sample is colorless. The index of refraction is 1.454.

Interplanar spacings and intensity measurements. The *d*-values of the Cork pattern were calculated from Bragg angle data and the *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	220	331	321
Cork	400	220	533
Swanson, Gilfrich, and Cook	220	331	321

Structural data. Cork [2] in 1927 found rubidium aluminum sulfate dodecahydrate to be an alpha alum having space group T_h^6–Pa3, and $4[RbAl(SO_4)_2 \cdot 12H_2O]$ per unit cell. The structure of the alpha alums was determined by Wyckoff [3] in 1923.

Two unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1927	Cork [2]	12.22
1935	Lipson and Beevers [4]	12.245
1956	Swanson, Gilfrich, and Cook.	12.243 at 25° C

The density of rubidium aluminum sulfate dodecahydrate calculated from the NBS lattice constant is 1.885 at 25° C.

Ref erences

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

[2] J. M. Cork, The crystal structure of the alums, Phil. Mag. **4,** 688–698 (1927).

[3] R. W. G. Wyckoff, The crystal structure of the alums, Am. J. Sci. **5,** 209–217 (1923).

[4] H. Lipson and C. A. Beevers, The crystal structure of the alums, Proc. Roy. Soc. London **148** [A], 664–680 (1935).

Rubidium Aluminum Sulfate Dodecahydrate, $RbAl(SO_4)_2 \cdot 12H_2O$ (cubic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1927 Cork Mo, 0.7107 A			1956 Swanson Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
111	------	--	------	7. 20	4	12. 5	7. 06	3	12. 23
200	------	--	------	6. 14	7	12. 3	6. 12	8	12. 24
210	5. 5	27	12. 3	------	----	------	5. 47	23	12. 22
211	5. 0	10	12. 2	------	----	------	4. 995	12	12. 22
220	4. 35	100	12. 30	4. 32	84	12. 2	4. 329	100	12. 24
221	4. 10	23	12. 30	------	----	------	4. 079	24	12. 24
222	------	--	------	3. 56	13	12. 3	3. 532	6	12. 24
302	------	--	------	------	----	------	3. 391	3	12. 23
321	3. 29	50	12. 31	------	----	------	3. 271	36	12. 24
400	3. 08	33	12. 32	3. 059	100	12. 24	3. 060	22	12. 24
410	------	--	------	------	----	------	2. 968	7	12. 24
411	------	--	------	------	----	------	2. 886	6	12. 22
331	2. 82	67	12. 29	------	----	------	2. 809	45	12. 24
420	2. 74	13	12. 24	------	----	------	2. 736	22	12. 24
421	------	--	------	------	----	------	2. 672	5	12. 22
332	2. 63	13	12. 25	------	----	------	2. 611	6	12. 25
422	2. 51	23	12. 30	------	----	------	2. 501	1	12. 25
431	2. 36	23	------	2. 382	35	------	2. 398	11	12. 22
511							2. 355	11	12. 24
502	2. 26	3	------	------	----	------	2. 274	2	12. 25
521							2. 239	4	12. 26
440	2. 16	3	------	2. 160	10	------	2. 166	1	12. 25
522							2. 132	4	12. 25
433	------	--	------	------	----	------	2. 099	<1	12. 24
531	------	--	------	------	----	------	2. 071	1	12. 25
600	2. 04	17	12. 24	------	----	------	2. 042	8	12. 25
610	------	--	------	------	----	------	2. 014	3	12. 25
611	1. 99	33	12. 27	------	----	------	1. 986	4	12. 24
620	------	--	------	------	----	------	1. 938	13	12. 25
533	1. 87	13	12. 26	1. 861	54	12. 20	1. 867	7	12. 25
622	------	--	------	------	----	------	1. 846	4	12. 25
630	------	--	------	------	----	------	1. 825	<1	12. 24
631	------	--	------	1. 793	3	12. 16	1. 803	1	12. 23
444	------	--	------	------	----	------	1. 769	1	12. 23
543	------	--	------	------	----	------	1. 732	1	12. 25
711	1. 70	13	------	------	----	------	1. 715	3	12. 25
640							1. 698	5	12. 25
702	------	--	------	------	----	------	1. 683	<1	12. 25
721	------	--	------	------	----	------	1. 666	<1	12. 24
642	1. 64	27	12. 27	------	----	------	1. 636	9	12. 25
722	------	--	------	------	----	------	1. 622	3	12. 25
731	------	--	------	------	----	------	1. 595	2	12. 25
-------	------	--	------	1. 533	2	------	---------	----	---------
820	1. 491	20	12. 30	------	----	------	1. 485	6	12. 247
822	------	--	------	1. 441	18	12. 23	1. 443	4	12. 245
-------	------	--	------	1. 432	3	------	---------	----	---------
-------	1. 413	3	------	------	----	------	---------	----	---------
840	1. 368	3	12. 24	------	----	------	1. 3686	2	12. 241
841	------	--	------	------	----	------	1. 3600	1	12. 240
911	------	--	------	------	----	------	1. 3440	1	12. 244
902	1. 332	3	12. 28	------	----	------	1. 3284	<1	12. 247
664	1. 305 [a]	3	12. 24	1. 308 [b]	6	12. 27	1. 3052	1	12. 244
Average of last five lines			12. 27	------	----	12. 21	---------	----	12. 243

[a] One additional line was omitted. [b] Eight additional lines were omitted.

Rubidium Chlorostannate, Rb_2SnCl_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium chlorostannate was precipitated from rubidium chloride and stannic chloride solutions by hydrochloric acid. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of potassium;[5] 0.01 to 0.1 percent each of aluminum, sodium, and silicon; 0.001 to 0.01 percent each of calcium, iron, and magnesium; and 0.0001 to 0.001 percent each of barium, chromium, copper, manganese, and strontium.

The sample is colorless. The index of refraction is 1.665.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	220	111	400

Structural data. Engel [1] in 1933 determined that rubidium chlorostannate has potassium chloroplatinate-type structure, the space group O_h^5–Fm3m, and 4(Rb_2SnCl_6) per unit cell.

The unit-cell measurement reported by Engel has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1935	Engel [1]	10.120
1956	Swanson, Gilfrich, and Cook.	10.118 at 25° C

The density of rubidum chlorostannate calculated from the NBS lattice constant is 3.221 at 25° C.

References

[1] G. Engel, Die Kristallstruktur einiger Verbindungen vom K_2PtCl_6–Typ, Naturwissenschaften **21,** 704 (1933).

