NBS CIRCULAR 539

VOLUME 8

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

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Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, Nancy T. Gilfrich, Marlene I. Cook,
Roger Stinchfield, and Paul C. Parks

National Bureau of Standards Circular 539
Volume 8, Issued April 1, 1959

For sale by the Superintendent of Documents, U. S. Government Printing Office, Washington 25, D. C.
Price 45 cents

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Errata

Vol. 1. Page 45, the D-value in the NBS pattern of 1.1329 should be 1.1140.
Vol. 3. Page 53, under Lattice constant, D^{16}_{2h}–Pbnm (Pnma) should read D^{16}_{2h}–Pmcn (Pnma).
Page 54, *hkl* 012 should be added to *d*-value 2.700 and *hkl* 031 should be added to *d*-value 2.409, also *hkl's* 230 and 410 should be deleted, *hkl* 040 should be changed to 211.
Vol. 7. Page ii, Errata Vol. 6 page 41, D^3d should read D^3_{3d}.
Page 50, under Structural data, should read calcium sulfate-type structure.

Standard X-ray Diffraction Powder Patterns

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. 8—Data for 61 Substances

Howard E. Swanson, Nancy T. Gilfrich,[1] Marlene I. Cook,[1]
Roger Stinchfield,[1] and Paul C. Parks[1]

Sixty-one standard X-ray diffraction powder patterns are presented. Thirty-three are to replace thirty-nine patterns already represented in the X-ray Powder Data File, and twenty-eight are for substances not previously represented. The X-ray Powder Data 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 sixty-one substances: $Al_2O_3 \cdot 6CaO \cdot 3SO_3 \cdot 31H_2O$, $(NH_4)_2SeBr_6$, $(NH_4)_2TeBr_6$, $(NH_4)_2IrCl_6$, $(NH_4)_2PdCl_6$, $(NH_4)_2TeCl_6$, NH_4VO_3, $(NH_4)_3PO_4$-$(MoO_3)_{12} \cdot 4H_2O$, Be_2SiO_4, BiOBr, $CaBr_2 \cdot 6H_2O$, $Ca(HCO_2)_2$, CeF_3, $CsBrO_3$, Cs_2PtBr_6, Cs_2SeBr_6, $CsClO_3$, $CsCr(SO_4)_2 \cdot 12H_2O$, $CsBF_4$, $CsGa(SO_4)_2 \cdot 12H_2O$, Er_2O_3, $GaPO_4$ (α-quartz type), GeO_2 (tetragonal), $InPO_4$, $Pb(HCO_2)_2$, Pb_3O_4 (minimum), $Pb_5(PO_4)_3OH$ (lead hydroxyapatite), $LiClO_4 \cdot 3H_2O$, NdF_3, NdOCl, $NiSiF_6 \cdot 6H_2O$, $NbSi_2$, K_2PtBr_6, K_2SeBr_6, $KReO_4$, $K_3PO_4(MoO_3)_{12} \cdot 4H_2O$, KCNS, $RbBrO_3$, Rb_2TeBr_6, $RbClO_3$, Rb_2TeCl_6, Rb_2SO_4, $ScPO_4$, AgI (iodyrite), $AgReO_4$, $Na_2CO_3 \cdot H_2O$ (thermonatrite), $Sr(HCO_2)_2$, $Sr(CHO_2)_2 \cdot 2H_2O$, $SrI_2 \cdot 6H_2O$, $TaSi_2$, $TlBrO_3$, $TlClO_3$, $TlIO_3$, TlCNS, Ti_5Si_3, WS_2, V_2O_5, YPO_4 (xenotime), $ZnCO_3$ (smithsonite), $ZnSiF_6 \cdot 6H_2O$, and $ZnSO_4 \cdot 7H_2O$ (goslarite).

INTRODUCTION

The National Bureau of Standards in its program[2] for the revision and evaluation of published X-ray data for the X-ray Powder Data File, presents data for 61 compounds. This paper is the eighth of the series of "Standard X-ray Diffraction Powder Patterns." These patterns are recommended to replace 39 cards now in the file. The patterns for 28 compounds not represented in the file have been added. These compounds are ammonium bromotellurate, ammonium chloroiridate, ammonium chloropalladate, ammonium chlorotellurate, cesium bromate, cesium bromoplatinate, cesium bromoselenate, cesium chlorate, cesium chromium sulfate dodecahydrate, cesium fluoborate, cesium gallium sulfate dodecahydrate, gallium phosphate (α-quartz type), indium phosphate, lithium perchlorate trihydrate, niobium silicide, potassium bromoplatinate, potassium bromoselenate, potassium phosphomolybdate tetrahydrate, rubidium bromate, rubidium bromotellurate, rubidium chlorate, rubidium chlorotellurate, scandium phosphate, tantalum silicide, thallium(I) bromate, thallium(I) chlorate, thallium(I) iodate, and titanium silicide.

The experimental procedure and general plan of these reports have not changed from that of the previous volumes of the NBS Circular.[3] However, the basic technique is discussed, in this section, under the same headings that appear in the text of this volume.

ASTM cards. Each section of this Circular contains a table listing the ASTM file card numbers, the three strongest lines, the radiations used, and the literature references for each card. Cards listed in the 1956 index to the Powder Data File [1][4] are included in the table.

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

NBS sample. Many of the samples used to make the NBS patterns were special preparations (of exceptionally high purity) obtained or prepared only in small quantities. The limit of detection for the alkali elements is 0.05 percent for the spectrographic analysis. Unless otherwise noted, the spectrographic analysis was done at NBS after recrystallization or heat treatment. A phase-purity check was made on the nonopaque materials during the refractive index determination. Another excellent check of phase-purity was provided by the X-ray pattern itself, since it was indexed by comparison with theoretical *d*-values. 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 give satisfactory intensity patterns usually have a particle-size average well within the range of 5 to 10 μ, as suggested by Alexander, Klug, and Kummer [2]. A special cell with one open end was

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[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; Vol. 5, October 1955; Vol. 6, September 1956; and Vol. 7, September 1957.

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

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 vertical position, the sample was drifted in 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 were measured as peak height above background and are expressed as percentages of the strongest line. Additional patterns were obtained for *d*-value measurements. These specimens were prepared by packing, into a shallow holder, a sample containing an internal standard approximately 5-weight percent of tungsten powder. The lattice constant used for tungsten at 25°C is 3.1648 A, as determined by Jette and Foote [3]. All of the NBS patterns, unless otherwise noted, are made at 25°C with 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 [4]. The conversions were from Bragg angle data, from *d*-values in kX units using the factor 1.00202, or from *d*-values based on wavelengths given in other than kX units. In each case, the type of conversion is indicated. The wavelength values in the tables of *d*-values and intensities are given in angstrom units, whereas the wavelengths listed under the first section of each report are the original values taken from the literature. The tables of patterns contain data based on the original work rather than that data reported on the ASTM cards.

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

Structural data. Although the NBS lattice constants of cubic materials were calculated for each *d*-value, the constant reported is that obtained by averaging the last five lines because of the greater accuracy of measurement in the large-angle part of the pattern. The unit-cell values for each noncubic substance were determined by means of a least-squares calculation made by the IBM 704 from the latter half of the pattern, using those *d*-values for which there was only one possible Miller index. The number of significant figures reported in the NBS pattern is limited by the quality of each sample and by its structural symmetry.

Published unit-cell data were converted to angstrom units in the same manner as were the published *d*-values. When cell values based upon more than one cell configuration have been taken from the literature, corrections that were made to make them comparable have been indicated. The limits of error generally published with unit-cell data have not been included in the table because the number of determinations and their accuracy and variations were such that a statistical evaluation would be unjustified.

Starting with this volume 8 we have adopted a variation in our routine for presenting the space group. In place of both the Schoenflies symbol and the International symbol previously listed, we have dropped the Schoenflies symbol and added the space group number given in the International Tables for X-ray Crystallography. It is felt that this number has become useful in locating space group data, while the use of the Schoenflies symbol has diminished.

We have also decided to present orthorhombic cell dimensions only in the "standard" arrangement of a, b, c, as given in the International Tables, rather than with a permutation as is occasionally given in the literature.

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 [5] in 1956 and the Avogadro number (6.0240×10^{23}) reported by Straumanis [6] in 1954. The refractive index measurements were made by grain-immersion methods in white light using oils standardized in sodium light.

References

[1] Cumulative alphabetical and grouped numerical index of X-ray diffraction data, American Society for Testing Materials, Philadelphia, Pa. (1956).

[2] 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).

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

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

[5] E. Wichers, Report of the Committee on Atomic Weights of the American Chemical Society, J. Am. Chem. Soc. **78**, 3235 (1956).

[6] M. E. Straumanis, Remark concerning the absolute value of Avogadro's number, Phys. Rev. **95**, 566 (1954).

Alumium Calcium Sulfate Hydrate (ettringite), $Al_2O_3 \cdot 6CaO \cdot 3SO_3 \cdot 31H_2O$ (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
2–0059	9.8 2.79 5.7	Molybdenum	Imperial Chemical Industries, Northwich, England, and British Museum.

Additional published patterns

Source	Radiation
Feitknecht and Buser [1] 1949	Copper

NBS sample. The sample of ettringite was prepared by Edwin S. Newman at NBS. His analysis shows the following chemical composition: 2.995 moles of CaO: 1 mole of Al_2O_3: 2.915 moles of $CaSO_4$: 31.05 moles of H_2O. Spectrographic analysis shows the following impurities: 0.1 to 1.0 percent each of silicon and strontium; 0.01 to 0.1 percent each of silver, chromium, copper, magnesium, sodium, and lead; and 0.001 to 0.01 percent each of boron, barium, cesium, iron, manganese, nickel, tin, zinc, and zirconium.

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

Interplanar spacings and intensity measurements. The *d*-values of the combined pattern reported by the Imperial Chemical Industries and the British Museum were converted from kX to angstrom units, and the *d*-values reported by Feitknecht and Buser were calculated from reported Bragg angle data. The indices of the three strongest lines for each pattern are as follows:

Pattern	1	2	3
Imperial Chemical Industries and the British Museum	100	304	110
Feitknecht and Buser	100	110	114
National Bureau of Standards	100	110	114

Structural data. Bannister, Hey, and Bernal [2] in 1936 determined that ettringite has the space group P6$_3$/mmc (No. 194) and $2(Al_2O_3 \cdot 6CaO \cdot 3SO_3 \cdot 31H_2O)$ per unit cell.

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

hkl	Imperial Chemical Industries and British Museum Mo, 0.7107 A		1949 Feitknecht and Buser Cu, ----		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
100	9.8	100	9.62	100	9.73	100
101	----	---	-----	---	8.86	12
110	5.7	80	5.60	90	5.61	81
112	4.9	60	4.95	40	4.98	24
200	----	---	-----	---	4.86	6
104	4.67	70	4.69	60	4.69	36
314	4.34	20	-----	---	4.41	3
203	----	---	-----	---	4.02	10
114	3.87	80	3.87	90	3.88	51
210	----	---	-----	---	3.67	7
204	3.60	30	3.60	30	3.60	14
212	3.45	60	3.48	70	3.48	31
213	3.26	40	3.24	40	3.27	4
300					3.240	19
116	3.02	30	3.015	20	3.016	6
220	----	---	-----	---	2.806	6
304	2.79	90	2.772	80	2.773	38
222	----	---	-----	---	2.714	6
310	2.67	30	-----	---	2.697	12
008					2.680	7
312	----	---	-----	---	2.616	21
216	2.57	80	2.559	80	2.564	45
313	----	---	-----	---	2.524	4
224	----	---	-----	---	2.487	3
400	----	---	-----	---	2.434	2
118	2.43	30	-----	---	2.422	2
306	2.36	10	-----	---	2.401	10
208					2.347	4
320	----	---	-----	---	2.230	20
226	2.20	80	2.207	90	2.209	43
322	----	---	-----	---	2.185	8
316	2.14	60	2.140	9	2.154	23
323	----	---	-----	---	2.130	2
410	----	---	-----	---	2.124	5
412	----	---	-----	---	2.081	4
324	2.06	30	-----	---	2.062	5
413	----	---	-----	---	2.033	1
317	----	---	-----	---	2.027	1
325	----	---	-----	---	1.979	2
414	----	---	-----	---	1.975	3
500	1.94	30	-----	---	1.946	10
407	1.89	30	-----	---	1.905	1
503					1.875	2
2·1·10	1.84	40	-----	---	1.853	6
332					1.845	8
421	----	---	-----	---	1.829	4
504						
422	1.80	10	-----	---	1.812	4
2·0·11					1.809	3
0·0·12	----	---	-----	---	1.786	2
334	1.75 (a)	40	-----	---	1.768	4

---

[a] Nine additional lines were omitted.

Lattice constants

		a	c
		A	A
1936	Bannister, Hey, and Bernal [2]	11.26	21.48
1949	Feitknecht and Buser [1]	11.2	21.4
1958	National Bureau of Standards	11.23	21.44 at 25°C

The density of ettringite calculated from the NBS lattice constants is 1.754g/cm^3 at 25°C.

References

[1] W. Feitknecht and H. Buser, Zur Kenntnis der nadeligen Calcium-Aluminum-hydroxysalze, Helv. Chim. Acta **32**, 2298–2305 (1949).

[2] F. A. Bannister, M. H. Hey, and J. D. Bernal, Mineral. Mag. **24**, 324–329 (1936).

Ammonium Bromoselenate, $(NH_4)_2SeBr_6$ (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
2–1438	1.17 3.03 2.62	Chromium	Sieg [1] 1932.

Additional published patterns. None.

NBS sample. The sample of ammonium bromoselenate was prepared at NBS from selenium dioxide, ammonium bromide, and hydrobromic acid. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of iron, sodium, and silicon.

The color of the sample was orange-red. The index of refraction could not be determined by the usual liquid grain immersion method because it was too highly colored.

Interplanar spacings and intensity measurements. The *d*-values of the Sieg pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Sieg	840	222	400
National Bureau of Standards	222	400	200

Structural data. Sieg [1] in 1932 determined that ammonium bromoselenate has potassium chloroplatinate-type structure, the space group Fm3m (No. 225), and 4[$(NH_4)_2SeBr_6$] per unit cell.

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

hkl	1932 Sieg Cr, 2.291 A			1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
111	6.08	vw	10.5	6.06	31	10.49
200	5.29	w–vw	10.5	5.24	64	10.49
220	-----	----	-----	3.71	3	10.49
311	3.18	vvw	10.5	3.160	12	10.48
222	3.03	vs	10.5	3.027	100	10.49
400	2.63	vs	10.5	2.621	87	10.48
331	-----	----	-----	2.406	4	10.48
420	2.35	s	10.5	2.344	36	10.48
422	-----	----	-----	2.137	<1	10.47
511	2.03	<vvw	10.5	2.017	8	10.48
440	1.86	vs	10.5	1.853	50	10.48
531	-----	----	-----	1.771	6	10.48
600	1.75	vvw	10.5	1.746	17	10.48
620	-----	----	-----	1.658	<1	10.48
533	-----	----	-----	1.5983	<1	10.481
622	1.58	s–vs	10.5	1.5800	27	10.480
444	1.51	s–w	10.5	1.5127	14	10.480
711	1.468	vvw	10.48	1.4679	4	10.483
640	1.455	vvw	10.48	1.4531	4	10.478
731	1.364	<vvw	10.48	1.3640	1	10.477
800	1.309	w–s	10.48	1.3100	6	10.480
820	1.270	s	10.48	1.2710	6	10.481
751	1.210	vvw	10.48	1.2097	1	10.476
662	1.201	vs	10.48	1.2018	6	10.477
840	1.170	vvs	10.48	1.1715	10	10.478
911	-----	----	-----	1.1498	1	10.475
842	-----	----	-----	1.1430	4	10.476
931	-----	----	-----	1.0982	<1	10.476
844	-----	----	-----	1.0694	7	10.478
933	-----	----	-----	1.0532	1	10.479
10·0·0	-----	----	-----	1.0475	1	10.475
951	-----	----	-----	1.0130	1	10.479
10·2·2	-----	----	-----	1.0085	2	10.481
953	-----	----	-----	0.9773	<1	10.480
10·4·0	-----	----	-----	.9730	1	10.480
880	-----	----	-----	.9262	1	10.479
11·3·1	-----	----	-----	.9157	<1	10.481
10·4·4	-----	----	-----	.9121	1	10.479
10·6·2	-----	----	-----	.8856	2	10.479
12·0·0	-----	----	-----	.8733	3	10.480
12·2·0	-----	----	-----	.8615	<1	10.481
12·4·0	-----	----	-----	.8286	3	10.481
12·4·2	-----	----	-----	.8182	3	10.478
10·6·6	-----	----	-----	.7989	1	10.477
12·4·4	-----	----	-----	.7900	2	10.480
12·6·0	-----	----	-----	.7810	1	10.478
Average value of last five lines			10.48	------	--	10.478

Lattice constants

		A
1932	Sieg [1]	10.48
1958	National Bureau of Standards	10.478 at 25°C

The density of ammonium bromoselenate calculated from the NBS lattice constant is 3.431 g/cm^3 at 25°C.

References

[1] L. Sieg, Die Kristallstruktur des Ammoniumhexabromoselenats, Z. anorg. u. allgem. Chem. **207**, 93–96 (1932).

Ammonium Bromotellurate, $(NH_4)_2TeBr_6$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium bromotellurate was prepared at NBS from tellurium oxide, hydrobromic acid, and ammonium bromide. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of iron and sodium; and 0.0001 to 0.001 percent each of calcium and silicon.

The color of the sample was bright orange. The index of refraction was too high to be determined by the usual liquid grain-immersion method.

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

Pattern	1	2	3
National Bureau of Standards	400	200	222

Structural data. Although there are no references to the crystal structure of ammonium bromotellurate in the literature, it appears to have potassium chloroplatinate-type structure, the space group Fm3m (No. 225), and $4[(NH_4)_2TeBr_6]$ per unit cell. The NBS unit-cell measurement is as follows:

Lattice constant

		A
1958	National Bureau of Standards	10.731 at 26°C

The density of ammonium bromotellurate calculated from NBS lattice constant is 3.456 at 26°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 26°C		
	d	*I*	*a*
	A		A
111	6.19	26	10.72
200	5.36	67	10.73
311	3.23	34	10.72
222	3.10	58	10.73
400	2.68	100	10.72
331	2.460	16	10.724
420	2.398	54	10.722
511	2.064	14	10.724
440	1.897	44	10.730
531	1.813	19	10.726
600	1.788	28	10.725
533	1.635	9	10.723
622	1.618	14	10.730
444	1.548	14	10.721
711	1.502	8	10.730
640	1.4875	6	10.726
731	1.3966	8	10.728
800	1.3406	7	10.725
733	1.3111	7	10.732
820	1.3012	9	10.730
822	1.2644	4	10.728
751	1.2388	6	10.728
662	1.2303	3	10.726
840	1.1995	12	10.729
911	1.1780	5	10.732
842	1.1708	9	10.731
931	1.1252	3	10.734
844	1.0950	8	10.729
933	1.0787	2	10.733
10·0·0	1.0733	2	10.733
951	1.0376	2	10.733
10·2·2	1.0324	2	10.729
10·4·0	0.9966	4	10.734
11·1·1	.9674	<1	10.729
880	.9483	2	10.729
11·3·1	.9375	<1	10.730
10·4·4	.9340	<1	10.731
10·6·2	.9070	<1	10.732
12·0·0	.8942	2	10.730
11·5·3	.8617	1	10.728
12·4·0	.8482	2	10.729
12·4·2	.8380	2	10.732
13·1·1	.8206	<1	10.731
12·4·4	.8087	<1	10.729
13·3·1	.8022	<1	10.733
12·6·0	.7998	<1	10.730
Average value of last five lines			10.731

Ammonium Chloroiridate, $(NH_4)_2IrCl_6$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium chloroiridate was prepared at NBS by R. Gilchrist. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent of sodium; and 0.0001 to 0.001 percent of silicon.

The color of the sample was brown-black. The indices of refraction were not obtained because the sample was too highly colored.

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

Pattern	1	2	3
National Bureau of Standards	111	200	311

Structural data. Boky and Ussikov [1] in 1940 determined that ammonium chloroiridate has potassium chloroplatinate-type structure, the space group Fm3m (No. 225), and $4[(NH_4)_2IrCl_6]$ per unit cell.

The unit-cell measurement reported by Boky and Ussikov was converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1940	Boky and Ussikov [1]	9.89
1958	National Bureau of Standards	9.860 at 25°C

The density of ammonium chloroiridate calculated from the NBS lattice constant is 3.055 g/cm³ at 25°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*
	A		*A*
111	5.70	100	9.87
200	4.93	68	9.87
220	3.48	27	9.86
311	2.973	48	9.861
222	2.846	5	9.860
400	2.465	38	9.859
331	2.262	16	9.859
420	2.205	28	9.862
422	2.013	10	9.861
511	1.897	17	9.859
440	1.743	19	9.859
531	1.666	14	9.859
600	1.643	12	9.857
620	1.559	3	9.859
533	1.504	6	9.860
444	1.423	6	9.860
711	1.381	8	9.860
640	1.3670	4	9.860
642	1.3180	3	9.863
731	1.2837	6	9.860
800	1.2327	1	9.862
733	1.2044	1	9.858
820	1.1954	2	9.858
822	1.1617	<1	9.857
751	1.1384	2	9.858
840	1.1021	2	9.859
911	1.0820	2	9.858
842	1.0757	1	9.859
664	1.0510	1	9.859
931	1.0340	<1	9.860
844	1.0063	<1	9.860
933	0.9911	5	9.861
10·0·0	.9861	<1	9.861
10·2·0	.9668	1	9.860
951	.9532	2	9.860
953	.9192	1	9.857
10·4·0	.9153	1	9.858
11·1·1	.8890	2	9.860
880	.8715	<1	9.860
11·3·1	.8614	1	9.859
10·4·4	.8582	1	9.860
10·6·0	.8455	<1	9.860
11·3·3	.8364	<1	9.861
12·0·0	.8217	<1	9.860
12·2·2	.7997	<1	9.859
11·5·3	.7920	<1	9.860
Average value of last five lines			9.860

References

[1] G. B. Boky and P. I. Ussikov, X-ray studies of the structure of $(NH_4)_2IrCl_6$, Compt. rend. acad. sci. U.R.S.S. **26,** 782–784 (1940).

Ammonium Chloropalladate, $(NH_4)_2PdCl_6$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium chloropalladate was prepared at NBS by R. Gilchrist. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of silver, platinum, and silicon; and 0.0001 to 0.001 percent each of calcium, magnesium, and lead.

The color of the sample was deep red. The index of refraction was too high to be determined by the usual liquid grain immersion method.

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

Pattern	1	2	3
National Bureau of Standards	111	200	400

Structural data. Ketelaar and van Walsem [1] in 1938 determined that ammonium chloropalladate has potassium chlorostannate-type structure, the space group Fm3m (No. 225), and $4[(NH_4)_2PdCl_6]$ per unit cell.

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

Lattice constants

		A
1938	Ketelaar and van Walsem [1]	9.83
1953	Sharpe [2]	9.84
1958	National Bureau of Standards	9.826 at 26°C

The density of ammonium chloropalladate calculated from the NBS lattice constant is 2.486 g/cm³ at 26°C.

References

[1] J. A. A. Ketelaar and J. F. van Walsem, Die Kristallstruktur des Ammonium-, Kalium-, Rubidium- und Cäsiumpalladiumhexachlorids und- Bromids, Rec. trav. chim. **57**, 964–966 (1938).

[2] A. G. Sharpe, Chemistry of the platinum metals. Part III. Lattice constants of some chloropalladates, bromopalladates, and bromoplatinates, J. Chem. Soc. 4177–4179 (1953).

Ammonium Chloropalladate, $(NH_4)_2PdCl_6$ (cubic)

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 26°C		
	d	*I*	*a*
	A		A
111	5.68	100	9.84
200	4.91	73	9.82
220	3.47	19	9.82
311	2.962	40	9.822
222	2.836	24	9.824
400	2.455	53	9.820
331	2.254	10	9.823
420	2.196	31	9.822
422	2.006	7	9.825
511	1.890	18	9.823
440	1.737	27	9.824
531	1.661	15	9.826
600	1.637	13	9.823
620	1.554	1	9.826
533	1.4984	4	9.826
622	1.4809	3	9.823
444	1.4180	9	9.824
711	1.3757	7	9.824
640	1.3627	6	9.827
642	1.3133	2	9.828
731	1.2790	5	9.824
800	1.2282	4	9.826
820	1.1914	5	9.824
822	1.1579	1	9.825
751	1.1342	3	9.822
840	1.0981	5	9.822
911	1.0786	2	9.826
842	1.0719	2	9.824
664	1.0471	1	9.823
931	1.0298	2	9.824
844	1.0025	4	9.822
933	0.9874	<1	9.824
10·0·0	.9828	<1	9.828
10·2·0	.9633	<1	9.824
951	.9496	2	9.823
953	.9161	2	9.824
880	.8684	<1	9.825
11·3·1	.8584	1	9.825
10·4·4	.8553	<1	9.827
11·3·3	.8334	1	9.826
12·0·0	.8188	3	9.826
12·2·0	.8077	<1	9.826
11·5·3	.7892	3	9.826
Average of last five lines			9.826

Ammonium Chlorotellurate, $(NH_4)_2TeCl_6$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The ammonium chlorotellurate was prepared at NBS by dissolving TeO_2 in concentrated HCl. To the H_2TeCl_6 a solution of NH_4Cl was added in stoichiometric proportions and the solution was crystallized on a steam bath. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of iron, sodium, and silicon; and 0.0001 to 0.001 percent each of boron and magnesium. The color of the sample was yellow. The index of refraction is 1.895.

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

Pattern	1	2	3
National Bureau of Standards	111	200	400

Structural data. Engel [1] in 1935 determined that ammonium chlorotellurate has potassium chloroplatinate-type structure, the space group Fm3m (No. 225), and $4[(NH_4)_2TeCl_6]$ 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]	10.199
1958	National Bureau of Standards	10.203 at 25°C

The density of ammonium chlorotellurate calculated from the NBS lattice constant is 2.353g/cm^3 at 25°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*
	A		A
111	5.90	100	10.22
200	5.12	90	10.20
220	3.61	25	10.21
311	3.080	66	10.22
222	2.948	20	10.21
400	2.554	74	10.20
331	2.343	28	10.21
420	2.285	47	10.22
422	2.084	13	10.21
511	1.965	21	10.21
440	1.804	37	10.205
531	1.725	20	10.205
600	1.700	20	10.200
620	1.6133	4	10.203
533	1.5565	7	10.207
444	1.4731	8	10.206
711	1.4293	9	10.207
640	1.4152	5	10.205
642	1.3644	4	10.210
731	1.3289	6	10.207
800	1.2754	5	10.203
733	1.2468	5	10.205
820	1.2376	9	10.206
822	1.2023	5	10.202
751	1.1782	4	10.204
840	1.1411	8	10.206
911	1.1201	2	10.205
842	1.1137	5	10.207
664	1.0874	2	10.201
931	1.0697	4	10.204
844	1.0414	3	10.204
933	1.0255	3	10.204
10·0·0	1.0207	3	10.207
10·2·0	1.0005	3	10.203
951	0.9865	4	10.204
953	.9516	3	10.205
10·4·0	.9474	4	10.204
11·1·1	.9201	4	10.204
880	.9018	2	10.203
11·3·1	.8915	3	10.204
10·4·4	.8881	4	10.203
10·6·0	.8749	3	10.203
11·3·3	.8656	3	10.205
12·0·0	.8503	5	10.204
11·5·1	.8415	3	10.203
12·2·0	.8388	4	10.204
12·2·2	.8276	5	10.203
11·5·3	.8195	7	10.203
12·4·0	.8066	6	10.203
991	.7991	3	10.202
12·4·2	.7967	10	10.203
10·8·2	.7871	3	10.202
Average value of last five lines			10.203

References

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

Ammonium Metavanadate, NH_4VO_3 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0762	3.17 4.14 4.92	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of ammonium metavanadate was obtained from the Vanadium Corp. of America, New York, N. Y. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, and silicon; and 0.0001 to 0.001 percent each of chromium and iron.

The sample was colorless and optically negative. The indices of refraction are $N_\alpha=1.828$, $N_\beta=1.90$, $N_\gamma=1.925$, and $2V\cong 57°$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	121	021	100
National Bureau of Standards	121	021	100

Structural data. Lukesh [2] in 1950 determined that ammonium metavanadate has the space group Pbcm (No. 57) and $4(NH_4VO_3)$ per unit cell. The unit-cell measurements reported by Lukesh are compared with the NBS values.

Ammonium Metavanadate, NH_4VO_3 (orthorhombic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		A	
020	5.9	33	5.88	49
100	4.94	66	4.90	73
021	4.16	84	4.14	96
120	3.79	23	3.77	38
111	-----	---	3.57	9
121	3.18	100	3.164	100
002	2.92	42	2.912	60
131	2.73	13	2.710	26
041	2.63	27	2.628	44
140	-----	---	2.523	7
102	-----	---	2.504	6
200	2.46	23	2.451	32
112				
141	-----	---	2.318	2
220	-----	---	2.263	1
211	-----	---	2.221	6
150	2.12	10	2.125	9
132	-----	---	2.111	19
042	-----	---	2.073	10
060	-----	---	1.965	5
231	-----	---	1.960	2
142	-----	---	1.910	2
202	-----	---	1.876	9
061	1.86	3	1.862	6
023	-----	---	1.844	10
160	-----	---	1.823	1
241	1.79	3	1.793	10
161	-----	---	1.740	5
123	1.72	3	1.727	10
250	-----	---	1.700	3
133	-----	---	1.640	5
300	-----	---	1.634	6
062	-----	---	1.623	11
043	1.63	10	1.622	8
170	-----	---	1.592	<1
242	-----	---	1.583	1
311	-----	---	1.558	<1
162	1.55	6	1.546	11
260	-----	---	1.534	3
321	1.52	3	1.520	6
330	-----	---	1.508	<1
261	-----	---	1.482	3
223	-----	---	1.474	4
080				
331	1.463	3	1.461	8
004	-----	---	1.457	6
340	1.423	3	1.429	3
081				
302	-----	---	1.426	1
233	-----	---	1.420	<1
312	-----	---	1.415	4
024				
104	1.393	3	1.396	2
270	-----	---	1.388	3
341				
114				
322	-----	---	1.385	2
181	-----	---	1.371	1
124	-----	---	1.358	1
262	-----	---	1.357	2
243	-----	---	1.353	2
350	-----	---	1.343	2
163	-----	---	1.330	<1
082	-----	---	1.315	3
182	-----	---	1.270	2

Lattice constants

		a	b	c
		A	A	A
1950	Lukesh [2]	4.97	11.84	5.64
1958	National Bureau of Standards	4.902	11.79	5.827 at 25°C

The density of ammonium metavanadate calculated from the NBS lattice constants is 2.307 g/cm^3 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] J. S. Lukesh, The unit cell and space group of ammonium metavanadate, NH_4VO_3, Acta Cryst. **3**, 476–477 (1950).

Ammonium Phosphomolybdate Tetrahydrate, $(NH_4)_3PO_4(MoO_3)_{12}\cdot 4H_2O$ (cubic)

ASTM cards.

Card number	Index lines	Radiation	Source
1–0636[a]	3.39 1.48 8.3	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

[a] This card is labeled ammonium phosphomolybdate trihydrate; diffraction data on this card is in agreement with the tetrahydrate.

Additional published patterns. None.

NBS sample. The sample of ammonium phosphomolybdate tetrahydrate was prepared at NBS by heating dilute solutions of ammonium molybdate and phosphoric acid at about 75°C. The salt was precipitated by slowly adding dilute nitric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of silicon; 0.001 to 0.01 percent each of aluminum, calcium, iron, and magnesium; and 0.0001 to 0.001 percent each of copper and manganese.

The color of the sample was deep yellow. The index of refraction is 1.977.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	222	732	110
National Bureau of Standards	222	110	400

Structural data. Keggin [2] in 1934 determined the structure of 12-phosphotungstic acid. Ferrari and Nanni [3] in 1939 showed that ammonium phosphomolybdate tetrahydrate has this structure, the space group Pn3m (No. 224), and $2[(NH_4)_3PO_4(MoO_3)_{12}\cdot 4H_2O]$ per unit cell.

Lattice constant

		A
1958	National Bureau of Standards	11.666 at 25°C

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*	*d*	*I*	*a*
	A		A	A		A
110	8.32	50	11.8	8.25	55	11.66
111	-----	---	-----	6.74	3	11.65
200	5.81	25	11.6	5.84	24	11.67
211	4.83	10	11.8	4.76	10	11.67
220	4.19	25	11.8	4.128	32	11.68
310	3.71	14	11.2	3.688	10	11.66
222	3.40	100	11.1	3.364	100	11.65
321	-----	---	-----	3.120	6	11.67
400	2.93	50	11.7	2.914	35	11.66
411	2.76	16	11.7	2.750	11	11.67
420	-----	---	-----	2.609	5	11.67
332	2.50	50	11.7	2.487	30	11.66
510	2.29	30	11.7	2.288	18	11.67
511	-----	---	-----	2.245	3	11.67
432	-----	---	-----	2.166	3	11.66
521	-----	---	-----	2.130	6	11.67
440	2.06	25	11.6	2.0624	15	11.667
522	-----	---	-----	2.0307	2	11.665
600	1.94	12	11.6	1.9442	7	11.665
611	1.89	25	11.6	1.8919	13	11.662
620	1.84	12	11.6	1.8444	5	11.665
621	-----	---	-----	1.8216	3	11.664
541	1.80	20	11.7	1.7997	11	11.663
622	1.76	20	11.7	1.7580	10	11.661
444	1.69	12	11.7	1.6842	6	11.668
710	1.65	40	11.7	1.6493	22	11.662
640	-----	---	-----	1.6182	2	11.669
721	1.59	12	11.7	1.5878	7	11.668
642	-----	---	-----	1.5589	1	11.666
730	-----	---	-----	1.5317	2	11.665
732	1.483	60	11.68	1.4816	19	11.666
811	1.443	30	11.72	1.4359	10	11.665
820	-----	---	-----	1.4148	1	11.667
653	-----	---	-----	1.3942	1	11.665
822	-----	---	-----	1.3749	4	11.666
661	1.363	12	11.64	1.3651	2	11.663
831	-----	---	-----	1.3562	1	11.666
910	1.293	8	11.71	1.2889	1	11.663
921	1.263	4	11.71	1.2577	1	11.663
930	1.232	2	11.69	1.2297	<1	11.666
932	1.207	12	11.70	1.2033	6	11.666
941	1.182	8	11.70	1.1781	3	11.663
10·0·0	-----	---	-----	1.1665	5	11.665
10·1·1	1.158	12	11.70	1.1549	6	11.664
10·2·0	-----	---	-----	1.1438	1	11.664

Ammonium Phosphomolybdate Tetrahydrate, $(NH_4)_3PO_4(MoO_3)_{12}\cdot 4H_2O$ (cubic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*
950	1.137	8	11.71	1.1330	5	11.665
10·3·1	-----	---	-----	1.1118	<1	11.661
871	-----	---	-----	1.0924	2	11.664
10·4·0	-----	---	-----	1.0832	2	11.666
11·1·0	1.057	6	11.68	1.0562	4	11.666
11·2·1	-----	---	-----	1.0394	2	11.667
11·2·2	-----	---	-----	1.0272	<1	11.667
10·4·4	-----	---	-----	1.0154	<1	11.666
11·3·2	1.007	4	11.66	1.0076	3	11.664
883	-----	---	-----	0.9965	2	11.664
12·1·1	-----	---	-----	.9652	<1	11.663
11·5·2	-----	---	-----	.9526	<1	11.667
12·2·2	-----	---	-----	.9463	1	11.667
12·4·1	-----	---	-----	.9195	<1	11.667
12·3·3	-----	---	-----	.9166	2	11.666
11·6·3	-----	---	-----	.9052	1	11.663
13·1·0	-----	---	-----	.8949	<1	11.668
13·2·1	-----	---	-----	.8844	4	11.666
13·3·0	-----	---	-----	.8745	3	11.667
13·3·1	-----	---	-----	.8715	2	11.660
12·6·1	-----	---	-----	.8667	3	11.660
13·3·2	-----	---	-----	.8649	1	11.668
12·6·2	-----	---	-----	.8599	2	11.664
10·9·3	-----	---	-----	.8460	<1	11.661
13·5·0	-----	---	-----	.8374	1	11.664
14·0·0	-----	---	-----	.8332	1	11.665
14·1·1	-----	---	-----	.8290	1	11.665
12·7·3	-----	---	-----	.8205	2	11.662
14·2·2	-----	---	-----	.8166	1	11.663
14·3·1	-----	---	-----	.8129	4	11.667
13·5·4	-----	---	-----	.8068	2	11.664
14·4·0	-----	---	-----	.8014	1	11.668
14·4·2	-----	---	-----	.7935	<1	11.662
15·5·1	-----	---	-----	.7831	1	11.668
Average value of last five lines			11.69	------	---	11.666

The density of ammonium phosphomolybdate tetrahydrate calculated from the NBS lattice constant is 4.075 g/cm³ 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] J. F. Keggin, The structure and formula of 12-phosphotungstic acid, Proc. Roy. Soc. **144**, 75–100 (1934).