[5] This amount of potassium can be expected to enter into solid solution with the rubidium compound decreasing the size of the cell by not more than one-thousandth of an angstrom.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25°C		
	d	*I*	*a*
	A		A
111	5. 84	90	10. 11
200	5. 06	4	10. 12
220	3. 58	100	10. 12
311	3. 051	42	10. 12
222	2. 919	63	10. 11
400	2. 529	87	10. 11
331	2. 322	14	10. 12
422	2. 066	40	10. 12
511	1. 948	18	10. 12
440	1. 7885	54	10. 117
531	1. 7095	17	10. 114
620	1. 5999	14	10. 119
533	1. 5428	5	10. 117
622	1. 5253	12	10. 118
444	1. 4600	15	10. 115
711	1. 4163	8	10. 114
642	1. 3518	14	10. 116
731	1. 3170	6	10. 116
800	1. 2648	6	10. 118
822	1. 1922	6	10. 116
751	1. 1682	3	10. 117
662	1. 1604	1	10. 116
840	1. 1314	10	10. 120
911	1. 1106	4	10. 118
664	1. 0786	3	10. 118
931	1. 0606	3	10. 118
844	1. 0326	7	10. 116
933	1. 0169	4	10. 118
10·2·0	0. 9921	5	10. 118
951	. 9782	4	10. 119
10·2·2	. 9736	1	10. 118
953	. 9435	2	10. 118
10·4·2	. 9236	3	10. 118
880	. 8943	1	10. 118
11·3·1	. 8840	2	10. 118
10·6·0	. 8676	3	10. 118
11·3·3	. 8582	3	10. 118
12·0·0	. 8431	5	10. 117
12·2·2	. 8206	4	10. 117
11·5·3	. 8127	1	10. 118
12·4·0	. 7999	4	10. 118
10·8·2	. 7806	2	10. 118
Average value of last five lines			10. 118

Rubidium Chromium Sulfate Dodecahydrate, $RbCr(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium chromium sulfate dodecahydrate was prepared at the NBS from rubidium sulfate and chromium sulfate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of nickel; 0.001 to 0.01 percent each of aluminum, calcium, magnesium, sodium, and silicon; and 0.0001 to 0.001 percent each of barium, copper, and iron.

The sample has a pale lavender color. The index of refraction is 1.481.

Interplanar spacings and intensity measurements. The three strongest lines for the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	220	321	331

Structural data. Klug and Alexander [2] in 1940 found rubidium chromium sulfate dodecahydrate to be a beta alum having the space group T_h^6–Pa3, and $4[RbCr(SO_4)_2 \cdot 12H_2O]$ per unit cell. The structure of the beta alums was determined by Lipson [1] in 1935.

The unit-cell measurement reported by Klug and Alexander has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1940	Klug and Alexander [2]	12.281 at 25° C
1956	Swanson, Gilfrich, and Cook.	12.279 at 25° C

The density of rubidium chromium sulfate dodecahydrate calculated from the NBS lattice constant is 1.958 at 25° C.

References

[1] H. Lipson, Existence of three alum structures, Nature, **135**, 912 (1935).

[2] H. P. Klug and L. Alexander, Crystal-chemical studies of the alums. II. The purple chrome alums, J. Am. Chem. Soc. **62**, 2992–2993 (1940).

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
200	6. 13	16	12. 3
210	5. 49	24	12. 3
211	5. 01	13	12. 3
220	4. 342	100	12. 28
221	4. 088	22	12. 26
222	3. 545	10	12. 28
321	3. 282	32	12. 28
400	3. 069	29	12. 28
410	2. 976	9	12. 27
331	2. 818	30	12. 29
420	2. 745	25	12. 28
421	2. 678	7	12. 27
332	2. 620	6	12. 29
422	2. 506	20	12. 28
511	2. 363	4	12. 28
440	2. 171	6	12. 28
522	2. 139	3	12. 29
600	2. 048	13	12. 29
610	2. 018	4	12. 27
611	1. 991	2	12. 28
620	1. 942	19	12. 28
533	1. 873	5	12. 28
622	1. 851	6	12. 28
630	1. 829	2	12. 27
631	1. 810	3	12. 28
444	1. 771	4	12. 27
543	1. 737	3	12. 28
640	1. 703	8	12. 28
642	1. 642	11	12. 29
722	1. 627	3	12. 28
732	1. 559	1	12. 27
820	1. 4890	9	12. 279
653	1. 4675	5	12. 278
622	1. 4082	4	12. 276
840	1. 3725	5	12. 276
841	1. 3647	4	12. 282
842	1. 3397	1	12. 279
664	1. 3090	2	12. 280
Average of last five lines			12. 279

Rubidium Fluoplatinate, Rb_2PtF_6 (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium fluoplatinate used for the NBS pattern was prepared by T. P. Perros, George Washington University, Washington, D. C. The rubidium content of this sample was found by flame spectrometer analysis at George Washington University to be 35.5 percent. The computed theoretical value is 35.60 percent.

The sample has a yellow color and is optically negative. The indices of refraction N_o–1.542 and N_e–1.512.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	101	110	201

Structural data. Mellor and Stephenson [1] in 1951 determined that rubidium fluoplatinate has potassium fluogermanate-type structure, the space group D^3_{3d}–$P\bar{3}m1$, and $1(Rb_2PtF_6)$ per unit hexagonal cell, or $3(Rb_2PtF_6)1$ per unit rhombohedral cell.

The unit-cell measurements reported by Sharpe [2] are given in angstrom units.

Lattice constants

		a	*c*
		A	*A*
1953	Sharpe [2]	5. 96	4. 83
1956	Swanson, Gilfrich, and Cook.	5. 954	4.805 at 25° C

The density of the rubidium fluoplatinate calculated from the NBS lattice constants is 5.404 at 25° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*
	A	
100	5. 16	41
001	4. 81	24
101	3. 517	100
110	2. 978	58
200	2. 579	3
111	2. 532	12
002	2. 404	6
201	2. 273	42
102	2. 178	25
210	1. 950	4
112	1. 870	4
211	1. 806	20
202	1. 758	16
300	1. 718	10
301	1. 6184	4
003	1. 6016	4
103	1. 5299	3
212	1. 5131	12
220	1. 4884	8
113	1. 4104	8
302	1. 3985	2
311	1. 3710	8
203	1. 3606	2
400	1. 2898	2
401	1. 2453	2
213	1. 2373	4
312	1. 2290	2
004	1. 2013	3
303	1. 1715	4
104	1. 1696	2
321	1. 1485	3
402	1. 1362	2
410	1. 1253	2
114	1. 1142	3
411	1. 0960	<1
223	1. 0902	3
204	1. 0883	<1
313	1. 0665	<1
322	1. 0613	2
214	1. 0226	1
501	1. 0084	1
403	1. 0043	1
304	0. 9845	1
421	. 9548	2
105	. 9448	3
224	. 9346	1
413	. 9204	4
511	. 9094	<1
422	. 9029	<1
205	. 9005	1
404	. 8790	<1
512	. 8639	1
215	. 8619	2
600	. 8593	2
324	. 8429	1
423	. 8324	1
414	. 8210	1
432	. 7990	1
315	. 7975	2
106	. 7912	2

References

[1] D. P. Mellor and N. C. Stephenson, The crystal structure of potassium hexafluoroplatinate, Aust. J. Sci. Research. **A4**, 406–11 (1951).