[3] A. Ferrari and O. Nanni, Richerche sui sali degli eteropoliacidi, l. Structtura dei fosfo- e degli arsenidodecamolibdati e dei fosfo- e degli arsenidodecawolframati di ammonio, di potassio e di tallio, Gazz. chim. Ital. **69**, 301–314 (1939).

Beryllium Orthosilicate (phenacite), Be_2SiO_4 (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
3–0538	3.12 3.67 2.52	Molybdenum	The Dow Chemical Co.
3–1171	1.26 3.11 2.52	Iron	Schütz [1] 1936[a].

[a] Synthetic phenacite.

Additional published patterns

Source	Radiation
Zachariasen [2] 1926	Iron, 1.934 A
Schütz [1] 1936[b]	Iron, 1.936 A
Morgan and Hummel [3] 1949	Copper, 1.537 A

[b] Natural phenacite.

NBS sample. The sample of phenacite was obtained from Minas Gerais, Brazil. A similar sample, from Kragerö, Norway, produced the same *d*-values within the limit of error of our equipment. Spectrographic analysis of the Brazil sample showed the following impurities: 0.1 to 1.0 percent aluminum; 0.01 to 0.1 percent each of calcium, iron, magnesium, sodium, nickel, tin, titanium, and zinc; and 0.001 to 0.01 percent each of boron, chromium, copper, germanium, manganese, lead, strontium, and zirconium.

The sample was colorless and optically positive. The refractive indices are $N_0=1.653$ and $N_e=1.669$.

Interplanar spacings and intensity measurements. The *d*-values reported by the Dow Chemical Co. were converted from kX to angstrom units and the *d*-values of the Schütz patterns and the Zachariasen pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Zachariasen	713	220	113
The Dow Chemical Co.	220	211	113
Schütz, synthetic	713	220	113
Schütz, natural	713	220	113
Morgan and Hummel	220	113	211
National Bureau of Standards	220	211	113

Structural data. Bragg [4] in 1926 determined that phenacite has the space group $R\overline{3}$ (No. 148) and $18(Be_2SiO_4)$ per unit hexagonal cell or $6(Be_2SiO_4)$ per unit rhombohedral cell. Phenacite is used as a structure-type.

The "a" (7.19 kX) reported by Zachariasen was multiplied by the $\sqrt{3}$. 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	Zachariasen [2]	12.48	8.25
1926	Bragg [4]	12.46	8.24
1927	Gottfried [5]	12.52	8.28
1927	Gossner [6]	12.45	8.23
1936	Schütz [1] synthetic	12.44	8.25
1936	Schütz [1] natural	12.45	8.26
1958	National Bureau of Standards	12.472	8.252 at 25°C

The density of phenacite calculated from the NBS lattice constants is 2.960 g/cm³ at 25°C.

Beryllium Orthosilicate, (phenacite), Be_2SiO_4 (trigonal)

hkl hex.	1926 Zachariasen Fe, 1.934 A		---- The Dow Chem. Co. Mo, 0.7107 A		1936 Schütz (natural) Fe, 1.936 A		1936 Schütz (synthetic) Fe, 1.936 A		1950 Morgan and Hummel Cu, 1.537 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*	
110	-----	---	6.40	38	-----	---	-----	---	6.20	20	6.24	41
021	-----	---	-----	---	-----	---	-----	---	4.47	10	4.52	3
---	-----	---	-----	---	-----	---	-----	---	4.03	5	-----	---
---	-----	---	-----	---	-----	---	-----	---	3.97	6	-----	---
012	-----	---	3.89	15	3.86	10	3.85	40	3.86	20	3.86	26
211	3.65	w	3.68	75	-----	---	-----	---	3.65	70	3.66	82
300	-----	---	-----	---	3.60	60	3.60	20	3.60	30	3.601	30
---	-----	---	-----	---	-----	---	-----	---	3.58	30	-----	---
202	-----	---	-----	---	3.27	10	-----	---	-----	---	3.279	3
220	3.13	s	3.13	100	3.13	80	3.12	80	3.10	100	3.119	100
122	-----	---	2.93	15	-----	---	-----	---	2.90	15	2.903	16
131	-----	---	2.83	10	2.83	10	-----	---	2.81	13	2.817	12
---	-----	---	-----	---	2.76	10	-----	---	-----	---	-----	---
113	2.53	s	2.53	75	2.52	80	2.52	80	2.51	100	2.518	73
410	2.37	w–s	2.36	63	2.35	60	2.35	60	2.35	35	2.358	70
042	-----	---	-----	---	-----	---	-----	---	-----	---	2.262	5
303	2.19	s	2.18	75	2.19	80	2.18	80	2.18	47	2.187	60
330	2.09	s	2.07	50	2.08	60	2.07	60	2.08	34	2.079	51
104	-----	---	2.02	3	-----	---	-----	---	-----	---	2.026	3
241	-----	---	1.98	3	1.98	10	-----	---	1.98	4	1.982	8
502	-----	---	1.91	10	1.92	20	1.92	10	1.91	5	1.914	9
214	-----	---	1.84	3	1.84	10	-----	---	1.84	3	1.842	3
422	-----	---	-----	---	-----	---	-----	---	-----	---	1.829	3
600	-----	---	-----	---	-----	---	-----	---	-----	---	1.798	4
413	1.79	w	1.79	15	1.80	40	1.79	20	1.79	8	1.790	15

Beryllium Orthosilicate, (phenacite), Be$_2$SiO$_4$ (trigonal)—Continued

hkl hex.	1926 Zachariasen Fe, 1.934 A		---- The Dow Chem. Co. Mo, 0.7107 A		1936 Schütz (natural) Fe, 1.936 A		1936 Schütz (synthetic) Fe, 1.936 A		1950 Morgan and Hummel Cu, 1.537 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*	
152	-----	---	-----	---	-----	---	-----	---	1.75	4	1.755	2
431	1.74	w–s	1.73	20	1.73	40	1.72	20	1.73	10	1.735	7
520											1.730	11
333	1.66	s	1.66	20	1.64	60	1.64	40	1.66	11	1.6581	17
404	-----	---	-----	---	-----	---	-----	---	-----	---	1.6391	2
161	-----	---	-----	---	-----	---	-----	---	-----	---	1.6154	2
324	-----	---	-----	---	1.56	10	-----	---	-----	---	1.5850	1
612	-----	---	-----	---	-----	---	-----	---	1.53	3	1.5297	7
603	1.51	s	1.50	20	1.51	20	1.51	40	1.51	5	1.5062	24
054	-----	---	-----	---	-----	---	-----	---	-----	---	1.4916	1
621	1.47	vw	1.47	3	-----	---	-----	---	-----	---	1.4732	7
315	-----	---	-----	---	1.44	10	-----	---	-----	---	1.4458	1
072												
710	1.43	s	1.43	15	1.43	40	1.43	40	1.43	13	1.4306	25
514	-----	---	-----	---	-----	---	-----	---	-----	---	1.4129	1
045	-----	---	-----	---	-----	---	-----	---	-----	---	1.4080	1
262												
006	1.376	s	1.38	15	1.37	40	1.37	40	1.37	1	1.3755	8
235											1.3737	6
630	1.365	w	-----	---	1.36	10	-----	---	-----	---	1.3608	5
443	-----	---	-----	---	-----	---	-----	---	-----	---	1.3566	5
434	1.344	w	-----	---	1.34	10	-----	---	-----	---	1.3454	2
505	-----	---	1.31	3	-----	---	-----	---	-----	---	1.3113	2
425	-----	---	-----	---	1.28	10	-----	---	-----	---	1.2833	<1
802												
713	1.271	vs	1.27	50	1.259	100	1.275	100	1.27	24	1.2692	36
226	1.258	w–vw	-----	---	1.246	10	-----	---	1.25	5	1.2584	4
633	1.222	s	1.22	18	-----	---	-----	---	1.22	10	1.2200	11
345	-----	---	-----	---	1.207	60	1.206	60	-----	---	1.2094	2
182												
900	1.201	s	1.20	8	-----	---	-----	---	-----	---	1.2005	5
416	1.189	s	1.19	8	1.186	40	1.187	40	-----	---	1.1882	5
642	-----	---	1.17	3	1.177	40	1.176	40	-----	---	1.1852	3
336	-----	---	1.15	3	1.150	20	1.150	20	-----	---	1.1469	3
553	-----	---	1.14	5	-----	---	-----	---	-----	---	1.1358	3
084	-----	---	-----	---	1.118	40	1.117	20	-----	---	1.1296	4
265	-----	---	1.11	3	1.097	20	-----	---	-----	---	1.1092	2
562	-----	---	-----	---	1.091	20	-----	---	-----	---	1.0916	5
823	-----	---	-----	---	-----	---	-----	---	-----	---	1.0830	1
526	-----	---	1.08	5	1.079	20	-----	---	-----	---	1.0760	3
---	-----	---	-----	---	1.063	20	-----	---	-----	---	-----	---
018	-----	---	-----	---	-----	---	-----	---	-----	---	1.0266	1
571												
716	-----	---	0.994	5	-----	---	-----	---	-----	---	0.9915	3

References

[1] W. Schütz, Die kristallchemische Verwandtschaft zwischen Germanium und Silicium, Z. physik. Chem. **31B**, 292–308 (1936).

[2] W. Zachariasen, Notiz über die Kristallstruktur von Phenakit, Willemit und Verwandten Verbindungen, Norske Geol. Tidsskr. **B9**, 65–73 (1926).

[3] R. A. Morgan and F. A. Hummel, Reactions of BeO and SiO$_2$; Synthesis and decomposition of phenacite, J. Am. Ceram. Soc. **32**, 250–255 (1949).

[4] W. L. Bragg, The structure of phenacite, Be$_2$SiO$_4$, Proc. Roy. Soc. **A 113**, 642–657 (1926).

[5] C. Gottfried, Über die Struktur der Phenakit-Dioptasgruppe, Neues Jahrb. Mineral. Geol., Beilage Bd. **55A**, 392–400 (1927).

[6] B. Gossner, Röntgenographische Untersuchung von Silikaten, Centr. Mineral. Geol. **No. 2A**, 39–44 (1927).

Bismuth Oxybromide, BiOBr (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
3-0733	2.81 8. 1.79	Copper	British Museum

Additional published patterns. None.

NBS sample. The sample of bismuth oxybromide was prepared by heating bismuth iodide with bromine water. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon; 0.001 to 0.01 percent aluminum; and 0.0001- to 0.001-percent each of silver, boron, calcium, iron, magnesium, and lead.

The sample was colorless. The refractive indices are too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by the British Museum were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
British Museum	102	001	104
National Bureau of Standards	102	110	001

Structural data. Bannister and Hey [1] in 1935 determined that bismuth oxybromide has lead fluorochloride-type structure, the space group P4/nmm (No. 129), and 2(BiOBr) per unit cell.

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

Lattice constants

		a	*c*
		A	A
1935	Bannister and Hey [1]	3.93	8.13
1941	Sillén [2]	3.923	8.092
1958	National Bureau of Standards	3.926	8.103 at 25°C

The density of bismuth oxybromide calculated from the NBS lattice constants is 8.106 g/cm³ at 25°C.

hkl	---- British Museum Cu, 1.5405 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		A	
001	8.	80	8.11	40
002	4.05	60	4.05	10
101	3.50	60	3.537	30
102	2.82	100	2.821	100
110	2.77	40	2.776	63
003	2.71	40	2.702	5
111	----	---	2.629	5
112	2.28	40	2.286	14
103	----	---	2.229	2
004	2.02	60	2.026	7
200	1.95	40	1.963	27
113	1.93	40	1.937	10
201	----	---	1.907	5
104	1.79	80	1.800	13
211	1.71	40	1.715	9
114	1.64	70	1.6369	13
212	1.60	80	1.6113	36
203	----	---	1.5882	5
105	1.50	60	1.4977	5
204	1.41	50	1.4101	6
220	1.39	40	1.3882	9
006	1.35	50	1.3505	3
214	1.33	60	1.3264	10
106	1.28	40	1.2770	2
302	1.24	50	1.2456	11
310	----	---	1.2415	12
311	1.22	60	1.2232	6
116	----	---	1.2145	6
215	1.19	40	1.1907	5
007	1.15	20	1.1580	5
224	----	---	1.1450	6
313	1.13	20	1.1282	4
107	1.11 (a)	60	1.1123	4

[a] Four additional lines are omitted.

References

[1] F. A. Bannister and M. H. Hey, The crystal structure of bismuth oxyhalides, Mineral. Mag. **24,** 49–58 (1935).

[2] L. G. Sillén, X-ray studies on BiOCl, BiOBr, and BiOI, Svensk Kemisk Tidskrift. **53,** 39 (1941).

Calcium Bromide Hexahydrate, $CaBr_2 \cdot 6H_2O$ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0349	4.03 2.21 3.49	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

A pattern for calcium bromide hexahydrate by Herrmann [2] on card number 2-0296 was deleted from the ASTM card file in the 1955 index.

Additional published patterns. None.

NBS sample. The sample of calcium bromide was obtained from the City Chemical Corp., New York as the anhydrous salt. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of magnesium; 0.001 to 0.01 percent each of aluminum, barium, iron, potassium, manganese, silicon, and strontium; and 0.0001 to 0.001 percent each of copper and lithium.

The sample was colorless and optically negative. The indices of refraction could not be determined by the usual liquid grain immersion method because they were less than 1.41.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units and the *d*-values of the Herrmann pattern were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	110,001	211	200,101
Herrmann	110,001	200,101	210,201
National Bureau of Standards	110	111	101

Structural data. Calcium bromide hexahydrate was found to be isostructural with strontium chloride hexahydrate by Herrmann [2] in 1931. The structure of strontium chloride-type substances was determined by Jensen [3] in 1940. Calcium bromide hexahydrate has the space group P321 (No. 150) with 1($CaBr_2 \cdot 6H_2O$) per unit cell.

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

The density of calcium bromide hexahydrate calculated from the NBS lattice constants is 2.221 g/cm³ at 25°C.

Lattice constants

		a	c
		A	A
1931	Herrmann [2]	7.99	3.98
1958	National Bureau of Standards	8.138	4.015 at 25°C

hkl	1931 Herrmann Cu, 1.5418 A		1938 Hanawalt, Rinn, and and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I	d	I
	A		A		A	
110	3.97	s	4.04	100	4.07	100
001					4.02	14
200	3.44	s	3.50	50	3.52	5
101					3.49	52
111	2.81	m	2.86	50	2.86	54
210	2.63	s	2.66	50	2.663	4
201					2.648	40
300	2.32	m	2.34	50	2.350	35
211	2.20	s	2.21	60	2.220	52
220	----	--	----	--	2.034	19
002	1.99	m	2.01	16	2.008	13
310	----	--	----	--	1.954	1
102	1.91	m	1.92	8	1.931	7
221	1.79	s	1.80	16	1.814	2
112					1.800	11
311	1.73	m	1.75	24	1.758	16
202					1.744	7
401	1.58	m	1.60	16	1.613	4
212					1.603	6
410	1.51	s	1.53	24	1.538	14
302					1.526	9
321	1.47	m	1.498	8	1.500	8
411	----	--	1.433	16	1.436	7
222	----	--			1.429	4
312	1.40	w	1.398	4	1.401	3
330	1.37	w	1.358	8	1.357	3
402	----	--	----	--	1.324	3
103	1.30	m	1.315	4	1.315	3
---	----	--	1.288	4	------	--
421	----	--	1.262	8	1.264	1
203	----	--	----	--	1.251	1
412	1.23	m	1.221	8	1.221	1
511	1.20	m	----	--	1.207	<1
213	1.18	m	1.192	4	1.1961	1
600	----	--	----	--	1.1748	<1
520	1.13	w	----	--	1.1286	<1
431	----	--	----	--	1.1132	<1
313	1.10	w	----	--	1.1042	<1
521	1.09	s	----	--	1.0866	<1
512	----	--	----	--	1.0703	<1
403	1.05	w	----	--	1.0653	<1
611	----	--	----	--	1.0380	<1
323	----	--	----	--	1.0309	<1
440	1.01	m	----	--	1.0171	<1
602	----	--	----	--	1.0138	<1
104	----	--	----	--	0.9937	<1
522	----	--	----	--	.9835	<1
701	----	--	----	--	.9762	<1
204	----	--	----	--	.9651	<1
621	----	--	----	--	.9496	<1
423	----	--	----	--	.9440	<1
214	----	--	----	--	.9391	<1
710	----	--	----	--	.9336	<1
304	----	--	----	--	.9230	<1
513	----	--	----	--	.9194	<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] Z. Herrmann, Über die Strukturen der Strontiumjodid-, Calciumchlorid-, und Calciumbromid- Hexahydrate, Z. anorg. u. allgem. Chem. **197**, 212–218 (1931).