[2] A. G. Sharpe, The chemistry of platinum metals. Part II. Fluoropalladates and fluoroplatinates, J. Chem. Soc. **1953**, 197–199.

Rubidium Fluosilicate, Rb_2SiF_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium fluosilicate was prepared at the NBS from rubidium chloride, silica gel, and hydrofluoric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of potassium, cesium, and sodium; 0.001 to 0.01 percent each of aluminum, calcium, and iron; and 0.0001 to 0.001 percent each of barium, lead, and magnesium.

The sample is colorless. The index of refraction is too low to be determined by the conventional liquid grain immersion method.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	220	222	111

Structural data. Ketelaar [1] in 1935 determined that rubidium fluosilicate has potassium chloroplatinate-type structure, the space group O_h^5–Fm3m, and $4(Rb_2SiF_6)$ per unit cell.

The unit-cell measurement reported by Ketelaar has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1935	Ketelaar [1]	8.463
1956	Swanson, Gilfrich, and Cook.	8.452 at 25° C

The density of rubidium fluosilicate calculated from the NBS lattice constant is 3.443 at 25° C.

References

[1] J. A. A. Ketelaar, Die Kristallstruktur von K-, Rb-, Cs- und Tl- Silico fluorid und von $LiMnO_4 \cdot 3H_2O$, Z. Krist. **92,** 155–156 (1935).

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	4. 89	48	8. 46
200	4. 287	37	8. 457
220	2. 989	100	8. 453
311	2. 547	3	8. 448
222	2. 441	68	8. 455
400	2. 113	48	8. 454
331	1. 940	<1	8. 457
420	1. 890	25	8. 452
422	1. 725	29	8. 451
511	1. 627	8	8. 452
440	1. 494	17	8. 451
531	1. 428	2	8. 451
600	1. 4088	9	8. 453
620	1. 3360	15	8. 450
622	1. 2740	9	8. 451
444	1. 2197	5	8. 450
711	1. 1833	3	8. 450
640	1. 1717	3	8. 449
642	1. 1293	11	8. 451
731	1. 1006	<1	8. 454
800	1. 0565	2	8. 452
820	1. 0250	4	8. 452
822	0. 9962	4	8. 453
751	. 9759	<1	8. 452
662	. 9694	1	8. 451
840	. 9451	4	8. 453
842	. 9222	4	8. 452
662	. 9008	3	8. 450
844	. 8626	3	8. 452
10·2·0	. 8289	6	8. 453
10·2·2	. 8134	<1	8. 453
10·4·0	. 7847	2	8. 452
Average of last five lines			8. 452

Sodium Nitrate (soda-niter), $NaNO_3$ (trigonal)

ASTM cards

Card numbers	Index	Radiation	Source
1–0840	3. 03 2. 31 1. 89	Molybde-num.	Hanawalt, Rinn, and Frevel [1] 1938.
3–1324	[a]	[a]	Wyckoff [2] 1920.

[a] No powder data.

Additional published patterns

Source	Radiation	Wavelength
Kracek, Posnjak, and Hendricks [3] 1931.	Molybdenum	K_α
Bijvoet and Ketelaar [4] 1932.	Iron	

NBS sample. The sample of sodium nitrate was obtained from the Allied Chemical and Dye Corp., New York, N. Y. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of potassium; 0.001 to 0.01 percent each of aluminum and silicon; and 0.0001 to 0.001 percent each of barium, calcium, iron, lithium, and magnesium.

The sample is colorless and optically negative. The indices of refraction are $N_o = 1.608$. The N_e is too low to be determined by the conventional liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units and the *d*-values of the Kracek, Posnjak, and Hendricks, and the Bijvoet and Ketelaar patterns were calculated from Bragg angle data.

The three strongest lines of each of the patterns are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	104	113	018, 116
Kracek, Posnjak, and Hendricks.	104	018	113
Bijovoet and Ketelaar	104	018	110
Swanson, Gilfrich, and Cook	104	113	018

Structural data. Bragg [5] in 1914 determined that sodim nitrate has the space group D^6_{3d}–$R\bar{3}c$ and $2(NaNO_3)$ per unit rhombohedral cell, or $6(NaNO_3)$ per unit hexagonal cell. Sodium nitrate is used as a structure-type.

The rhombohedral cell measurements reported by Wyckoff and Kracek, Posnjak, and Hendricks have been converted to hexagonal values and all were converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1920	Wyckoff [2]	4. 86	16. 13
1931	Kracek, Posnjak, and Hendricks [3].	5. 06	16. 81 at 25° C.
1933	Weigle [6]	5. 064	16. 80 at 18° C.
1934	Saïm and Mercier [7]	5. 0702	16. 818 at 20° C.
1956	Swanson, Gilfrich, and Cook.	5. 0696	16. 829 at 25° C.

The density of sodium nitrate calcuated from the NBS lattice constants is 2.260 at 25° C.

References

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

[2] R. W. G. Wyckoff, The crystal structure of sodium nitrate, Phys. Rev. **16,** 149–157 (1920).

[3] F. C. Kracek, E. Posnjak, and S. B. Hendricks, Gradual transition in sodium nitrate. II. The structure at various temperatures and its bearing on molecular rotation, J. Am. Chem. Soc. **53,** 3339–3348 (1931).

[4] J. M. Bijvoet and J. A. A. Ketelaar, Note. Molecular rotation in solid sodium nitrate, J. Am. Chem. Soc. **54,** 625–628 (1932).

[5] W. L. Bragg, The analysis of crystals by the X-ray spectrometer, Proc. Roy. Soc. London **89,** 468–489 (1914).

[6] J. Weigle, Mesures de précision reseaux rhomboédriques: $NaNO_3$, Helv. Phys. Acta **7,** 46–50 (1933).

[7] H. Saïm and A. Mercier, Dealation thermique du nitrate de sodium mesuré aux rayons X, Helv. Phys. Acta **7,** 267–272 (1934).