[3] A. Tovbarg Jensen, On the structure of $SrCl_2 \cdot 6H_2O$, Kgl. Danske Videnskab. selskab. Mat. fys. Medd. **17**, no. 9 (1940).

Calcium Formate, $Ca(HCO_2)_2$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0197	5.6 3.43 2.99	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of calcium formate was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of potassium, magnesium, sodium, silicon, and strontium; and 0.0001 to 0.001 percent each of aluminum, barium, copper, iron, and manganese.

The sample was colorless and optically positive with the indices of refraction $N\alpha=1.509$, $N\beta=1.522$, and $N\gamma=1.556$. $2V\cong15°$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	210	311,221	012,321
National Bureau of Standards	210	321	221

Structural data. Nitta [2] in 1928 determined that calcium formate has the space group Pbca (No. 61) and $8[Ca(HCO_2)_2]$ per unit cell.

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

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1928	Nitta [2]	13.41	10.18	6.30
1958	National Bureau of Standards	13.40	10.18	6.282 at 25°C

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
200	6.6	8	6.70	7
210	5.6	100	5.59	100
111	5.0	50	4.96	59
021	----	---	3.95	<1
121	3.83	12	3.79	18
311	3.44	100	3.425	46
221			3.403	88
400	----	---	3.348	6
102	3.11	16	3.058	20
230	3.00	80	3.005	3
321			2.962	92
112	----	---	2.931	9
131	----	---	2.917	7
202	2.87	25	2.841	28
212	2.78	8	2.739	19
022	----	---	2.675	6
421	2.57	6	2.556	1
040	2.53	20	2.546	3
312	----	---	2.490	17
222	----	---	2.485	20
511	2.41	6	2.395	14
322	2.31	25	2.292	21
402				
132	2.25	40	2.272	2
600			2.232	29
610	2.19	12	2.181	18
332	----	---	2.050	6
113	----	---	2.027	8
440				
531	2.00	25	1.996	15
042			1.978	18
142	----	---	1.957	5
250	1.94	8	1.949	8
023	----	---	1.938	4
123	----	---	1.918	12
151				
630	1.88	12	1.866	10
313				
602	----	---	1.820	1
342	----	---	1.808	1
612	1.79	10	1.791	4
133	1.74	10	1.767	10
532	----	---	1.747	1
721	----	---	1.724	16
233				
442	----	---	1.703	4
640	----	---	1.678	10
423				
333	----	---	1.656	3
252				
810	----	---	1.653	3

Calcium Formate, $Ca(CHO_2)_2$ (orthorhombic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
513	----	---	1.629	2
161	----	---	1.626	3
043	----	---	1.616	<1
811	----	---	1.599	1
352	----	---	1.593	3
542				
433	----	---	1.573	<1
004	----	---	1.571	<1
361	----	---	1.539	3

The density of calcium formate calculated from the NBS lattice constants is 2.016 g/cm³ 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] I. Nitta, The crystal structure of some rhombic formates, Sci. Papers Inst. Phys. Chem. Research Tokyo **9**, 151–163 (1928).

Cerium(III) Fluoride, CeF_3 (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
3–1054	2.01 1.44 0.990	Copper	Oftedal [1] 1929.

Additional published patterns. None.

NBS sample. The sample of cerous fluoride was obtained from the City Chemical Corp., New York. It was annealed at 1,000°C in an argon atmosphere. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium and lanthanum; 0.001 to 0.01 percent each of magnesium and silicon; and 0.0001 to 0.001 percent of titanium.

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

hkl	1929 Oftedal Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
002	-----	---	3.64	40
110	-----	---	3.55	34
111	-----	---	3.195	100
112	-----	---	2.545	12
211	-----	---	2.219	4
300	2.06	m	2.054	44
113	2.01	s	2.004	52
004	-----	---	1.8202	5
302	1.78	m	1.7885	30
221	1.73	w	1.7275	18
114	-----	---	1.6197	4
222	-----	---	1.5975	3
214	1.44	s	1.4339	12
223				
304	1.36	m	1.3616	9
115	1.35	m	1.3473	8
410			1.3439	6
411	1.32	m	1.3216	14
224	-----	---	1.2715	2
412	-----	---	1.2612	2
006	-----	---	1.2135	2
330	-----	---	1.1854	4
404	-----	---	1.1755	12
413				
116	-----	---	1.1480	3
225	1.13	s$^-$	1.1268	10
332				
414	-----	---	1.0810	3
306	1.05	m	1.0443	5
600	-----	---	1.0264	3
226	-----	---	1.0021	2
117	-----	---	0.9981	3
334	-----	---	.9932	5
415	0.990	s	.9877	8
521	-----	---	.9774	5
522	-----	---	.9520	1
523	-----	---	.9136	5
416	-----	---	.9005	3
227	-----	---	.8976	3
604	-----	---	.8942	3
441	-----	---	.8825	3
524	-----	---	.8670	2
336	-----	---	.8478	4

Interplanar spacings and intensity measurements. The *d*-values of the Oftedal pattern were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Oftedal	113	223	415
National Bureau of Standards	111	113	300

Structural data. Oftedal [2] in 1931 determined that cerium fluoride has the space group $P6_3/mcm$ (No. 193) with $6(CeF_3)$ per unit cell. Cerium fluoride is used as a structure type.

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

Lattice constants

		a	c
		A	A
1929	Oftedal [1]	7.128	7.288
1958	National Bureau of Standards	7.112	7.279 at 25°C

The density of cerium fluoride calculated from the NBS lattice constants is 6.159 g/cm³ at 25°C.

References

[1] I. Oftedal, Über die Kristallstruktur von Tysonit und einigen künstlich dargestellten Lanthanidenfluoriden, Z. physik. Chem. (B) **5**, 272–291 (1929).

[2] I. Oftedal, Zur Kristallstruktur von Tysonit (Ce, La, . . .)F_3, Z. physik. Chem. (B) **13**, 190–200 (1931).

Cesium Bromate, $CsBrO_3$ (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium bromate was prepared at NBS by reaction of cesium bromide with silver bromate. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of rubidium; 0.01 to 0.1 percent of potassium; 0.001 to 0.01 percent each of silver, aluminum, sodium, and silicon; and 0.0001 to 0.001 percent each of calcium, iron, lithium, and magnesium.

The sample was colorless and optically negative. The refractive indices are $N_o=1.684$ and $N_e=1.601$.

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

Pattern	1	2	3
National Bureau of Standards	012	110	202

Structural data. The structure of cesium bromate has not been published but because of the similarity of the patterns, it is thought to have potassium bromate-type structure. The NBS pattern was indexed assuming the space group to be R3m (No. 160) with $1(CsBrO_3)$ per unit rhombohedral cell or $3(CsBrO_3)$ per unit hexagonal cell.

Lattice constants

		a	c
		A	A
1958	National Bureau of Standards	6.506	8.230 at 25°C

The density of cesium bromate calculated from the NBS lattice constants is 4.306 g/cm³ at 25°C.

hkl hex.	1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*
	A	
101	4.65	8
012	3.32	100
110	3.25	90
003	2.744	8
021	2.666	13
202	2.329	38
113	2.096	5
211	2.060	3
104	1.9332	13
122	1.8915	23
300	1.8779	12
024	1.6614	8
220	1.6268	9
015	1.5805	2
303	1.5475	1
131	1.5365	1
214	1.4798	10
312	1.4611	9
205	1.4215	4
223	1.3992	2
401	1.3897	1
006	1.3723	<1
042	1.3328	4
125	1.3028	1
116	1.2638	3
134	1.2443	4
232	1.2330	4
410	1.2299	6
404	1.1623	1
107	1.1511	1
315	1.1341	<1
413	1.1212	<1
306	1.1075	1
324	1.0946	<1
027	1.0845	1

Cesium Bromoplatinate, Cs_2PtBr_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium bromoplatinate was prepared at NBS from cesium bromide and bromoplatinic acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium; and 0.001 to 0.01 percent each of aluminum, barium, calcium, potassium, rubidium, silicon, and tin.

The color of the sample was orange. The index of refraction is 1.972.

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

Pattern	1	2	3
National Bureau of Standards	400	222	111

Structural data. The structure of cesium bromoplatinate has not been published. Because of the similarity of patterns, it is thought to be isostructural with cesium bromoselenate. The NBS pattern was indexed assuming the space group to be Fm3m (No. 225) with $4(Cs_2PtBr_6)$ per unit cell.

Lattice constants

		A
1953	Sharpe [1]	10.63
1958	National Bureau of Standards	10.643 at 26°C

The density of cesium bromoplatinate calculated from the NBS lattice constant is 5.180 g/cm³ at 26°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 26°C		
	d	*I*	*a*
	A		*A*
111	6.16	70	10.65
200	5.32	9	10.65
220	3.76	54	10.65
311	3.209	28	10.64
222	3.073	74	10.65
400	2.661	100	10.64
331	2.443	4	10.65
420	2.381	3	10.65
422	2.173	24	10.64
511	2.049	25	10.65
440	1.882	63	10.65
531	1.7987	18	10.641
600	1.7739	4	10.643
620	1.6828	12	10.643
533	1.6236	4	10.646
622	1.6044	21	10.642
444	1.5363	20	10.644
711	1.4905	13	10.644
642	1.4221	11	10.642
731	1.3855	1	10.642
800	1.3303	9	10.642
822	1.2543	6	10.643
751	1.2289	6	10.643
662	1.2208	7	10.643
840	1.1899	15	10.643
911	1.1681	6	10.642
664	1.1346	5	10.643
931	1.1158	5	10.644
844	1.0864	12	10.644
933	1.0700	4	10.644
10·2·0	1.0439	7	10.646
951	1.0290	8	10.644
953	0.9924	16	10.643
10·4·2	.9716	17	10.643
880	.9408	17	10.643
11·3·1	.9299	20	10.643
10·6·0	.9127	13	10.643
11·3·3	.9028	6	10.644
10·6·2	.8994	11	10.642
12·0·0	.8869	33	10.643
12·2·2	.8633	15	10.644
11·5·3	.8549	9	10.643
12·4·0	.8414	22	10.643
991	.8336	9	10.643
10·8·2	.8212	10	10.643
13·1·1	.8139	15	10.643
10·6·6	.8116	6	10.644
12·4·4	.8022	20	10.643
13·3·1	.7955	13	10.643
12·6·2	.7846	5	10.642
Average value of last five lines			10.643

References

[1] A. G. Sharpe, Chemistry of the platinum metals. Part III. Lattice constants of some chloropalladates, bromopalladates, and bromoplatinates, J. Chem. Soc. 4177–4179 (1953).

Cesium Bromoselenate, Cs_2SeBr_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium bromoselenate was prepared at NBS by dissolving SeO_2 in HBr and mixing with a solution of CsBr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of iron and rubidium; and 0.001 to 0.01 percent each of aluminum, bismuth, chromium, sodium, nickel, and silicon.

The color of the sample was reddish-orange. The refractive index was too high to be determined by the usual liquid immersion technique.

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

Pattern	1	2	3
National Bureau of Standards	222	400	440

Structural data. The structure of cesium bromoselenate has not been published, but because of the similarity of patterns, it is thought to be isostructural with ammonium bromoselenate, $(NH_4)_2SeBr_6$. The NBS pattern was indexed assuming the space group to be Fm3m (No. 225) and $4(Cs_2SeBr_6)$ per unit cell.

Lattice constant

		A
1958	National Bureau of Standards	10.722 at 25°C

The density of cesium bromoselenate calculated from the NBS lattice constant is 4.440 g/cm³ at 25°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*
	A		*A*
111	6.19	17	10.73
200	5.36	2	10.74
220	3.79	23	10.72
311	3.231	9	10.72
222	3.095	100	10.72
400	2.679	74	10.72
331	2.462	2	10.73
420	2.398	1	10.72
422	2.188	10	10.72
511	2.063	6	10.72
440	1.8949	47	10.72
531	1.8117	4	10.72
600	1.7878	<1	10.73
620	1.6949	4	10.72
533	1.6348	<1	10.72
622	1.6160	31	10.72
444	1.5473	16	10.72
711	1.5014	3	10.72
642	1.4328	4	10.72
731	1.3950	2	10.72
800	1.3404	6	10.72
820	1.2999	<1	10.72
822	1.2633	2	10.72
662	1.2300	10	10.72
840	1.1989	12	10.72
844	1.0946	8	10.72
951	1.0366	2	10.722
10·2·2	1.0318	5	10.723
880	0.9478	2	10.723
10·6·2	.9061	4	10.722
12·0·0	.8934	5	10.721
12·2·2	.8697	<1	10.723
12·4·0	.8475	2	10.721
10·6·6	.8176	1	10.723
12·4·4	.8081	1	10.721
Average value of last five lines			10.722

Cesium Chlorate, $CsClO_3$ (trigonal)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium chlorate was prepared at NBS by reaction of solutions of cesium bromide and silver chlorate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of sodium and rubidium; 0.001 to 0.01 percent each of calcium and potassium; and 0.0001 to 0.001 percent each of silver, aluminum, barium, copper, iron, magnesium, silicon, and strontium.

The sample was colorless and optically negative. The refractive indices are $N_o=1.587$ and $N_e=1.508$.

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

Pattern	1	2	3
National Bureau of Standards	012	110	101

Structural data. The structure of cesium chlorate has not been published but because of the similarity of the patterns, it is thought to have potassium bromate-type structure. The NBS pattern was indexed assuming the space group to be R3m (No. 160) with 1($CsClO_3$) per unit rhombohedral cell or 3($CsClO_3$) per unit hexagonal cell.

Lattice constant

		a	c
		A	A
1958	National Bureau of Standards	6.424	8.254 at 25°C

The density of cesium chlorate calculated from the NBS lattice constants is 3.653 g/cm³ at 25°C.

Cesium Chlorate, $CsClO_3$ (trigonal)

hkl hex.	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		*hkl* hex.	1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*		*d*	*I*
	A			A	
101	4.61	45	321	1.2615	2
102	3.316	100	134	1.2357	3
110	3.215	82	232	1.2195	6
003	2.751	16	410	1.2143	5
021	2.636	35	107 404	1.1534	2
202	2.305	43			
113	2.091	18	315	1.1272	2
211	2.039	17	413	1.1106	3
104	1.9367	11	306	1.1048	3
122	1.8743	24	051	1.1023	2
300	1.8546	13	027 324	1.0851	1
024	1.6573	8			
220	1.6062	8	502	1.0743	2
015	1.5823	5	330	1.0706	1
303	1.5377	5	045	1.0638	1
			226	1.0448	2
131	1.5165	6	241	1.0430	2
214	1.4729	10			
312	1.4453	12	217	1.0284	2
205	1.4198	3	422	1.0190	2
223	1.3871	4	018	1.0143	<1
			235	1.0097	1
006	1.3757	1	333	0.9978	1
401	1.3714	2			
042	1.3177	2	511	.9918	<1
125	1.2985	3	054	.9793	1
116	1.2647	4	152	.9711	2
			208	.9676	1

Cesium Chromium Sulfate Dodecahydrate, $CsCr(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium chromium sulfate dodecahydrate was prepared at NBS from cesium nitrate 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, cobalt, potassium, magnesium, and rubidium; and 0.0001 to 0.001 percent each of barium, copper, iron, manganese, and silicon.

The color of the sample was bright green. The index of refraction is 1.482.

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

Pattern	1	2	3
National Bureau of Standards	220	331	420

Structural data. Klug and Alexander [1] in 1940 determined that cesium chromium sulfate do-

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*
	A		A
111	7.2	11	12.4
200	6.21	49	12.42
210	5.56	28	12.43
211	5.07	13	12.42
220	4.386	100	12.40
221	4.137	29	12.41
222	3.577	33	12.39
302	3.4410	10	12.406
321	3.3164	28	12.409
400	3.1014	63	12.406
410	3.0084	18	12.404
331	2.8447	78	12.400
420	2.7736	69	12.404
421	2.7064	11	12.402
422	2.5327	47	12.408
511	2.3864	26	12.400
440	2.1933	19	12.407
600	2.0678	34	12.407
620	1.9608	47	12.401
533	1.8915	13	12.403

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	I	a
	A		A
622	1.8700	14	12.404
444	1.7898	9	12.401
711	1.7366	7	12.402
640	1.7196	20	12.400
642	1.6573	46	12.402
731	1.6151	9	12.406
800	1.5506	7	12.405
820	1.5041	23	12.403
822	1.4621	6	12.406
831	1.4421	18	12.405
751	1.4326	7	12.407
662	1.4230	10	12.405
832	1.4135	6	12.403
840	1.3864	11	12.400
911	1.3611	7	12.400
842	1.3536	7	12.406
664	1.3224	6	12.405
931	1.3004	6	12.405
844	1.2660	6	12.404
10·0·0	1.2405	4	12.405
10·2·0	1.2163	12	12.404
10·2·2	1.1936	3	12.404
953	1.1567	3	12.404
10·4·0	1.1519	6	12.406
10·6·0	1.0640	3	12.408
11·3·3	1.0523	6	12.406
10·6·2	1.0483	2	12.404
12·0·0	1.0340	4	12.408
12·2·2	1.0060	3	12.403
12·4·2	0.9687	5	12.406
Average of last five lines			12.405

decahydrate is a beta alum. Lipson [2] in 1935 had determined that the beta alums have methyl ethyl aluminum sulfate dodecahydrate-type structure, the space group Pa3 (No. 205), and $4[CsCr(SO_4)_2 \cdot 12H_2O]$ per unit cell.

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]	12.403 at 25°C
1958	National Bureau of Standards	12.405 at 25°C

The density of cesium chromium sulfate dodecahydrate calculated from the NBS lattice constant is 2.063 g/cm³ at 25°C.

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).

Cesium Fluoborate, $CsBF_4$ (orthorhombic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium fluoborate was prepared at NBS by precipitation from CsBr and HBF_4. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of sodium; 0.01 to 0.1 percent each of calcium and rubidium; 0.001 to 0.01 percent each of potassium and strontium; and 0.0001 to 0.001 each of aluminum, barium, copper, iron, magnesium, and silicon.

The sample was colorless. The indices of refraction are too low to be determined by the usual liquid immersion methods.

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

Pattern	1	2	3
National Bureau of Standards	122	211	210

Structural data. Klinkenberg [1] in 1937 determined that cesium fluoborate is isomorphous with barium sulphate ($BaSO_4$). The space group is Pnma (No. 62), and $4(CsBF_4)$ per unit cell.

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

Lattice constants

		a	b	c
		A	A	A
1937	Klinkenberg [1]	9.45	5.84	7.67
1958	National Bureau of Standards	9.658	5.895	7.636 at 25°C

The density of cesium fluoborate calculated from the NBS lattice constants is 3.355 g/cm³ at 25°C.

References

[1] L. J. Klinkenberg, The crystal structure of $NaOH \cdot BF_2$ and of the alkali fluoborates and $TIBF_4$, Rec. Trav. Chim. Pays-Bas **56**, 36–40 (1937).

Cesium Fluoborate, $CsBF_4$ (orthorhombic)

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I
	A	
200	4.83	23
011	4.66	40
111	4.20	47
201	4.08	21
002	3.816	33
210	3.734	62
102	3.550	53
211	3.353	83
112	3.041	25
301	2.962	20
020	2.947	34
212	2.670	9
311	2.648	6
220	2.515	23
302 103	2.461	27
221	2.390	19
401	2.302	26
122	2.268	100
410	2.234	26
411	2.145	3
222	2.101	10
321	2.091	10
303	1.996	12
412	1.928	5
004	1.908	11
031	1.903	12
313	1.890	8
501 104	1.873	9
421	1.815	8
511 114	1.785	6
204	1.775	5
231	1.770	6
403	1.751	2
132	1.720	9
214	1.700	4
512	1.654	19
304	1.642	8
331	1.637	4
024	1.6025	5
314	1.5813	13
503	1.5386	10
610	1.5532	7
332	1.5359	15
430	1.5244	12
105	1.5087	1
513	1.4890	1
015	1.4784	7
115	1.4613	5
205	1.4564	8
414	1.4515	5
612	1.4379	3
432	1.4158	7
215	1.4135	7
333	1.4011	2
621	1.3893	5
241	1.3862	1
523	1.3640	8
622	1.3245	3
711 514	1.3229	3
225	1.3056	5
702	1.2976	5
532	1.2955	2
405	1.2908	5
006	1.2726	5
342 143	1.2644	4
415	1.2610	4
325	1.2497	5
630	1.2453	5
441	1.2411	4
631	1.2295	2
800	1.2074	3

Cesium Gallium Sulfate Dodecahydrate, $CsGa(SO_4)_2 \cdot 12H_2O$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium gallium sulfate dodecahydrate was prepared at NBS from cesium chloride, gallium and sulfuric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, potassium, magnesium, nickel, and rubidium; 0.001 to 0.01 percent each of barium, iron, molybdenum, sodium, and silicon; and 0.0001 to 0.001 percent each of chromium and manganese. The sample was colorless. The index of refraction is 1.461.

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

Pattern	1	2	3
National Bureau of Standards	220	420	200

Structural data. Klug and Kieffer [1] in 1943 determined that cesium gallium sulfate dodecahydrate is a beta alum. Lipson [2] in 1935 had determined that the beta alums have methyl ethyl aluminum sulfate dodecahydrate-type structure, the space group Pa3 (No. 205), and $4[CsGa(SO_4)_2 \cdot 12H_2O]$ per unit cell.

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

Cesium Gallium Sulfate Dodecahydrate, $CsGa(SO_4)_2\cdot 12H_2O$ (cubic)

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	I	a
	A		A
111	7.17	7	12.4
200	6.21	48	12.4
210	5.56	27	12.4
211	5.07	8	12.4
220	4.39	100	12.4
221	4.13	19	12.4
222	3.578	31	12.40
302	3.438	5	12.40
321	3.315	20	12.40
400	3.101	35	12.41
410	3.008	12	12.40
331	2.845	45	12.40
420	2.772	50	12.40
421	2.706	8	12.40
422	2.532	32	12.40
511	2.386	10	12.40
432	2.304	4	12.41
440	2.1928	15	12.404
531	2.0961	<1	12.401
600	2.0664	20	12.398
611	2.0111	<1	12.397
620	1.9612	24	12.404
621	1.9367	<1	12.401
533	1.8912	5	12.401
622	1.8688	8	12.396
630	1.8478	1	12.396
631	1.8284	<1	12.401
444	1.7898	3	12.400
711	1.7360	<1	12.398
640	1.7196	13	12.400
721	1.6876	1	12.401
642	1.6570	9	12.400
722	1.6423	1	12.399
731	1.6146	1	12.402
800	1.5502	3	12.402
810	1.5382	1	12.401
733	1.5147	1	12.398
820	1.5043	13	12.405
822	1.4619	9	12.405
830	1.4517	1	12.403
831	1.4419	1	12.404
751	1.4316	1	12.401
662	1.4223	4	12.399
832	1.4131	1	12.400
840	1.3862	5	12.399
911	1.3613	1	12.402
842	1.3530	4	12.400
664	1.3219	6	12.401
931	1.3000	2	12.401
Average of last five lines			12.401

Lattice constants

		A
1943	Klug and Kieffer [1]	12.402 at 25°C
1958	National Bureau of Standards	12.401 at 25°C

The density of cesium gallium sulfate dodecahydrate calculated from the NBS lattice constant is 2.127 g/cm³ at 25°C.

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

Erbium Sesquioxide, Er_2O_3 (cubic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0827	3.06 1.87 1.59	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Staritzky [2] 1956	Copper, K_α

NBS sample. The sample of erbium sequioxide was prepared at NBS by Ernest L. Weise. It was annealed at 1,000°C for 2 hr before using. Spectrographic analysis detected no impurities greater than 0.01 percent. The color of the sample was pink. The index of refraction is 1.932.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	222	440	622
Staritzky	222	440	622
National Bureau of Standards	222	440	400

Structural data. Zachariasen [3] in 1927 determined that erbium sesquioxide has the thallium oxide-type structure, the space group $I2_13$ (No. 199) and $16(Er_2O_3)$ per unit cell.

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

Lattice constants

		a
		A
1925	Goldschmidt, Barth, and Lunde [4]	10.56
1927	Zachariasen [3]	10.56
1930	Pauling and Shappell [5]	10.56
1939	Bommer [6]	10.53
1954	Templeton and Dauben [7]	10.547
1956	Staritzky [2]	10.550
1958	National Bureau of Standards	10.548 at 25°C

The density of erbium sesquioxide calculated from the NBS lattice constant is 8.654 g/cm³ at 25°C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1956 Staritzky Cu, 1.5418 A			1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
211	4.32	7	10.6	4.29	12	10.51	4.308	15	10.552
222	3.07	100	10.6	3.04	100	10.53	3.045	100	10.550
321	----	--	----	2.810	2	10.51	2.818	3	10.546
400	2.65	27	10.6	2.631	40	10.52	2.637	40	10.550
411	2.49	3	10.6	2.481	9	10.55	2.486	8	10.549
420	----	--	----	2.352	2	10.52	2.3575	2	10.543
332	2.25	3	10.6	2.243	10	10.52	2.2488	6	10.448
422	----	--	----	2.148	2	10.52	2.1532	2	10.548
510	2.07	13	10.6	2.064	16	10.52	2.0687	10	10.548
521	----	--	----	1.922	8	10.53	1.9258	4	10.545
440	1.87	50	10.6	1.861	62	10.527	1.8645	44	10.547
530	1.81	7	10.6	1.806	5	10.531	1.8094	3	10.550
600	----	--	----	1.755	1	10.530	1.7590	1	10.554
611	1.71	7	10.5	1.710	10	10.541	1.7113	7	10.549
620	----	--	----	1.665	2	10.530	1.6681	1	10.550
541	----	--	----	1.626	9	10.538	1.6276	5	10.548
622	1.59	42	10.6	1.589	53	10.540	1.5903	32	10.549
631	----	--	----	1.553	12	10.533	1.5558	8	10.552
444	1.52	7	10.5	1.521	14	10.538	1.5228	7	10.550
710	----	--	----	1.490	5	10.536	1.4918	3	10.549
640	----	--	----	1.462	3	10.543	1.4629	2	10.549
721	----	--	----	1.434	7	10.538	1.4359	4	10.552
642	----	--	----	1.409	4	10.544	1.4099	2	10.551
732	----	--	----	(a)	--	------	1.3398	3	10.550
800	1.325	3	10.60	------	--	------	1.3189	5	10.551

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A			1956 Staritzky Cu, 1.5418 A			1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
811	----	--	----	------	--	------	1.2988	4	10.552
820	----	--	----	------	--	------	1.2795	2	10.551
653	----	--	----	------	--	------	1.2608	3	10.549
822	----	--	----	------	--	------	1.2436	2	10.552
831	----	--	----	------	--	------	1.2266	3	10.552
662	1.222	7	10.65	------	--	------	1.2102	8	10.550
840	1.187	3	10.62	------	--	------	1.1794	6	10.549
910	----	--	----	------	--	------	1.1650	1	10.550
842	1.147	3	10.51	------	--	------	1.1511	2	10.550
921	----	--	----	------	--	------	1.1377	3	10.550
930	----	--	----	------	--	------	1.1119	3	10.548
932	1.089	7	10.56	------	--	------	1.0833	2	10.551
844	----	--	----	------	--	------	1.0768	4	10.550
941	----	--	----	------	--	------	1.0656	3	10.549
10·0·0	----	--	----	------	--	------	1.0547	2	10.547
10·1·1	----	--	----	------	--	------	1.0444	1	10.548
10·2·0	----	--	----	------	--	------	1.0345	3	10.550
950	----	--	----	------	--	------	1.0246	<1	10.550
10·2·2	----	--	----	------	--	------	1.0150	4	10.548
10·3·1	----	--	----	------	--	------	1.0058	3	10.550
871	----	--	----	------	--	------	0.9881	2	10.550
10·4·0	----	--	----	------	--	------	.9794	3	10.549
10·3·3	----	--	----	------	--	------	.9710	2	10.548
10·4·2	----	--	----	------	--	------	.9630	2	10.549
11·1·0	----	--	----	------	--	------	.9551	1	10.549
11·2·1	----	--	----	------	--	------	.9398	3	10.549
880	----	--	----	------	--	------	.9322	2	10.547
10·4·4	----	--	----	------	--	------	.9182	3	10.549
11·3·2	----	--	----	------	--	------	.9113	2	10.548
10·6·0	----	--	----	------	--	------	.9045	<1	10.548
11·4·1	----	--	----	------	--	------	.8978	1	10.547
10·6·2	----	--	----	------	--	------	.8914	3	10.547
965	----	--	----	------	--	------	.8853	1	10.550
12·0·0	----	--	----	------	--	------	.8789	1	10.547
12·1·1	----	--	----	------	--	------	.8730	3	10.549
12·2·0	----	--	----	------	--	------	.8671	2	10.549
11·5·2	----	--	----	------	--	------	.8613	2	10.549
12·2·2	----	--	----	------	--	------	.8555	3	10.547
12·3·1	----	--	----	------	--	------	.84987	1	10.547
11·6·1	----	--	----	------	--	------	.83921	2	10.548
12·4·0	----	--	----	------	--	------	.83389	2	10.548
12·3·3	----	--	----	------	--	------	.82877	1	10.548
12·4·2	----	--	----	------	--	------	.82367	4	10.548
11·6·3	----	--	----	------	--	------	.81874	2	10.548
10·8·2	----	--	----	------	--	------	.81380	3	10.548
13·1·0	----	--	----	------	--	------	.80893	2	10.547
10·6·6	----	--	----	------	--	------	.80429	1	10.5482
13·2·1	----	--	----	------	--	------	.79963	1	10.5478
12·4·4	----	--	----	------	--	------	.79507	1	10.5478
13·3·0	----	--	----	------	--	------	.79062	1	10.5482
12·6·0	----	--	----	------	--	------	.78622	4	10.5482
13·3·2	----	--	----	------	--	------	.78189	2	10.5483
Average value of last five lines--			10.59	------	--	------	------	--	10.5481

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[a] More than 50 additional lines were not published [2].

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. Staritzky, Erbium Sesquioxide, Er_2O_3, Anal. Chem. **28,** No. 12, 2023–2024 (1956).

[3] W. Zachariasen, The crystal structure of the modification C of the sesquioxides of the rare earth metals, and of indium and thallium, Norsk Geol. Tidssk. **9,** 310–316 (1927).

[4] V. M. Goldschmidt, T. Barth, and G. Lunde, Isomorphie und Polymorphie der Sesquioxide, die Lanthaniden-Kontraktion und ihre Konsequenzen, Skrifter Norske Videnskaps-Akad. Oslo I. Mat. Naturv. Kl. No. **7,** 1–59 (1925).

[5] L. Pauling and M. D. Shappell, The crystal structure of Bixbyite and the C-modification of the sesquioxides, Z. Krist. **75,** 128–142 (1930).

[6] H. Bommer, Die Gitterkonstanten der C-Formen der Oxyde der seltenen Erdmetalle, Z. anorg. allgem. chem. **241,** 273–280 (1939).

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

Gallium Phosphate, (α-quartz type) $GaPO_4$ (trigonal)

ASTM cards. None.

Additional published patterns. A pattern listing lines common to α-quartz was published by Shafer and Roy [1] in 1956.

NBS sample. The gallium phosphate was prepared by Alvin Perloff at NBS in a hydrothermal bomb using gallium metal and an excess of dilute phosphoric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, chromium, sodium, and nickel; 0.001 to 0.01 percent each of copper and silicon; and 0.0001 to 0.001 percent each of calcium, magnesium, manganese, molybdenum, lead, and tin.

The color of the sample was pale yellow and it was optically positive. The indices of refraction are N_o=1.598 and N_e=1.593.

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

Pattern	1	2	3
National Bureau of Standards	102	100	104

Structural data. Perloff [2] in 1956 reported gallium phosphate (α-quartz type) as being isostructural with the berlinite form of aluminum phosphate, the space groups $P3_121$ (No. 152) or $P3_221$ (No. 154), and 1($GaPO_4$) per unit cell. $GaPO_4$ is also reported to exist in the low and high cristobalite forms [1], [2], and [3].

hkl. hex.	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		*hkl.* hex.	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		*hkl.* hex.	1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*		*d*	*I*		*d*	*I*
	A			*A*			*A*	
100	4.24	25	214	1.3870	10	321	.9702	1
101	3.96	8	302	1.3703	7	322	.9591	2
003	3.68	3	108	1.3136	6	309	.9271	1
102	3.37	100	215	1.2986	1			
103	2.783	2				410	.9264	<1
			304	1.2600	3	0·0·12	.9206	1
110	2.450	11	220	1.2261	2	406	.9196	2
111	2.393	3	221	1.2179	1	324	.9185	2
104	2.316	19	216	1.2099	2	412	.9135	1
112	2.240	10	118	1.2036	1			
200	2.123	15				2·1·10	.9111	2
			222	1.1963	1	1·0·12	.9000	2
201	2.085	1	310	1.1774	3	318	.8962	1
113	2.041	2	311	1.1709	<1	414	.8783	1
202	1.982	2	312	1.1517	1	3·0·10	.8711	<1
105	1.961	4	217	1.1255	<1			
203	1.839	11				1·1·12	.8623	1
			313	1.1217	1	2·0·12	.8449	2
114	1.834	12	119	1.0978	<1	408	.8418	1
106	1.690	6	314	1.0834	4	502	.8395	1
204	1.684	6	1·0·10	1.0699	2	416	.8276	<1
115	1.6417	3	400	1.0615	1			
210	1.6050					2·2·10	.8207	2
			218	1.0471	2	330	.8170	<1
211	1.5880	3	402	1.0423	1	504	.8115	1
212	1.5405	12	226	1.0205	1	3·1·10	.8057	1
107	1.4790	2	1·1·10	1.0076	3	420	.8023	<1
213	1.4713	4	316	0.9921	4			
301	1.4029	1				2·1·12	.7987	2
			404	.9909	1	328	.7959	1
206	1.3908	11	308	.9888	<1	422	.7939	1

The unit-cell measurements reported by Perloff and Shafer and Roy are used for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1956	Perloff [2]	4.917	11.10
1956	Shafer and Roy [1]	4.92	11.10
1958	National Bureau of Standards	4.902	11.05 at 25°C

The density of gallium phosphate calculated from the NBS lattice constants is 3.567 g/cm³ at 25°C.

References

[1] E. Shafer and R. Roy, Studies of silica-structure phases: I, $GaPO_4$, $GaAsO_4$, and $GaSbO_4$, J. Am. Ceram. Soc. **39**, No. 10, 330–336 (1956).

[2] A. Perloff, Temperature inversions of anhydrous gallium orthophosphate, J. Am. Ceram. Soc. **39**, No. 3, 83–88 (1956).

[3] R. C. L. Mooney, The crystal structure of aluminum phosphate and gallium phosphate, low-cristobalite type, Acta Cryst **9**, 728–734 (1956).

Germanium Dioxide, GeO_2 (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
3–0552	3.11 1.62 1.00	Copper	Goldschmidt [1] 1932.

Additional published patterns

Source	Radiation
Laubengayer and Morton [2] 1932	--------

NBS sample. The sample of germanium dioxide was prepared at NBS by Charles E. Weir. Tetragonal germanium dioxide was formed by heating hexagonal germanium dioxide hydrothermally at 800°C and 20,000 psi for two days. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of aluminum, calcium, iron, palladium, and platinum; and 0.01 to 0.1 percent each of magnesium, nickel, and tin.