Sodium Nitrate (soda-niter), $NaNO_3$ (trigonal)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1931 Kracek, Posnjak, and Hendricks Mo, 0.7107 A		1932 Bijvoet and Ketelaar Fe, ----------		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
012	3. 91	2	3. 88	20	3. 81	32	3. 89	6
104	3. 04	100	3. 04	>100	3. 00	>100	3. 03	100
006	2. 81	6	2. 81	40	2. 85	25	2. 81	15
110	2. 54	6	2. 54	30	2. 46	34	2. 53	9
113	2. 31	30	2. 31	50–70	2. 26	<5	2. 311	24
202	2. 11	8	2. 13	40	2. 07	24	2. 125	9
024	1. 94	2	1. 946	10	------	----	1. 947	4
018	1. 89	25	1. 896	70	1. 90	77	1. 898	16
116			1. 882	30	1. 86	22	1. 880	7
211	1. 65	7	1. 653	30	------	----	1. 652	4
122	1. 63	4	1. 630	20	1. 60	<5	1. 629	4
214	1. 54	3	1. 539	10+	1. 58	12	1. 544	2
208	------	--	------	----	------	----	1. 519	<1
119	1. 50	1	1. 506	10	1. 50	11	1. 505	1
125	1. 493	3	1. 491	20	------	----	1. 4884	1
030	1. 464	6	1. 462	20	1. 45	<5	1. 4633	4
0·0·12	1. 403	2	1. 402	20	1. 41	12	1. 4018	1
217	1. 370	2	1. 367	20	------	----	1. 3652	<1
0·2·10	1. 335	1	1. 335	5	------	----	1. 3360	<1
128	1. 303	2	1. 301	10	1. 28	5	1. 3035	<1
220	1. 268	1	1. 268	5	------	----	1. 2682	<1
1·1·12	1. 226	1	1. 227	10	1. 22	5–10	1. 2268	<1
------	------	--	1. 224	5	------	----	------	----
2·1·10	------	--	1. 187	30	------	----	1. 1812	<1
134	1. 172	4	------	----	------	----	1. 1698	1
226	------	--	------	----	1. 14	11	1. 1558	<1
1·2·11	------	--	1. 124	5	------	----	1. 1244	<1
042	------	--	1. 088	5	------	----	1. 0881	<1
404	------	--	1. 063	5	------	----	1. 0620	1
2·0·14	------	--	1. 056	20	------	----	1. 0546	<1
318	------	--	------	----	------	----	1. 0540	1
1·0·16	------	--	------	----	1. 032	11	1. 0229	<1
3·0·12	------	--	------	----	------	----	1. 0126	<1
324	------	--	------	----	------	----	0. 9796	<1
1·2·14	------	--	------	----	------	----	. 9738	<1
048	------	--	------	----	------	----	. 9731	<1
140	------	--	------	----	------	----	. 9581	<1
0·2·16	------	--	------	----	------	----	. 9487	<1
2·2·12	------	--	------	----	------	----	. 9406	<1
327	------	--	------	----	------	----	. 9288	<1
4·0·10	------	--	------	----	------	----	. 9194	<1
238	------	--	------	----	------	----	. 9084	<1
2·1·16	------	--	------	----	------	----	. 8884	<1

Strontium Peroxide, SrO_2 (tetragonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
3-0872	2. 51 1. 99 1. 86	Copper	Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward [1] 1935.
1-1113	2. 52 3. 13 2. 00	Molybdenum.	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns. None.

NBS sample. The sample of strontium peroxide was precipitated by adding sodium peroxide to a solution of strontium chloride. The precipitate was dried in an oven at about 150° C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of calcium; 0.001 to 0.01 percent each of silver, aluminum, barium, iron, magnesium, silicon, and tin; and 0.0001 to 0.001 percent each of boron, copper, manganese, and lead.

The sample is colorless. The particle size was too small to determine the indices of refraction by the conventional liquid grain immersion-method.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern and the *d*-values of the Benal, Djatlowa, Kasarnowsky, Reichstein, and Ward pattern were converted from kX to angstrom units.

The three strongest lines of each of the patterns are as follows:

Pattern	1	2	3
Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward.	200	202	113
Hanawalt, Rinn, and Frevel	200	111	202
Swanson, Gilfrich, and Cook	111	200	002

Structural data. Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward [1] in 1935 determined that strontium peroxide has calcium carbide-type structure, the space group D_{4h}^{17}–F4/mmm, and 4(SrO_2) per unit cell.

The unit-cell measurements reported by Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1935	Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward [1].	5. 03	6.56
1956	Swanson, Gilfrich, and Cook.	5. 0445	6.6161 at 24° C

The density of strontium peroxide calculated from the NBS lattice constants is 4.719 at 24° C.

hkl	1935 Bernal, Djatlowa, Kasarnowsky, Reichstein, and Ward Cu, 1.5418 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 24° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
002	3. 25	w	3. 31	40	3. 31	70
111	3. 09	m	3. 14	88	3. 14	100
200	2. 516	vs	2. 52	100	2. 52	96
202	1. 994	s	2. 00	50	2. 006	55
113	1. 866	s	1. 87	50	1. 876	49
220	1. 774	m	1. 78	15	1. 784	29
004	---	---	----	--	1. 654	4
222	---	---	1. 57	30	1. 570	22
131	1. 558	m	1. 55	30	1. 551	24
--	1. 542	m	----	--	----	--
204	1. 380	vvw	1. 378	5	1. 3832	7
133	1. 291	s	1. 293	35	1. 2928	21
400	1. 260	vvw	1. 263	5	1. 2609	7
115	1. 241	w	----	--	1. 2409	9
224	1. 214	vvw	1. 212	5	1. 2127	4
402	1. 176	w	1. 178	10	1. 1786	7
331	---	---	----	--	1. 1704	5
240	1. 126	w	1. 129	10	1. 1279	7
006	---	---	----	--	1. 1026	<1
242	1. 066	m	1. 068	10	1. 0676	7
333	---	---	1. 047	5	1. 0467	5
135	---	---	1. 017	10	1. 0184	9
206	---	---	----	--	1. 0106	2
404	0. 999 [a]	---	----	--	1. 0029	1
151	. 977	---	----	--	0. 9785	6
226	---	---	----	--	. 9379	4
244	. 931	---	----	--	. 9316	4
153	. 899	---	----	--	. 9025	6
440	---	---	----	--	. 8916	<1
335	---	---	----	--	. 8844	2
442	. 858	---	----	--	. 8607	4
351	---	---	----	--	. 8579	5
600	---	---	----	--	. 8409	<1
602	---	---	----	--	. 8149	3
137	---	---	----	--	. 8131	4
353	---	---	----	--	. 8055	7
260	---	---	----	--	. 7977	3

[a] Intensity values were not given for the following *d*-spacings.