The sample was colorless. The indices of refraction were too high to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by Goldschmidt and those reported by Laubengayer and Morton have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Goldschmidt	110	211	411
Laubengayer and Morton	110	101	211
National Bureau of Standards	110	101	211

hkl	1932 Goldschmidt Cu, 1.5405 A		1932 Laubengayer and Morton ----------		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
110	3.11	100	3.10	100	3.108	100
101	2.40	60	2.390	61	2.399	61
200	2.20	30	2.194	21	2.199	15
111	2.11	20	2.104	9	2.106	12
210	1.97	15	1.965	2	1.967	5
211	1.62	100	1.618	61	1.620	52
220	1.56	70	1.556	15	1.5546	16
002	1.43	30	1.424	7	1.4314	8
310	1.39	60	1.389	11	1.3900	11
301	1.31	80	-----	---	1.3045	19
112	1.30	40	1.299	44	1.3004	17
311	1.25	5	-----	---	1.2506	1
202	1.20	40	1.195	3	1.1995	4
212	-----	---	-----	---	1.1572	2
321	1.12	70	1.117	7	1.1219	7
400	1.10	50	1.096	3	1.0990	3
410	1.07	2	-----	---	1.0666	1
222	1.05	60	-----	---	1.0531	6
330	1.04	60	-----	---	1.0362	3
411	1.00	90	-----	---	0.9991	9
312	-----	---	-----	---	.9972	9
420	0.984	60	-----	---	.9830	4
103	.933	40	-----	---	.9324	2
113	-----	---	-----	---	.9122	<1
402	.872	60	-----	---	.8717	4
510	.863	60	-----	---	.8622	5
213	.859	70	-----	---	.8584	8
501	.841	90	-----	---	.8405	11
332	-----	---	-----	---	.8394	6
422	.811	70	-----	---	.8103	8
303	-----	---	-----	---	.7996	6
521	-----	---	-----	---	.7851	8

Structural data. van Arkel [3] in 1925 proposed that germanium dioxide had rutile-type structure. Goldschmidt [1] in 1932 verified this structure and gave the space group as P4mnm (No. 136), with $2(GeO_2)$ per unit cell. Laubengayer and Morton [2] reported that the insoluble tetragonal form of germanium dioxide inverts to the soluble hexagonal form at 1,033°±10°C. Several unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	A
1932	Goldschmidt [1]	4.399	2.865
1932	Laubengayer and Morton [2]	4.404	2.857
1956	Baur [4]	4.395	2.860
1958	National Bureau of Standards	4.3963	2.8626 at 25°C

The density of germanium dioxide calculated from the NBS lattice constants is 6.277 g/cm³ at 25°C.

References

[1] V. M. Goldschmidt, Die Rutilmodifikation des germanium-dioxyds, Z. physik. Chem **17B**, 172–176 (1932).

[2] A. W. Laubengayer and D. S. Morton, Germanium. XXXIX. The polymorphism of germanium dioxide, J. Am. Chem. Soc. **54**, 2303–2320 (1932).

[3] A. E. van Arkel, Kristalstructuur van magnesium-fluoride en andere verbindingen van hetzelfde kristaltype, Physica **5**, 162–171 (1925).

[4] W. H. Baur, Über die Verfeinerung der Kristallstrukturbestimmung einiger Vertreter des Rutiltyps; TiO_2, SnO_2, GeO_2, and MgF_2, Acta Cryst. **9**, 515–520 (1956).

Indium Phosphate, $InPO_4$ (orthorhombic)

ASTM cards. None.

Additional published patterns. A calculated powder pattern with observed intensities has been published by Mooney [1].

NBS sample. The indium phosphate was prepared at NBS by Alvin Perloff. The crystals were obtained by heating in a hydrothermal bomb a mixture of indium oxide and dilute phosphoric acid for approximately a week at temperatures between 350° and 400°C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium and iron; and 0.001 to 0.01 percent each of aluminum, copper, magnesium, manganese, sodium, neodymium, titanium, and thallium; and 0.0001 to 0.001 percent each of silver, barium, chromium, gallium, molybdenum, silicon, and tin.

The sample was colorless and optically negative. The indices of refraction are $N_\alpha = 1.608$, $N_\beta = 1.618$, and $N_\gamma = 1.623$. $2V \cong 80°$.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		*hkl*	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		*hkl*	1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*		*d*	*I*		*d*	*I*
	A			A			A	
110	4.43	81	152	1.3952	9	353	1.0517	5
020	4.00	42	134	1.3822	13	404	1.0456	3
111	3.71	22				136	1.0212	1
021	3.445	13	332	1.3532	5	424	1.0117	1
002	3.394	14	224	1.3471	2	512	1.0062	8
			400	1.3297	7			
112	2.694	100	044	1.2934	5	008	0.9981	9
200	2.660	30	153	1.2671	3	530	.9874	1
022	2.586	13				264	.9739	3
130	2.382	34	420	1.2614	5	354	.9720	4
220	2.216	8	062	1.2399	3	082	.9586	<1
			402	1.2376	3			
202	2.094	22	314	1.2115	4	513	.9573	<1
040	1.9993	15	260	1.1901	5	532	.9481	3
023	1.9697	6				316	.9462	4
132	1.9505	17	350	1.1870	5	460	.9405	3
222	1.8546	26	422	1.1831	4	280	.9344	1
			261	1.1722	3			
310	1.7311	17	351	1.1695	3	444	.9265	1
042	1.7220	14	244	1.1625	3	281		
004	1.6975	14				246	.9229	9
311	1.6774	9	154	1.1357	7	156	.9092	9
133	1.6409	5	045	1.1225	7	462	.9062	4
			352	1.1198	3	533		
240	1.5970	5	170	1.1168	8			
114	1.5846	10	334	1.1129	6	282	.9008	3
024	1.5618	9				336	.8982	3
312	1.5414	13	440	1.1066	7	265	.8950	3
150	1.5305	7	116	1.0955	7			
			026	1.0881	7	600	.8858	4
330	1.4760	9	172	1.0598	4	550		
242	1.4453	20	263	1.0537	3	373	.8849	4
204	1.4304	9				190	.8751	4

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

Pattern	1	2	3
National Bureau of Standards	112	110	020

Structural data. Mooney [1] in 1956 determined that indium phosphate has the space group Cmcm (No. 63) and 4($InPO_4$) per unit cell.

The unit-cell measurements of the Mooney pattern have been converted from kX to angstrom units.

Lattice constants

		a	b	c
		A	A	A
1956	Mooney [1]	5.319	7.867	6.781
1958	National Bureau of Standards	5.320	7.993	6.785 at 25°C

The density of the indium phosphate calculated from the NBS lattice constants is 4.828 g/cm^3 at 25°C.

References

[1] R. C. Mooney, Crystal structure of anhydrous indium phosphate and thallic phosphate by X-ray diffraction, Acta Cryst. **9**, 113–117 (1956).

Lead Formate, $Pb(HCO_2)_2$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0231	5.2 5.7 3.02	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of lead formate was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of bismuth and calcium; 0.001 to 0.01 percent each of aluminum, chromium, magnesium, silicon, and zinc; and 0.0001 to 0.001 percent each of silver, boron, barium, copper, and iron.

The sample was colorless and optically negative with the refractive indices Nα =1.789, Nβ =1.852, and Nγ=1.877. 2V≅80°.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	110	011	210, 112
National Bureau of Standards	110	200	112

Structural data. Nitta [2] in 1928 determined that lead formate has the space group $P2_12_12_1$ (No. 19) and 4[$Pb(HCO_2)_2$] per unit cell.

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		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		A	
011	5.7	80	5.66	42
110	5.2	100	5.24	100
020	4.37	40	4.38	20
111	----	---	4.28	30
002	3.71	40	3.71	37
120	----	---	3.64	14
200	3.26	60	3.265	69
210	3.03	80	3.058	25
112			3.025	59
201	----	---	2.988	36
022	2.83	20	2.827	31
211				
031	2.72	40	2.717	49
220	2.60	20	2.617	10
122			2.597	15
221	2.45	20	2.469	14
202			2.449	19
013	2.36	20	2.380	13
212			2.3587	10
113	2.22	10	2.2344	12
040	2.18	10	2.1897	9
230			2.1761	18
222	----	---	2.1382	17
231	----	---	2.0882	18
301				
140	2.07	10	2.0759	9
123	2.02	40	2.0442	21
311			2.0307	23
141	----	---	1.9987	20
203	----	---	1.9709	9
320	----	---	1.9485	14
213	----	---	1.9236	4
033	1.87	30	1.8867	15
232			1.8771	16
302				
004	----	---	1.8538	5
240	----	---	1.8181	4
014	1.80	10	1.8127	5
133				
223			1.7973	2

Lead Formate, $Pb(HCO_2)_2$ (orthorhombic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
241	----	---	1.7659	2
114	1.74	20	1.7474	9
330			1.7446	3
322	1.71	20	1.7250	11
024				
051			1.7048	5
150	----	---	1.6920	4
124	----	---	1.6507	4
151				
233	1.63	20	1.6332	9
303				
242				
204			1.6122	9
313	----	---	1.6055	10
410				
401	1.59	30	1.5935	9
143			1.5901	12
250	1.54	20	1.5433	7
340				
152			1.5393	11
251	----	---	1.5114	2
341				
421	----	---	1.4971	3
060	----	---	1.4605	3
333, 160	----	---	1.4244	12
252, 430				
342				
044	----	---	1.4148	6
234	----	---	1.4116	3
304				
125	----	---	1.3733	3
403	----	---	1.3616	4
062	----	---	1.3583	4
324	----	---	1.3419	7
351				
162	----	---	1.3298	3
432				
261	----	---	1.3115	4
510	----	---	1.2907	2
441	----	---	1.2882	1
511	----	---	1.2714	3
334				
262	----	---	1.2540	3
520	----	---	1.2505	2
154				
006	----	---	1.2362	3
170	----	---	1.2284	1
045				
305	----	---	1.2254	3
235				
404				
512	----	---	1.2190	3
106, 315	----	---	1.2131	2
414, 171				
360				
145	----	---	1.2071	2
116	----	---	1.2036	2

Lattice constants

		a	b	c
		A	A	A
1928	Nitta [2]	6.53	8.77	7.42
1932	Halla and Zimmermann [3]	6.51	8.77	7.52
1958	National Bureau of Standards	6.525	8.759	7.418 at 25°C

The density of lead formate calculated from the NBS lattice constants is 4.656 g/cm³ 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] I. Nitta, The crystal structure of some rhombic formates, Sci. Pap. Inst. Phys. Chem. Res. Tokyo **9**, 151–163 (1928).

[3] F. Halla and L. Zimmermann, Zur struktur des Bleiformats $Pb(HCO_2)_2$, Z. Krist. **83**, 497–498 (1932).

Lead(II,III) Oxide (minium), Pb_3O_4 (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1-0654	3.35 2.88 2.76	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		A	
110	----	---	6.23	11
201	----	---	3.66	3
211	3.36	100	3.38	100
002	----	---	3.28	7
220	----	---	3.113	19
112	2.89	43	2.903	48
310	2.77	43	2.787	45
202	2.63	28	2.632	30
320	----	---	2.444	2
321	----	---	2.289	4
222	----	---	2.260	8
400	----	---	2.205	1
330	----	---	2.076	1
411	----	---	2.032	12
420	1.95	14	1.970	12
213	1.89	28	1.903	22
421	----	---	1.887	<1
402	1.82	28	1.829	21
332	1.74	43	1.755	30
510	----	---	1.729	1
431	----	---	1.7025	2
422	----	---	1.6897	2
004	1.62	14	1.6417	8
323	----	---	1.6302	<1
521	} 1.58	14	1.5876	12
114				
440	----	---	1.5580	7
512	} 1.51	14	1.5292	8
413				
530	----	---	1.5116	2
531	----	---	1.4744	<1
600	----	---	1.4687	4
224	----	---	1.4521	2
611	1.405	14	1.4144	13
314				
620	----	---	1.3944	<1
532	----	---	1.3728	1
541	----	---	1.3471	4
523	----	---	1.3109	4
622	----	---	1.2830	3
424	----	---	1.2614	4
710	} ----	---	1.2461	4
215				
720	----	---	1.2110	<1
613	----	---	1.2088	1
641	----	---	1.2019	<1
721	} ----	---	1.1906	2
514				
712	} ----	---	1.1654	4
543				
730	----	---	1.1575	4
642	----	---	1.1457	4
444	----	---	1.1302	3
415	----	---	1.1190	1
615	} ----	---	1.1122	2
534				
604	----	---	1.0948	3
811	} ----	---	1.0781	2
116				
820	----	---	1.0682	<1
652	} ----	---	1.0671	<1
643				
624	} ----	---	1.0621	2
206				
660	----	---	1.0388	<1
226	----	---	1.0324	<1
750	} ----	---	1.0245	2
525				
822	----	---	1.0163	<1
653	----	---	1.0034	<1
714	----	---	0.9930	<1
644	} ----	---	.9800	4
406				
752	} ----	---	.9781	3
813				
336	----	---	.9682	5
426	----	---	.9566	<1
545	----	---	.9502	2
921	} ----	---	.9460	7
734				
851	} ----	---	.9249	4
516				
931	----	---	.9198	<1
217	----	---	.9126	3
932	----	---	.8940	4
664	} ----	---	.8777	3
606				
327	----	---	.8756	2
626	----	---	.8606	2
722	} ----	---	.8593	6
853				
10·0·2	----	---	.8513	1
844	----	---	.8450	<1
871	} ----	---	.8224	2
716				
008	----	---	.8206	2
646	----	---	.8153	4
527	} ----	---	.8136	1
118				
228	----	---	.7936	4
617	} ----	---	.7872	4
318				

Additional published patterns. None.

NBS sample. The sample of lead oxide was prepared from PbO maintained at 470° for 30 hr at NBS by Robert S. Roth. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent bismuth; 0.001 to 0.01 percent each of silver, aluminum, sodium, and silicon; and 0.0001 to 0.001 percent each of barium, calcium, iron, and magnesium.

The color of the sample was bright orange-red. The indices of refraction could not be determined by the usual liquid grain immersion method because the sample was too fine-grained.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	211	112	310
National Bureau of Standards	211	112	310

Structural data. Gross [2] and Byström and Westgren [3] independently in 1943 determined that lead oxide has the space group $P4_2/mbc$ (No. 135) and $4(Pb_3O_4)$ per unit cell. Pb_3O_4 has been used as a structure-type.

Several unit-cell measurements have been compared with the NBS values. The values reported by Gross [4] and Straumanis [5] were converted from kX to angstrom units.

Lattice constants

		a	*c*
		A	*A*
1941	Gross [4]	8.88	6.67
1942	Straumanis [5]	8.89	6.52
1947	Bystrom [6]	8.806	6.564
1958	National Bureau of Standards	8.815	6.565 at 25°C

The density of lead oxide calculated from the NBS lattice constants is 8.924 g/cm³ 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, The crystal structure of Pb_3O_4, J. Am. Chem. Soc. **65**, 1107–1110 (1943).

[3] A. Byström and A. Westgren, The crystal structure of Pb_3O_4 and $SnPb_2O_4$, Arkiv Kemi **16**, No. 14 (1943).

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

[5] M. Straumanis, Die Gitterkonstanten der Mennige, Z. physik. Chem. **52B**, 127 (1942).

[6] A. Byström, On the stereochemistry of lead and some metals with similar atomic structure, Arkiv. Kemi **25**, No. 13 (1947).

Lead Phosphate Hydrate (lead hydroxyapatite), $Pb_5(PO_4)_3OH$ (hexagonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
2-0700	2.96 1.85 2.06	Molybdenum	Klement [1] 1938.
1-0924	2.91 4.03 3.61	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns. None.

NBS sample. The sample of lead hydroxyapatite was prepared by Alvin Perloff at NBS by heating stoichiometric proportions of lead acetate, $(NH_4)_2HPO_4$, and water in a hydrothermal bomb at 300° for one week [3]. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of boron, bismuth, and sodium; 0.001 to 0.01 percent each of aluminum, copper, molybdenum, silicon, and zinc; and 0.0001 to 0.001 percent each of silver, barium, calcium, iron, and magnesium.

The sample was colorless. The indices of refraction were too high, above 2.00, to be determined by the usual liquid grain immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units and the d-values of the Klement pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Klement	211	004	222
Hanawalt, Rinn, and Frevel	211	111	002
National Bureau of Standards	211	111	300

Structural data. Klement [1] in 1938 found that lead hydroxyapatite has apatite-type structure. Mehmel [4] in 1930 determined that the apatites have the space group $P6_3/m$ (No. 176) and $2[Pb_5(PO_4)_3OH]$ per unit cell.

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

Lead Phosphate Hydrate (lead hydroxyapatite), $Pb_5(PO_4)_3OH$ (hexagonal)

hkl	1938 Klement Cu, 1.5418 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I	d	I
	A		A		A	
110	----	--	----	--	4.93	18
200	4.30	w	----	--	4.28	26
111	4.14	w	4.04	24	4.11	40
002	----	--	3.62	16	3.71	10
102	3.37	w	3.32	16	3.41	22
210	3.23	w	3.19	16	3.23	32
211	2.96	vs	2.92	100	2.965	100
300	2.85	w	2.83	8	2.852	38
202	----	--	----	--	2.806	<1
220	----	--	----	--	2.469	<1
310	----	--	----	--	2.371	<1
302	----	--	----	--	2.261	3
113	----	--	----	--	2.214	9
400	----	--	2.15	8	2.138	6
222	2.05	m	2.02	16	2.056	18
312	2.00	vw			2.000	13
213	1.96	w	1.96	8	1.965	18
321	1.90	w	1.91	16	1.898	16
303	----	--	----	--	1.868	10
410	----	--	1.86	8	1.866	13
004	1.85	ms	1.82	16	1.856	20
114	----	--	----	--	1.737	<1
204	----	--	----	--	1.704	<1
412	----	--	----	--	1.670	<1
501	----	--	----	--	1.666	<1
420	----	--	----	--	1.612	5
214	1.60	w	----	--	1.610	7
304	1.55	w	1.57	8	1.555	6
502					1.553	7
510	1.53	vw	----	--	1.536	6
511	1.50 (a)	w	1.51	16	1.503	9

---

[a] Nine additional lines are omitted.