References

[1] J. D. Bernal, E. Djatlowa, I. Kasarnowsky, S. Reichstein and A. G. Ward, The structure of strontium and barium peroxides SrO_2 and BaO_2, Z. Krist. **92,** 344–354 (1935).

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

Thallium Aluminum Sulfate Dodecahydrate, $TlAl(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of thallium aluminum sulfate dodecahydrate was prepared at the NBS from thallium nitrate and aluminum sulfate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of lead; 0.001 to 0.01 percent each of chromium, magnesium, palladium, and silicon; and 0.0001 to 0.001 percent each of barium, calcium, iron, and manganese.

The sample is colorless. The index of refraction is 1.501.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	220	331	111

Structural data. Lipson [1] in 1935 determined that thallium aluminum sulfate dodecahydrate was an alpha alum having the space group T_h^6–Pa 3 and $4[TlAl(SO_4)_2 \cdot 12H_2O]$ per unit cell. The structure of the alpha alums was determined by Wyckoff [2] in 1923.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1927	Cork [3]	12.23
1935	Lipson and Beevers [4]	12.231
1940	Klug and Alexander [5]	12.231 at 25° C
1956	Swanson, Gilfrich, and Cook.	12.230 at 25° C

The density of thallium aluminum sulfate dodecahydrate calculated from the NBS lattice constant is 2.322 at 25° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	7.06	39	12.24
200	6.12	31	12.24
210	5.47	10	12.24
211	5.00	6	12.24
220	4.32	100	12.23
221	4.079	13	12.24
311	3.688	31	12.23
222	3.532	20	12.24
321	3.269	19	12.23
400	3.060	28	12.24
410	2.968	6	12.24
411	2.884	4	12.24
331	2.807	60	12.24
420	2.736	35	12.24
421	2.668	4	12.23
332	2.608	4	12.23
422	2.500	28	12.25
511	2.354	26	12.23
432	2.271	2	12.23
440	2.163	7	12.24
522	2.129	2	12.23
433	2.098	2	12.23
531	2.067	13	12.23
600	2.039	18	12.23
611	1.983	2	12.22
620	1.934	20	12.23
533	1.865	13	12.23
622	1.843	9	12.23
444	1.766	3	12.22
543	1.729	1	12.22
711	1.713	5	12.23
640	1.696	9	12.23
642	1.634	14	12.23
722	1.620	5	12.23
731	1.592	7	12.23
733	1.494	3	12.23
820	1.484	9	12.24
822	1.4411	6	12.228
831	1.4209	2	12.223
751	1.4120	4	12.228
662	1.4026	5	12.228
832	1.3939	1	12.231
840	1.3670	3	12.227
911	1.3422	4	12.228
842	1.3344	3	12.230
664	1.3035	3	12.228
931	1.2822	3	12.231
844	1.2483	3	12.231
933	1.2291	2	12.229
Average of last five lines			12.230

References

[1] H. Lipson, The relation between the alum structures, Proc. Roy. Soc. London **151,** 347–356 (1935).

[2] R. W. G. Wyckoff, The crystal structure of the alums, Am. J. Sci. **5,** 209–217 (1923).

[3] J. M. Cork, The crystal structure of some of the alums, Phil. Mag. **4,** 688–698 (1927).

[4] H. Lipson and C. A. Beevers, The crystal structure of the alums, Proc. Roy. Sci. London **148,** 664–680 (1935).

[5] H. P. Klug and L. Alexander, Crystal-chemical studies of the alums. III. Further solid solution studies, J. Am. Chem. Soc. **62,** 2993–2995 (1940).

Thallium Chlorostannate, Tl_2SnCl_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of thallium chlorostannate was precipitated from thallium chloride and tin chloride solutions by hydrochloric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, cobalt, sodium, and silicon; 0.001 to 0.01 percent each of aluminum, barium, and magnesium; and 0.0001 to 0.001 percent each of boron, copper, iron, and lead.

The sample is colorless. The index of refraction is 1.886.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	220	222	400

Structural data. Engel [1] in 1935 determined that thallium chlorostannate has potassium chloroplatinate-type structure, the space group O_h^5—Fm3m, and $4(Tl_2SnCl_6)$ per unit cell.

The unit-cell measurement reported by Engel has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1934	Engel [1]	9.990
1956	Swanson, Gilfrich, and Cook.	9.992 at 25° C

The density of thallium chlorostannate calculated from the NBS lattice constant is 4.927 at 25° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	5. 77	27	9. 99
200	4. 998	24	9. 996
220	3. 532	100	9. 991
311	3. 013	13	9. 994
222	2. 886	50	9. 997
400	2. 498	50	9. 992
331	2. 293	6	9. 994
420	2. 235	9	9. 995
422	2. 040	37	9. 995
511	1. 923	6	9. 993
440	1. 766	25	9. 991
531	1. 689	5	9. 991
600	1. 665	3	9. 990
620	1. 580	11	9. 992
533	1. 524	<1	9. 993
622	1. 507	9	9. 996
444	1. 4423	6	9. 992
711	1. 3994	2	9. 994
640	1. 3853	1	9. 990
642	1. 3350	9	9. 990
731	1. 3010	2	9. 993
800	1. 2488	3	9. 990
820	1. 2118	<1	9. 993
822	1. 1774	4	9. 991
751	1. 1537	1	9. 991
662	1. 1461	2	9. 992
840	1. 1172	6	9. 992
911	1. 0968	2	9. 992
664	1. 0650	2	9. 991
931	1. 0474	1	9. 992
844	1. 0197	4	9. 991
933	1. 0040	<1	9. 990
10·2·0	0. 9797	3	9. 991
951	. 9662	1	9. 994
10·2·2	. 9617	1	9. 994
10·4·0	. 9315	<1	9. 989
10·4·2	. 9122	2	9. 993
880	. 8829	<1	9. 990
11·3·1	. 8729	1	9. 991
10·6·0	. 8567	1	9. 991
11·3·3	. 8475	<1	9. 992
10·6·2	. 8445	<1	9. 992
12·0·0	. 8326	2	9. 991
12·2·2	. 8104	<1	9. 991
11·5·3	. 8026	2	9. 992
12·4·0	. 7899	1	9. 992
Average of last five lines			9. 992

References

[1] G. Engel, Die Kristallstrukturen einiger Hexachlorokomplexsalze, Z. Krist. **90,** 341–373 (1935).