Lattice constants

		a	c
		A	A
1938	Klement [1]	9.91	7.30
1958	National Bureau of Standards	9.877	7.427 at 25°C

The density of lead hydroxyapatite calculated from the NBS lattice constants is 7.079 g/cm³ at 25°C.

References

[1] R. Klement, Basische Phosphate zweiwertiger Metalle II. Blei-Hydroxylapatit, Z. anorg. Chem. **237,** 161–171 (1938).

[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] A. S. Posner and A. Perloff, Apatites deficient in divalent cations, J. Research NBS **58,** 279–286 (1957) RP 2761.

[4] M. Mehmel, Über die Struktur des Apatits, I., Z. Krist. **75,** 323–331 (1930).

Lithium Perchlorate Trihydrate, $LiClO_4 \cdot 3H_2O$ (hexagonal)

ASTM cards. None.

Additional published patterns. None.

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

The sample was colorless and optically negative. The indices of refraction are $N_o=1.482$ and $N_e=1.447$.

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

Pattern	1	2	3
National Bureau of Standards	101	201	110

Structural data. West [1] in 1934 determined that lithium perchlorate trihydrate has the space group $P6_3mc$ (No. 186) and $2(LiClO_4 \cdot 3H_2O)$ per unit cell. Lithium perchlorate trihydrate is used as a structure-type.

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

Lithium Perchlorate Trihydrate, $LiClO_4 \cdot 3H_2O$ (hexagonal)

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		*hkl*	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		*hkl*	1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*		*d*	*I*		*d*	*I*
	A			A			A	
100	6.69	19	500	1.3372	<1	440	.9649	<1
101	4.23	100	322			700	.9548	<1
110	3.862	74	501	1.2988	3	612		
200	3.344	6	313			504		
201	2.850	89	330	1.2866	5	701	.9404	2
002	2.726	27	412			433		
210	2.528	32	420	1.2632	<1	315		
102			204			620	.9268	<1
211	2.292	17	421	1.2304	2	424		
300	2.228	1	403			621	.9136	<1
112			502	1.2000	1	405		
202	2.113	3	214			702	.9012	<1
301	2.062	1	511	1.1729	3	514		
220	1.930	6	323			613	.8888	1
310	1.854	10	332	1.1637	2	325		
212			304			710	.8852	<1
311	1.756	14	224	1.1136	1	116		
103			430	1.0992	1	662	.8779	<1
302	1.725	1	512			540	.8557	<1
400	1.672	3	431	1.0772	1	434		
401	1.598	7	503			216		
203			105			703	.8452	<1
222	1.575	<1	520	1.0703	<1	505		
320	1.5345	1	521	1.0501	<1	712	.8422	<1
312			423	1.0374	<1	630		
321	1.4760	4	205			524		
213			610	1.0196	1	720, 542	.8164	<1
410	1.4588	3	432			614, 316		
402	1.4244	2	611	1.0018	1	721	.8075	<1
411	1.4097	2	513			515		
303			215					
004	1.3640	1	522	0.9961	<1			
			414					

Lattice constants

		a	*c*
		A	A
1934	West [1]	7.73	5.43
1958	National Bureau of Standards	7.719	5.455 at 25°C

The density of lithium perchlorate trihydrate calculated from the NBS lattice constants is 1.892 g/cm³ at 25°C.

References

[1] C. D. West, Crystal structures of some hydrated compounds, Z. Krist. **88,** 193–204 (1934).

Neodymium Fluoride, NdF_3 (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
3–1064	1.99 1.77 2.03	Copper	Oftedal [1] 1929.

Additional published patterns. None.

NBS sample. The sample of neodymium fluoride was prepared at NBS by reaction of ammonium bifluoride with neodymium chloride. It was annealed at 800°C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of lead, silicon, calcium, and iron; 0.001 to 0.01 percent each of aluminum, magnesium, and manganese; and 0.0001 to 0.001 percent of nickel.

The color of the sample was light red-brown. 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 Oftedal pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Oftedal	113	302	300
National Bureau of Standards	111	113	002

Structural data. Oftedal [2] in 1931 determined that neodymium fluoride has cerium fluoride-type structure, the space group $P6_3/mcm$ (No. 193), and 6(NdF_3) per unit cell.

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

Lattice constants

		a	c
		A	A
1929	Oftedal [1]	7.035	7.211
1958	National Bureau of Standards	7.030	7.199 at 25°C

The density of neodymium fluoride calculated from the NBS lattice constants is 6.506 g/cm³ at 25°C.

hkl	1929 Oftedal Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		A	
002	----	----	3.60	45
110	----	----	3.52	31
111	----	----	3.158	100
112	----	----	2.516	12
300	2.03	s	2.030	45
113	1.98	s+	1.9819	53
004	----	----	1.7994	7
302	1.76	s+	1.7678	30
221	1.71	m	1.7083	21
114	----	----	1.6016	5
222	----	----	1.5788	3
214	1.42	m	1.4180	14
223				
304	1.35	m−	1.3462	12
115	1.33	w+	1.3322	9
411	1.30	m+	1.3065	15
224	----	----	1.2572	3
412	----	----	1.2463	3
006	----	----	1.2002	4
330	----	----	1.1719	4
413	1.16	s	1.1624	10
404				
116	----	----	1.1354	3
225	1.11	s	1.1141	11
332				
414	----	----	1.0690	2
306	1.03	s	1.0328	5
600	----	----	1.0147	2
226	----	----	0.9911	1
117	----	----	.9870	4
334	----	----	.9818	5
415	0.975	m(D)	.9766	11
521	.965	m+	.9661	5

References

[1] I. Oftedal, Über die Kristallstruktur von Tysonit und einigen künstlich dargestellten Lanthanidenfluoriden, Z. physik. Chem. **B5**, 272–291 (1929).

[2] I. Oftedal, Zur Kriskallstruktur von Tysonit (Ce, La, . . .)F_3, Z. physik. Chem. **B13**, 190–200 (1931).

Neodymium Oxychloride, NdOCl (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–1094	2.59 3.47 2.85	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of neodymium oxychloride was prepared by heating neodymium chloride hydrate at a temperature sufficiently high to drive off the water. Further annealing at 1,000°C improved the diffraction pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum and silicon; 0.001 to 0.01 percent each of calcium, iron, and magnesium; and 0.0001 to 0.001 percent each of chromium, manganese, and copper. The color of the sample was pale blue. The indices of refraction were not determined because the sample was too fine-grained.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and Frevel pattern were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	102	101	110
National Bureau of Standards	102	101	110

Structural data. Zachariasen [2] in 1949 determined that neodymium oxychloride has lead fluoride-type structure, the space group P4/nmm (No. 129), and 2(NdOCl) per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1949	Zachariasen [2]	4.04	6.77
1958	National Bureau of Standards	4.025	6.775 at 25°C

The density of neodymium oxychloride calculated from the NBS lattice constants is 5.919 g/cm^3 at 25°C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
001	6.8	20	6.77	31
101	3.48	75	3.46	94
002	-----	--	3.384	11
110	2.86	75	2.844	77
111	-----	--	2.620	6
102	2.60	100	2.592	100
003	2.25	4	2.258	9
112	2.18	30	2.179	27
200	2.00	50	2.012	40
103	1.96	1	1.9705	4
201	1.92	7	1.9290	8
113	1.77	25	1.7694	21
211	1.73	30	1.7397	28
212	1.59	50	1.5890	38
104	1.56	15	1.5610	15
203	1.50	10	1.5027	9
114	1.456	6	1.4562	8
220	1.423	13	1.4230	12
213	-----	--	1.4069	4
221	1.393	1	1.3926	2
301	1.316	7	1.3161	6
222	-----	--	1.3125	5
204	-----	--	1.2958	5
105	-----	--	1.2840	2
310	1.273	8	1.2725	10
311	1.251	6	1.2503	4
302	-----	--	1.2474	11
214	1.232	10	1.2333	12
115	-----	--	1.2231	5
223	1.204	1	1.2041	4
312	1.192	6	1.1913	7
205	1.126	4	1.1237	4
313	1.105	7	1.1089	7
321			1.1015	6
215	1.082	3	1.0826	1
322	1.062	7	1.0603	8
304	1.052	7	1.0518	3
116			1.0497	6
314	-----	--	1.0178	3
400	-----	--	1.0062	5
206	-----	--	0.9849	6
225	-----	--	.9815	4
411	-----	--	.9664	5
330	-----	--	.9488	3
107	-----	--	.9412	7
412	-----	--	.9382	6
324	-----	--	.9322	7
315	-----	--	.9277	4
403	-----	--	.9191	1
420	-----	--	.9002	6
226	-----	--	.8848	7

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] W. H. Zachariasen, Crystal chemical studies of the 5f-series of elements; XII, New compounds representing known structure types, Acta Cryst. **2**, 388–390 (1949).

Nickel Fluosilicate Hexahydrate, $NiSiF_6 \cdot 6H_2O$ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0309	4.67 4.16 2.58	Molybdenum	Dow Chemical Co.

Additional published patterns. None.

NBS sample. The sample of nickel fluosilicate hexahydrate was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, cobalt, iron, and magnesium; 0.001 to 0.01 percent each of chromium, copper, manganese, titanium, and zinc; and 0.0001 to 0.001 percent each of barium and lead.

The color of the sample was green and it was optically positive. The indices of refraction were too low to be determined by the liquid grain immersion method.

Interplanar spacings and intensity measurements. The d-values reported by the Dow Chemical Co. were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Dow Chemical Co.	110	102	212
National Bureau of Standards	110	102	212

Structural data. Hassel [1] in 1927 determined that nickel fluosilicate hexahydrate has nickel chlorostannate-type structure, the space group $R\bar{3}$ (No. 148), and $1(NiSiF_6 \cdot 6H_2O)$ per unit rhombohedral cell and $3(NiSiF_6 \cdot 6H_2O)$ per unit hexagonal cell. The unit-cell measurements reported by Hassel and Salvesen [2] have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
		A	A
1927	Hassel and Salvesen [2]	9.28	9.524
1958	National Bureau of Standards	9.310	9.618 at 25°C

The density of nickel fluosilicate hexahydrate calculated from the NBS lattice constants is 2.130 g/cm³ at 25°C.

hkl hex.	---- Dow Chemical Co. Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		A	
110	4.68	100	4.65	100
012	4.17	50	4.13	62
---	3.91	2	------	--
---	3.71	1	------	--
202	3.10	8	3.09	7
211	2.91	18	2.905	13
---	2.78	1	------	--
113	2.66	5	2.641	6
122	2.59	40	2.574	34
---	2.46	1	------	--
---	2.36	7	------	--
104	----	--	2.306	3
---	2.23	1	------	--
131	2.18	3	2.178	3
024	2.07	8	2.065	8
312	2.03	3	2.028	3
401	1.98	5	1.973	6
---	1.94	1	------	--
214	1.90	13	1.8878	12
015	----	--	1.8699	2
042	1.87	2	1.8599	7
321	1.82	3	1.8164	3
410	1.77	3	1.7590	4
232	1.73	5	1.7266	6
---	1.68	1	------	--
134	1.64	13	1.6371	10
051	1.60	1	1.5901	4
330	1.55	2	1.5518	3
404	----	--	1.5440	<1
413	----	--	1.5424	3
116	1.52	2	1.5154	2
---	1.50	1	------	--
324	1.47	2	1.4654	3
422	1.44	2	1.4521	1
511	1.42	1	1.4324	2
152	----	--	1.3868	3
306	----	--	1.3776	3
600	----	--	1.3442	2
226	----	--	1.3200	3
342	----	--	1.2784	3

References

[1] O. Hassel, Vorläufige Notiz über die Kristallstruktur einiger Verbindungen von der Zusammensetzung $MG_6 \cdot LR_6$, Z. physik. Chem. **126,** 118–126 (1927).

[2] O. Hassel and J. R. Salvesen, Über den Kristallbau der trigonal kristallisierenden heteropolaren Verbindungen von der Zusammensetzung $MG_6 \cdot LR_6$, $MG_5D \cdot LR_6$ und $MG_4D_2LR_6$, Z. physik. Chem. **128,** 345–361 (1927).

Niobium Silicide, $NbSi_2$ (hexagonal)

ASTM cards. None.

Additional published patterns

Source	Radiation
Wallbaum [1] 1941	Cobalt, Kα

NBS sample. The sample of niobium silicide was prepared at NBS by Raymond Walker and Sylvanus Holley as a solid state reaction of the elements maintained in vacuum at 1,350°C for 1 hr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, iron, magnesium, titanium, and vanadium; 0.001 to 0.01 percent each of molybdenum, nickel, and zirconium, and 0.0001 to 0.001 percent each of boron, calcium, copper, and manganese. The sample was a gray metallic powder.

Interplanar spacings and intensity measurements. The *d*-values of the Wallbaum pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Wallbaum	114, 301	111	302
National Bureau of Standards	111	101	112

Structural data. Wallbaum [1] in 1941 determined that niobium silicide has $CrSi_2$-type structure, the space group $P6_222$ (No. 180), and 3($NbSi_2$) per unit cell. The unit-cell measurements reported by Wallbaum have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1941	Wallbaum [1]	4.795	6.589
1958	National Bureau of Standards	4.7971	6.592 at 25°C

The density of niobium silicide calculated from the NBS lattice constants is 5.652 g/cm³ at 25°C.

hkl	1941 Wallbaum Co, 1.7902 A *d*	*I*	1958 National Bureau of Standards Cu, 1.5405 A at 25°C *d*	*I*
	A		*A*	
100	-----	----	4.17	11
101	3.51	mw	3.52	72
102	2.58	w	2.587	32
110	2.40	w−	2.401	19
111	2.25	m	2.255	100
003	2.196	mw	2.199	35
200	2.076	w	2.079	21
112	1.936	m−	1.941	64
113	1.618	w−	1.621	10
210	-----	----	1.571	4
104	-----	----	1.532	10
211	1.522	w+	1.528	14
203	1.506	w	1.509	12
212	1.415	w	1.418	8
300	-----	----	1.384	4
114	1.354	m+	1.358	22
301			1.355	25
204	-----	----	1.292	1
302	1.274	m	1.277	13
105	-----	----	1.257	5
220	1.197	m−	1.200	10
303	-----	----	1.171	3
115	-----	----	1.156	8
214	1.135	m−	1.1363	4
311			1.1347	5
006	1.098	w−	1.0989	2
312	1.085	w	1.0877	2
304	1.059	w+	1.0600	7
223	1.050	m+	1.0528	16
400	-----	----	1.0387	<1
116	-----	----	0.9985	1
206	-----	----	.9711	3
305	-----	----	.9549	5
314	-----	----	.9442	4
321	-----	----	.9434	5
403	-----	----	.9390	4
107	-----	----	.9184	1
322	-----	----	.9157	1
410	-----	----	.9065	<1
411	-----	----	.8982	9
117	-----	----	.8766	5
412	-----	----	.8741	10
315	-----	----	.8676	2
306	-----	----	.8608	<1
413	-----	----	.8380	3
324	-----	----	.8250	4
226	-----	----	.8100	9
217	-----	----	.8080	4
414	-----	----	.7943	12
331	-----	----	.7937	8
420	-----	----	.7851	4

References

[1] H. J. Wallbaum, Disilizide des Niobs, Tantals, Vanadiums und Rheniums, Z. Metallkunde **33**, 378–381 (1941).

Potassium Bromoplatinate, K_2PtBr_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium bromoplatinate was prepared at NBS from bromoplatinic acid and potassium bromide. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of cesium, sodium, and rubidium; and 0.0001 to 0.001 percent each of barium, calcium, iron, magnesium, and silicon.

The color of the sample was red. The index of refraction was too high to be determined by the usual liquid immersion techniques.

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

Pattern	1	2	3
National Bureau of Standards	400	111	200

Structural data. Mathieu [1] in 1929 determined that potassium bromoplatinate has potassium chloroplatinate-type structure, the space group Fm3m (No. 225), and 4(K_2PtBr_6) per unit cell.

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

Lattice constants

		A
1929	Mathieu [1]	10.371
1953	Sharpe [2]	10.27
1958	National Bureau of Standards	10.293 at 26°C

The density of potassium bromoplatinate calculated from the NBS lattice constant is 4.584 g/cm^3 at 26°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 26°C		
	d	*I*	*a*
	A		A
111	5.95	86	10.30
200	5.15	74	10.29
220	3.64	15	10.30
311	3.10	49	10.29
222	2.97	59	10.29
400	2.57	100	10.30
331	2.36	15	10.30
420	2.301	43	10.291
422	2.102	9	10.296
511	1.982	30	10.296
440	1.820	58	10.294
531	1.740	26	10.296
600	1.716	20	10.294
620	1.628	4	10.294
533	1.570	7	10.296
622	1.552	10	10.294
444	1.4854	17	10.291
711	1.4409	13	10.290
640	1.4269	6	10.290
642	1.3755	4	10.293
731	1.3399	8	10.292
800	1.2861	6	10.289
820	1.2480	9	10.291
822	1.2127	3	10.290
751	1.1885	6	10.293
840	1.1504	12	10.290
911	1.1295	7	10.290
842	1.1231	6	10.293
931	1.0790	5	10.293
844	1.0506	9	10.294
933	1.0347	5	10.295
10·0·0	1.0291	4	10.291
951	0.9951	6	10.294
953	.9597	5	10.292
10·4·0	.9557	5	10.293
10·4·2	.9396	<1	10.293
880	.9097	1	10.292
11·3·1	.8992	5	10.292
10·4·4	.8960	4	10.295
11·3·3	.8731	5	10.294
12·0·0	.8576	1	10.292
11·5·1	.8489	2	10.292
12·2·2	.8349	2	10.293
11·5·3	.8267	2	10.292
12·4·0	.8137	3	10.293
12·4·2	.8037	6	10.293
13·1·1	.7871	6	10.293
Average value of last five lines			10.293

References

[1] M. Mathieu, Determination of the length of the cube edge of potassium bromoplatinate, Compt. Rend. **188**, 1611 (1929).