Thallium Chromium Sulfate Dodecahydrate, $TlCr(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of thallium chromium sulfate dodecahydrate was prepared at the NBS from thallium nitrate and chromium sulfate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of barium, sodium, and silicon; 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, nickel, and vanadium; and 0.0001 to 0.001 percent each of silver, copper, and manganese.

The sample has a lavender color. The index of refraction is 1.523.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	220	331	420

Structural data. Klug and Alexander [1] in 1940 found thallium chromium sulfate dodecahydrate to be a beta alum having the space group T_h^6–Pa3 and $4[TlCr(SO_4)_2.12H_2O]$ per unit cell. The structure of the beta alums was determined by Lipson [2] in 1935.

The unit-cell measurement reported by Klug and Alexander has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1940	Klug and Alexander [1]	12.263
1956	Swanson, Gilfrich and Cook	12.263 at 25° C

The density of thallium chromium sulfate dodecahydrate calculated from the NBS lattice constant is 2.394 at 25° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	7.08	25	12.3
200	6.14	37	12.3
210	5.49	12	12.3
211	5.01	10	12.3
220	4.341	100	12.28
221	4.088	11	12.26
311	3.700	16	12.27
222	3.542	22	12.27
321	3.278	16	12.26
400	3.066	29	12.26
410	2.974	4	12.26
411	2.890	3	12.26
331	2.814	41	12.27
420	2.743	40	12.27
421	2.678	4	12.27
332	2.615	3	12.27
422	2.504	28	12.27
511	2.361	15	12.27
521	2.240	2	12.27
440	2.170	10	12.27
522	2.137	2	12.28
531	2.074	6	12.27
600	2.046	16	12.28
610	2.018	<1	12.27
611	1.991	<1	12.27
620	1.941	20	12.27
533	1.871	8	12.27
622	1.850	9	12.27
630	1.8297	1	12.274
631	1.8097	1	12.274
444	1.7714	2	12.273
711	1.7181	2	12.267
640	1.7019	9	12.273
642	1.6401	13	12.273
722	1.6242	<1	12.262
731	1.5974	4	12.270
800	1.5331	1	12.265
733	1.4981	1	12.262
820	1.4877	8	12.268
822	1.4453	6	12.264
751	1.4161	<1	12.264
662	1.4067	3	12.263
840	1.3710	3	12.263
841	1.3628	<1	12.265
911	1.3460	3	12.263
842	1.3380	3	12.263
664	1.3072	3	12.263
Average of last five lines			12.263

References

[1] H. P. Klug and L. Alexander, Crystal-chemical studies of the alums. II. The purple chrome alums, J. Am. Chem. Soc. **62,** 2992–2993 (1940).

[2] H. Lipson, Existence of three alum structures, Nature **135,** 912 (1935).

Thallium Fluosilicate, Tl_2SiF_6 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
2–1441[a]	1. 15 1. 01 1. 04	Iron-----	Tabet [1] 1933.

[a] Deleted in the 1955 index.

The Tabet pattern was made using iron rather than molybdenum radiation as indicated on the ASTM card.

Additional published patterns. None.

NBS sample. The sample of thallium fluosilicate was prepared at the NBS from thallium nitrate, silica gel and hydrofluoric acid. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of aluminum, barium, calcium, iron, and magnesium.

The sample is colorless. The index of refraction is 1.546.

Interplanar spacings and intensity measurements. The *d*-values of the Tabet pattern were calculated from Bragg angle data.

The three strongest lines of the two patterns are as follows:

Pattern	1	2	3
Tabet-----	642	822	820
Swanson, Gilfrich, and Cook-----	220	200	222

Structural data. Tabet [1] in 1933 determined that thallium fluosilicate has potassium chloroplatinate-type structure, the space group O_h^5–Fm3m, and $4(Tl_2SiF_6)$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1933	Tabet [1]-----	8. 62
1935	Ketelaar [2]-----	8. 580
1956	Swanson, Gilfrich, and Cook.	8. 568 at 25° C

The density of thallium fluosilicate calculated from the NBS lattice constant is 5.816 at 25° C.

hkl	1933 Tabet Fe, 1.9373 A			1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
111	----	--	----	4. 96	10	8. 59
200	----	--	----	4. 29	78	8. 58
220	3. 07	43	8. 68	3. 029	100	8. 568
222	2. 50	38	8. 66	2. 475	51	8. 572
400	2. 16	30	8. 64	2. 143	29	8. 570
420	1. 93	59	8. 63	1. 9163	35	8. 570
422	1. 76	51	8. 62	1. 7489	28	8. 568
511	----	--	----	1. 6490	3	8. 568
440	----	--	----	1. 5149	11	8. 567
600	1. 44	57	8. 64	1. 4281	12	8. 569
620	1. 36	62	8. 60	1. 3549	13	8. 569
622	1. 30	46	8. 62	1. 2920	7	8. 570
444	----	--	----	1. 2369	3	8. 570
640	----	--	----	1. 1883	3	8. 569
642	1. 15	100	8. 61	1. 1452	8	8. 570
800	----	--	----	1. 0710	1	8. 568
820	1. 04	65	8. 58	1. 0390	4	8. 568
822	1. 01	68	8. 57	1. 0098	3	8. 568
662	----	--	----	0. 9830	1	8. 570
840	----	--	----	. 9581	2	8. 570
842	----	--	----	. 9351	3	8. 570
664	----	--	----	. 9134	2	8. 568
844	----	--	----	. 8746	1	8. 569
10·0·0	----	--	----	. 8569	1	8. 569
10·2·0	----	--	----	. 8402	3	8. 568
10·2·2	----	--	----	. 8245	1	8. 568
10·4· 2	----	--	----	. 7955	2	8. 568
10·4· 0	----	--	----	. 7821	2	8. 568
Average of last five lines----		--	8. 60	------	----	8. 568

References

[1] M. Tabet, La strutturs del fluosilicato di tallio, Gazz. chim. ital. **63,** 679–680 (1933).

[2] J. A. A. Ketelaar, Die Kristallstruktur von K-, Rb-, Cs- und Tl- Silico-fluorid und von $LiMnO_4$, Z. Krist. **92,** 155–156 (1935).

Thallium Gallium Sulfate Dodecahydrate, $TlGa(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of thallium gallium sulfate dodecahydrate was prepared at the NBS from thallium nitrate, gallium and sulfuric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of magnesium; 0.001 to 0.01 percent each of aluminum, barium, calcium, molybdenum, and silicon; and 0.0001 to 0.001 percent each of chromium, iron, manganese, sodium, and nickel.

The sample is colorless. The index of refraction is 1.512.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	220	200	420

Structural data. Klug and Kieffer [1] in 1943 found thallium gallium sulfate dodecahydrate to be a beta alum having the space group T_h^6–Pa3 and $4[TlGa(SO_4)_2 \cdot 12H_2O]$ per unit cell. The structure of the beta alums was determined by Lipson [2] in 1935.

The unit-cell measurement reported by Klug and Kieffer has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1943	Klug and Kieffer [1]	12.258 at 25° C
1956	Swanson, Gilfrich, and Cook.	12.257 at 25° C

The density of thallium gallium sulfate dodecahydrate calculated from the NBS lattice constant is 2.461 at 25° C.

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C		
	d	*I*	*a*
	A		A
111	7.09	15	12.3
200	6.12	37	12.2
210	5.48	9	12.3
211	5.00	6	12.3
220	4.335	100	12.26
221	4.084	9	12.25
311	3.699	10	12.27
222	3.542	20	12.27
321	3.274	13	12.25
400	3.065	25	12.26
410	2.971	3	12.25
411	2.888	1	12.25
331	2.810	29	12.25
420	2.741	34	12.26
421	2.676	3	12.26
332	2.614	3	12.26
422	2.503	25	12.26
511	2.359	10	12.26
440	2.167	9	12.26
522	2.135	3	12.26
531	2.072	4	12.26
600	2.043	15	12.26
610	2.015	1	12.26
611	1.988	1	12.25
620	1.939	17	12.25
533	1.868	5	12.25
622	1.848	7	12.26
444	1.770	3	12.27
543	1.7329	<1	12.253
640	1.6992	8	12.253
642	1.6380	12	12.258
722	1.6228	2	12.252
731	1.5958	1	12.258
800	1.5322	<1	12.258
733	1.4975	<1	12.258
820	1.4862	7	12.256
821	1.4756	<1	12.257
822	1.4440	5	12.253
831	1.4250	<1	12.258
662	1.4058	3	12.256
840	1.3703	3	12.256
911	1.3458	<1	12.261
842	1.3372	<1	12.256
664	1.3063	4	12.254
Average of last five lines			12.257

References

[1] H. P. Klug and G. L. Kieffer, Crystal-chemical studies of the alums. V. The gallium alums, J. Am. Chem. Soc. **65**, 2071–2703 (1943).

[2] H. Lipson, Existence of three alum structures, Nature **135**, 912 (1935).

Thallium(I) Nitrate, $TlNO_3$ (orthorhombic)

ASTM cards. ASTM card number 4–0629 gives a pattern for cubic thallium nitrate. This form is reported as being stable between 150° and 210° C by Finbak and Hassel [1].

Additional published patterns. None.

NBS sample. The sample of thallous nitrate was obtained from the Johnson Matthey Co., Ltd., London. Their spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of calcium and magnesium; and 0.0001 to 0.001 percent of aluminum.

The sample is colorless. The indices of refraction could not be determined because the sample reacted with the index liquids.

Interplanar spacings and intensity measurements. The three strongest lines of the NBS pattern are as follows:

Pattern	1	2	3
Swanson, Gilfrich, and Cook	122	120	040

Structural data. Ferrari and Cavalca [2] in 1950 found that the structure of thallous nitrate belonged to one of two possible space groups, D_{2h}^{16}–Pbnm or C_{2v}^{9}–$Pbn2_1$, and $8(TlNO_3)$ per unit cell.

The unit-cell measurements reported by Rivoir and Abbad have been converted from kX to angstrom units for comparison with the NBS values. Their reported "*c*" value differs from the accepted value by a factor of two. The measurements reported by Ferrari and Cavalca are given in angstrom units.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1943	Rivoir and Abbad [3]	6. 17	12. 29	3. 99
1950	Ferrari and Cavalca [2].	6. 25	12. 46	7. 96
1956	Swanson, Gilfrich, and Cook.	6. 287	12. 31	8. 001 at 25° C

The density of thallous nitrate calculated from the NBS lattice constants is 5.714 at 25° C.

References

[1] C. Finbak and O. Hassel, Rotation von Anionpolyedern in Kubischen Kristallgittern. III. Die Nitrate, Z. physik. Chem. **35,** 25–28 (1937).

[2] A. Ferrari and L. Cavalca, Ricerche sulla struttura del nitrato talloso rombico, Gazz. chim. ital. **80,** 199–203 (1950).

[3] L. Rivoir and M. Abbad, La estructura del nitrato talioso rombico, Anales real soc. españ. fís. y quim. Madrid **39,** 306–325 (1943).

hkl	1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*
	A	
110	5. 60	4
021	4. 88	2
120	4. 40	68
002	4. 01	31
112	3. 259	5
200	3. 145	28
040	3. 080	34
210	3. 048	10
122	2. 962	100
141	2. 612	3
230	2. 495	5
202	2. 474	24
042	2. 442	29
212	2. 426	6
150	2. 293	1
240	2. 199	17
232	2. 118	3
310	2. 066	2
004	2. 004	9
320	1. 984	8
160	1. 951	10
250	1. 939	2
242	1. 928	14
312	1. 835	4
233	1. 824	14
322	1. 778	9
162	1. 754	13
252	1. 745	1
332	1. 691	6
204	1. 688	7
044	1. 678	7
350	1. 595	<1
400	1. 572	<1
410	1. 560	2
080	1. 539	2
333	1. 529	1
244	1. 480	7
360	1. 465	3
402	1. 463	2
135	1. 452	2
082	1. 436	4
324	1. 409	2
164	1. 397	5
280	1. 382	4
362	1. 377	3
334	1. 365	<1
006	1. 3346	<1
450	1. 3243	<1
442	1. 3210	<1
282	1. 3060	2
126, 372	1. 2764	3
452	1. 2570	<1
325	1. 2469	<1
046	1. 2242	<1
084	1. 2195	1

Thallium(I) Sulfate, Tl_2SO_4 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1-0784	3. 13 3. 53 2. 17	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of thallium sulfate was obtained from Johnson, Matthey, & Co., Ltd., London. Their spectrographic analysis showed the following impurities: 0.01 to 0.05 percent each of calcium and magnesium; and 0.0001 to 0.001 percent each of lead, aluminum, iron, and silicon.

The sample is colorless, and optically positive. The indices of refraction are $\alpha=1.862$, $\beta=1.865$ and $\gamma=1.887$. $2V\simeq 70°$.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel.	022, 112	121	231, 123, 222
Swanson, Gilfrich, and Cook.	112	130	121

Structural data. Gross [2] in 1941 found thallium sulfate to be isostructural with the alkaline sulfates having the space group D_{2h}^{16}–Pmcn and $4(Tl_2SO_4)$ per unit cell. The structure of the alkali sulfates was determined by Ogg [3] in 1928.

The unit-cell measurements reported by Gross have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1941	Gross [2]	6. 03	10. 70	7. 82
1956	Swanson, Gilfrich, and Cook.	5. 923	10. 66	7. 828 at 25° C

The density of thallium sulfate calculated from the NBS lattice constants is 6.783 at 25° C.

References

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

[2] S. T. Gross, Unit cell measurements of Pb_3O_4, Pb_2O_3, and Tl_2SO_4, J. Am. Chem. Soc. **63,** 1168 (1941).

[3] A. Ogg, The crystal structure of the isomorphous sulfates of potassium, ammonium, rubidium, and cesium, Phil. Mag. **5,** 354–367 (1928).

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*
	A		*A*	
020	------	----	5. 32	6
110	------	----	5. 17	9
021	4. 36	40	4. 40	17
111			4. 32	28
002	------	----	3. 91	2
012	------	----	3. 67	14
121	3. 54	48	3. 53	57
102	3. 27	16	3. 266	26
031	------	----	3. 237	21
022	3. 14	100	3. 154	53
112			3. 122	100
130	3. 04	32	3. 045	88
200	2. 96	40	2. 961	55
122	2. 78	8	2. 783	10
040	------	----	2. 664	1
032	2. 64	8	2. 630	15
013	2. 54	32	2. 533	26
221	2. 45	16	2. 457	15
141	2. 37	8	2. 321	12
212	2. 31	24	2. 308	10
042	2. 24	8	2. 200	9
231	2. 17	48	2. 186	13
123			2. 181	12
222			2. 158	27
033	2. 10	8	2. 103	9
051	2. 05	16	2. 056	16
232	1. 96	32	1. 966	12
004			1. 957	3
310	------	----	1. 941	7
213	1. 92	32	1. 926	17
311	1. 87	8	1. 884	4
052	------	----	1. 873	<1
104	------	----	1. 858	6
024	1. 83	24	1. 837	7
114			1. 832	13
321	------	----	1. 802	7
143	1. 78	32	1. 778	23
242	------	----	1. 767	4
312	------	----	1. 739	10
330	1. 72	16	1. 726	11
233			1. 715	7
251	1. 69	8	1. 689	12
161	------	----	1. 663	3
062	------	----	1. 618	1
252	------	----	1. 583	<1
224	1. 56	16	1. 561	8
260	------	----	1. 524	4
115	------	----	1. 499	4
261	------	----	1. 495	2
071				
234	1. 480	16	1. 484	8
400			1. 482	5
170	------	----	1. 475	3
	[a]			

[a] Five additional lines were omitted.

Zinc Fluoride, ZnF_2 (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0661 [a]	3. 33 2. 60 1. 75	Molybdenum.	Hanawalt, Rinn, and Frevel [1] 1938.

[a] Deleted from the 1955 index.

Additional published patterns

Source	Radiation	Wavelength
Ferrari [2] 1926	Copper	1.540 and 1.389 A

NBS sample. The sample of zinc fluoride was prepared at the NBS from zinc carbonate and hydrofluoric acid. It was then heated at 700° C at 20,000 psi pressure for 7 days. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon; 0.001 to 0.01 percent each of aluminum, boron, calcium, iron, magnesium, lead, and zirconium; 0.0001 to 0.001 percent each of copper and manganese; and less than 0.0001 percent silver.

The sample is colorless, and it is optically positive. The refractive indices are $N_o=1.502$ and $N_e=1.529$.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units, and the *d*-values of the Ferrari pattern were calculated from Bragg angle data.

The three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	110	101	211
Ferrari	211	110	101
Swanson, Gilfrich, and Cook	110	101	211

Structural data. Ferrari [2] in 1926 determined that zinc fluoride has rutile-type structure, the space group D_{4h}^{14}–$P4_2/mnm$, and $2(ZnF_2)$ per unit cell.

Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1926	Ferrari [2]	4. 726	3.137
1926	Goldschmidt, Barth, Holmsen, Lunde, and Zachariasen [3].	4. 73	3.15
1954	Stout and Reed [4]	4. 7034	3.1335 at 25° C
1956	Swanson, Gilfrich, and Cook.	4. 7108	3.1318 at 25° C

The density of zinc fluoride calculated from the NBS lattice constants is 4.939 at 25° C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1926 Ferrari Cu, 1.540 A		1956 Swanson, Gilfrich, and Cook Cu, 1.5405 A, 25° C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
110	3. 34	100	3. 22	s	3. 33	100
101	2. 61	80	2. 55	s	2. 608	95
200	2. 35	6	-----	----	2. 356	17
111	2. 27	20	2. 25	mw	2. 285	26
210	2. 10	5	2. 07	w	2. 108	10
211	2. 75	80	1. 73	vs	1. 748	80
220	1. 67	20	1. 65	m	1. 666	27
002	1. 56	8	1. 54	m	1. 565	17
310	1. 493	11	1. 47	mw	1. 490	14
112 301	1. 408	32	1. 41	s	1. 4173 1. 4039	12 22
311	-----	---	-----	----	1. 3451	1
202	1. 303	3	1. 29	w	1. 3039	6
212	1. 253	2	-----	----	1. 2567	3
321	1. 207	6	1. 20	mw	1. 2057	6
400	1. 179	2	-----	----	1. 1778	7
410	-----	---	-----	----	1. 1423	3
222	1. 137	6	1. 13	m	1. 1413	6
330	1. 114	2	-----	----	1. 1104	4
312	1. 077	6	1. 07	m	1. 0794	12
411	-----	---			1. 0734	6
420	-----	---	-----	----	1. 0532	2
103	-----	---	0. 998	w	1. 0192	2
113	-----	---	. 972	w	0. 9961	<1
402	-----	---			. 9413	5
213	-----	---	. 936	mw	. 9354	8
510	-----	---	-----	----	. 9239	4
332	-----	---	-----	----	. 9056	3
501	-----	---	. 896	w	. 9022	6
422	-----	---	-----	----	. 8740	4
303	-----	---	. 868	m	. 8693	5
521	-----	---	. 840	ms	. 8424	6
440	-----	---	-----	----	. 8329	2
323	-----	---	-----	----	. 8156	1
512	-----	---	-----	----	. 7957	4
600	-----	---	-----	----	. 7851	1

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CUMULATIVE INDEX TO VOLUMES 1, 2, 3, 4, 5, AND 6[6]

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

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