[2] A. G. Sharpe, Chemistry of the platinum metals. Part III. Lattice constants of some chloropalladates, bromopalladates, and bromoplatinates, J. Chem. Soc. 4177–4179 (1953).

Potassium Bromoselenate, K_2SeBr_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium bromoselenate was prepared at NBS from potassium iodide, selenium dioxide, and hydrobromic acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium, and 0.001 to 0.01 percent each of aluminum, calcium, iron, rubidium, and silicon.

The color of the sample was reddish-orange. The index of refraction could not be determined by the usual liquid grain immersion method because the sample was too highly colored.

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

Pattern	1	2	3
National Bureau of Standards	222	400	440

Structural data. Hoard and Dickinson [1] in 1933 determined that potassium bromoselenate has potassium chloroplatinate-type structure, the space group Fm3m (No. 225), and 4(K_2SeBr_6) per unit cell.

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

Lattice constants

		A
1933	Hoard and Dickinson [1]	10.384
1958	National Bureau of Standards	10.419 at 25°C

The density of potassium bromoselenate calculated from the NBS lattice constant is 3.738 g/cm^3 at 25°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	*I*	*a*
	A		A
111	6.01	23	10.41
200	5.21	30	10.42
311	3.138	11	10.41
222	3.007	100	10.42
400	2.604	81	10.42
331	2.391	4	10.424
420	2.331	20	10.424
511	2.006	6	10.421
440	1.842	44	10.419
531	1.7615	6	10.421
600	1.7366	8	10.420
622	1.5700	18	10.414
444	1.5034	11	10.416
711	1.4590	2	10.419
640	1.4449	2	10.419
731	1.3558	2	10.414
800	1.3023	3	10.418
820	1.2634	3	10.418
751	1.2026	<1	10.415
662	1.1951	3	10.419
840	1.1647	6	10.417
911	1.1437	2	10.420
842	1.1369	<1	10.420
931	1.0922	<1	10.419
844	1.0634	6	10.419
Average value of last five lines			10.419

References

[1] J. L. Hoard and B. N. Dickinson, The crystal structure of potassium bromoselenate, Z. Krist. **84**, 436–441 (1933).

Potassium Perrhenate, $KReO_4$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
3–0417	3.35 5.15 2.09	Copper	Broch [1] 1929.

Additional published patterns. None.

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

The sample was colorless and optically positive. The indices of refraction are $N_o=1.645$ and $N_e=1.675$.

Interplanar spacings and intensity measurements. The *d*-values of the Broch pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Broch	112, 103	101	204
National Bureau of Standards	112, 103	101	204

Structural data. Broch [1] in 1929 determined that potassium perrhenate has scheelite-type structure, the space group $I4_1/a$ (No. 88), and 4($KReO_4$) 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
1929	Broch [1]	5.626	12.53
1958	National Bureau of Standards	5.675	12.700 at 25°C

The density of potassium perrhenate calculated from the NBS lattice constants is 5.425 g/cm³ at 25°C.

Potassium Perrhenate, $KReO_4$ (tegragonal)

hkl	1929 Broch Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
101	5.03	vs	5.19	55
112	3.30	vvs	3.396	100
103				
004	3.11	m	3.175	16
200	2.78	m	2.837	19
114	2.43	m	2.491	14
211				
105	2.28	vw	2.318	2
213	2.13	m	2.177	7
204	2.07	vs	2.118	22
220	1.97	s	2.006	8
301	1.84	vs	1.873	12
116				
215	1.76	s	1.795	7
107	1.70	vs	1.727	18
303				
312				
206	1.67	s	1.697	8
224				
008	1.55	vvw	1.587	1
314	1.53	vw	1.562	2
321				
305	1.49	s	1.517	2
118	1.45	s	1.476	4
217				
400	1.40	vw	1.419	1
208	1.36	m	1.386	4
109	1.34	vs	1.369	8
316				
461				
325	1.31	vw	1.338	<1
307	1.29	m+	1.309	5
413				
332				
404	1.27	w	1.2952	2
420	1.25	w+	1.2693	2
228	1.23	w	1.2450	2
219	1.20	vvw	1.2332	1
334				
1·1·10	1.20	m	1.2108	1

Potassium Perrhenate, $KReO_4$ (tetragonal)—Continued

hkl	1929 Broch Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
406	1.16	m+	1.1784	2
424				
1·0·11, 309	1.11	m+	1.1310	2
336				
417, 503	1.08	s	1.0967	<1
512				
408	----	--	1.0577	<1
521, 329	----	--	1.0503	<1
514				
3·1·10	----	--	1.0363	2
505				
338	----	--	1.0227	<1
523				
440	----	--	1.0027	<1
2·0·12, 428	----	--	0.9911	2
442				
3·0·11, 419	----	--	0.9854	2
516				
525	----	--	.9735	<1
507	----	--	.9622	3
532				
444	----	--	.9568	1
4·0·10	----	--	.9462	<1
600				
2·2·12	----	--	.9360	1
3·2·11, 611	----	--	.9306	1
534				
3·3·10	----	--	.9210	1
3·1·12, 2·1·13	----	--	.9114	1
527, 518, 613				
446	----	--	.9066	1
604				
4·2·10	----	--	.8976	<1
620				
1·1·14, 4·1·11	----	--	.8844	3
509, 536, 541				
615	----	--	.8760	<1
3·0·13	----	--	.8678	1
543				
2·0·14	----	--	.8637	1
606, 624				
4·0·12	----	--	.8482	1
448				
1·0·15	----	--	.8371	2
5·1·10, 545				
3·2·13, 3·3·12	----	--	.8299	1
617, 538, 633				
4·2·12	----	--	.8128	4
608				
3·1·14, 5·0·11	----	--	.8095	3
701				
712, 703	----	--	.7964	5
547				
4·4·10	----	--	.7871	2
640				

References

[1] E. Broch, Die Kristallstruktur von Kaliumperrhenat, Z. physik. Chem. **6**, 22–26 (1929).

Potassium Phosphomolybdate Tetrahydrate, $K_3PO_4(MoO_3)_{12}\cdot 4H_2O$ (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium phosphomolybdate tetrahydrate was prepared at NBS by heating dilute solutions of potassium molybdate and phosphoric acid at about 75°C. The salt was precipitated by slowly adding dilute nitric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of cesium; 0.001 to 0.01 percent each of aluminum, sodium, rubidium, and silicon; and 0.0001 to 0.001 percent each of barium, calcium, magnesium, lead, and tin. The color of the sample was greenish-yellow. The index of refraction is 1.965.

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

Pattern	1	2	3
National Bureau of Standards	222	110	400

Structural data. Keggin [1] in 1934 determined the structure of 12-phosphotungstic acid. Ferrari and Nanni [2] in 1939 showed that potassium phosphomolybdate tetrahydrate has this structure, the space group Pn3m (No. 224), and $2[K_3PO_4(MoO_3)_{12}\cdot 4(H_2O)]$ per unit cell.

Lattice constants

		A
1939	Ferrari and Nanni [2]	11.72
1958	National Bureau of Standards	11.596 at 25°C

The density of potassium phosphomolybdate tetrahydrate calculated from the NBS lattice constant is 4.277 g/cm³ at 25°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C		
	d	I	a
	A		A
110	8.21	39	11.61
111	6.70	2	11.60
200	5.79	15	11.58
211	4.73	12	11.59
220	4.10	20	11.60
310	3.67	10	11.606
222	3.346	100	11.591
321	3.100	4	11.599
400	2.898	36	11.592
411	2.732	10	11.591
420	2.593	2	11.596
332	2.473	22	11.599
510	2.274	16	11.595
432	2.153	2	11.594
521	2.117	5	11.595
440	2.050	16	11.597
522	2.0187	2	11.597
600	1.9332	5	11.599
611	1.8812	13	11.596
620	1.8338	2	11.598
621	1.8104	3	11.592
541	1.7892	9	11.595
622	1.7486	12	11.599
444	1.6737	7	11.596
710	1.6396	17	11.594
640	1.6080	2	11.595
721	1.5786	6	11.600
730	1.5229	3	11.598
732	1.4725	17	11.594
811	1.4277	8	11.599
820	1.4067	2	11.600
653	1.3868	2	11.603
822	1.3663	3	11.593
661	1.3571	3	11.595
831	1.3479	3	11.595
662	1.3300	2	11.595
752	1.3133	1	11.599
910	1.2814	2	11.603
921	1.2500	3	11.592
930	1.2226	<1	11.599
932	1.1956	4	11.592
941	1.1710	3	11.592
10·1·1	1.1477	5	11.591
10·2·0	1.1374	<1	11.599
950	1.1260	4	11.593
10·2·2	1.1165	1	11.603
10·3·1	1.1055	<1	11.594
Average value of last five lines			11.596

References

[1] J. F. Keggin, The structure and formula of 12-Phosphotungstic acid, Proc. Roy. Soc. **144,** 75–100 (1934).

[2] A. Ferrari and O. Nanni, Richerche sui sali degli eteropolacidi, l. Struttura dei fosfo- e degli arsenidodecamolibdati e dei fosfo- e degli arsenidodecawolframati di ammonio, di potassio e di talli, Gazz. chim. Ital. **69,** 301–314 (1939).

Potassium Thiocyanate, KCNS (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0882	2.97 2.79 2.51	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns

Source	Radiation
Büssem, Günther, and Tubin [2] 1934	Copper, Kα

NBS sample. The sample of potassium thiocyanate was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, chromium, silicon, and tungsten; and 0.001 to 0.01 percent each of barium, magnesium, and rubidium. The sample was colorless and optically positive. The indices of refraction are Nα=1.619, Nβ=1.665, Nγ=1.74 and 2V=52°.

Interplanar spacings and intensity measurements. The d-values of the Büssem, Günther, and Tubin pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	112	211, 121	202, 022
Büssem, Günther, and Tubin	112	211, 121	200, 020
National Bureau of Standards	112	121	211

Structural data. Klug [3] in 1933 determined that potassium thiocyanate has the space group Pbcm (No. 57) and 4(KCNS) per unit cell. Potassium thiocyanate is used as a structure-type.

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
1933	Klug [3]	6.67	6.647	7.60
1934	Büssem, Günther, and Tubin [2]	6.68	6.66	7.56
1958	National Bureau of Standards	6.708	6.695	7.616 at 25°C

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1934 Büssem, Günther, and Tubin Cu Kα		1958 National Bureau of Standards Cu, 1.5405 A at 52°C	
	d	I	d	I	d	I
	A		A		A	
100	-----	---	-----	---	6.71	4
110	-----	---	-----	---	4.74	7
111	-----	---	-----	---	4.02	4
002	-----	---	-----	---	3.81	9
200	3.35	35	3.35	22	3.354	19
020					3.346	21
102	-----	---	-----	---	3.316	14
021	-----	---	-----	---	3.066	6
210	-----	---	-----	---	3.000	6
120	-----	---	-----	---	2.995	22
112	2.98	100	2.96	100	2.966	100
211	2.80	80	2.80	24	2.790	34
121					2.784	56
202	2.52	40	2.51	14	2.518	27
022					2.512	19
220	2.36	20	2.36	6	2.370	14
221	-----	---	-----	---	2.262	4
113	2.23	2	2.22	1	2.238	4
300						
310	-----	---	-----	---	2.121	19
130	-----	---	2.11	6	2.118	17
311	-----	---	-----	---	2.042	4
023	-----	---	-----	---	2.024	4
222	-----	---	-----	---	2.011	6
123	1.94	25	-----	---	1.936	17
302	-----	---	1.913	11	1.928	19
004					1.905	14
230	-----	---	-----	---	1.857	4
132	-----	---	-----	---	1.850	6
104	-----	---	-----	---	1.831	4
231	-----	---	-----	---	1.805	5
114	-----	---	-----	---	1.767	3
223	-----	---	-----	---	1.7323	2
232	1.66	20	1.657	4	1.6687	8
024					1.6546	5
133	-----	---	-----	---	1.6268	3
214	1.61	2	1.609	3	1.6070	5
124						
141	-----	---	-----	---	1.5883	2
042	1.53	16	1.531	4	1.5326	8
142	1.490	16	1.488	4	1.4946	11
224					1.4839	8
241	-----	---	-----	---	1.4700	10
332	1.460	16	1.454	3	1.4580	6
134	1.415	12	1.409	3	1.4161	12
215	-----	---	-----	---	1.3578	3
125						
430	-----	---	-----	---	1.3399	3
340						
106	-----	---	-----	---	1.2471	3
414	-----	---	-----	---	1.2368	3
135						
116	1.229	8	-----	---	1.2262	6
206	-----	---	-----	---	1.1870	2
026						

Potassium Thiocyanate, KCNS (orthorhombic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1934 Büssem, Günther, and Tubin Cu Kα		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
522	1.181	8	-----	---	1.1837	3
244	-----	---	-----	---	1.1765	3
344	-----	---	-----	---	1.0955	5
260	-----	---	-----	---	1.0585	2
542 452	-----	---	-----	---	1.0088	3
444	-----	---	-----	---	1.0053	1
416 146	-----	---	-----	---	1.0008	5
360	-----	---	-----	---	0.9985	3
361 336	-----	---	-----	---	.9896	2

The density of potassium thiocyanate calculated from the NBS lattice constants is 1.887 g/cm³ 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] W. Büssem, P. Günther, and R. Tubin, Die Struktur des Thallorhodanids und des Kaliumrhodanids, Z. phys. Chem. **24B,** 1–21 (1934).

[3] H. P. Klug, The crystal structure of potassium thiocyanate, Z. Krist. **85,** 214–222 (1933).

Rubidium Bromate, $RbBrO_3$ (trigonal)

ASTM cards. None.

Additional published patterns

Source	Radiation
Asensio Amor [1] 1954	Copper Kα

NBS sample. The sample of rubidium bromate was prepared at NBS by crystallization from a solution of rubidium chlorate and sodium bromate. It was recrystallized several times before using. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of potassium; 0.01 to 0.1 percent each of barium, calcium, cesium, nickel, strontium, and thallium.

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

Interplanar spacings and intensity measurements. The *d*-values of the Asensio Amor pattern were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Asensio Amor	012	202	214
National Bureau of Standards	012	110	202

hkl hex.	1954 Amor Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
101	4.35	20	4.48	9
012	3.18	100	3.23	100
110	3.00	50	3.108	81
---	2.81	5	------	--
003	2.68	10	2.699	9
021	2.41	10	2.554	8
202	2.19	100	2.242	51
113	2.01	10	2.039	4
211	1.95	10	1.974	3
---	1.91	10	------	--
104	1.88	50	1.896	15
122	1.77	50	1.819	25
300	1.73	20	1.795	14
024	1.60	50	1.6181	10
220	1.56	10	1.5543	12
015	1.54	5	1.5508	5
303	1.51	30	1.4957	3
---	1.46	10	------	--
214	1.41	100	1.4351	13
312	1.40	5	1.4013	13
205	1.39	5	1.3879	4
006	1.37	20	1.3493	3
223	1.36	20	1.3471	3
401	1.31	10	1.3282	3
---	1.30	5	------	--

hkl hex.	1954 Amor Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
042	1.27	5	1.2775	4
125	1.25	10	1.2678	2
116	1.24	10	1.2384	5
321	1.23	10	1.2213	1
134	1.19	5	1.2022	6
232	1.17	50	1.1816	5
410	1.15	30	1.1752	5
107	1.14	10	1.1310	3
404	1.13	10	1.1205	4
315	1.10	10	1.0981	2
306	1.08	10	1.0792	3
051	1.07	10	1.0680	<1
027	----	--	1.0631	2
324	----	--	1.0546	3
502	----	--	1.0407	1
330	----	--	1.0366	2
226	----	--	1.0192	2
217	----	--	1.0060	1
018	----	--	0.9951	1
422	----	--	.9871	2

Structural data. Asensio Amor [1] in 1954 determined that rubidium bromate has potassium bromate-type structure, the space group R3m (No. 160), and 1($RbBrO_3$) per unit rhombohedral cell or 3($RbBrO_3$) per unit hexagonal cell. The Asensio Amor pattern did not include lattice constants.

Lattice constants

		a	c
		A	A
1958	National Bureau of Standards	6.218	8.099 at 25°C

The density of rubidium bromate calculated from the NBS lattice constants is 3.919 g/cm^3 at 25°C.

References

[1] I. Asensio Amor, Contribución al estudio por rayos X del bromato de rubidio, Univ. Barcelona, Publs. dept. crist. y mineral. **1**, 173–175 (1954).

Rubidium Bromotellurate, Rb_2TeBr_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium bromotellurate was prepared at NBS from H_2TeBr_6 and Rb_2SO_4. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of potassium; 0.01 to 0.1 percent of sodium; and 0.001 to 0.01 percent each of calcium, chromium, cesium, copper, iron, nickel, silicon, and vanadium. The color of the sample was deep orange. The index of refraction was too high to be measured by the liquid immersion method.

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

Pattern	1	2	3
National Bureau of Standards	222	400	440

Structural data. The structure of rubidium bromotellurate has not been published. It is thought to have a potassium chloroplatinate-type structure because of similarity of patterns. The NBS pattern was indexed assuming the space group to be Fm3m (No. 225) with 4(Rb_2TeBr_6) per unit cell.

Lattice constants

		a
1958	National Bureau of Standards	10.771 at 26°C

The density of rubidium bromotellurate calculated from the NBS lattice constant is 4.134 g/cm^3 at 26°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 26°C		
	d	I	a
	A		A
111	6.22	32	10.77
200	5.387	16	10.775
220	3.809	19	10.775
311	3.248	26	10.771
222	3.109	100	10.770
400	2.693	93	10.772
331	2.472	11	10.775
420	2.4092	10	10.774
422	2.1999	11	10.777
511	2.0728	10	10.771
440	1.9038	52	10.770
531	1.8205	9	10.770
600	1.7948	7	10.769
622	1.6234	20	10.768
444	1.5541	14	10.767
711	1.5082	5	10.777
731	1.4020	5	10.769
800	1.3466	5	10.773
840	1.2041	10	10.770
844	1.0995	9	10.773
12·0·0	0.8976	1	10.773
Average value of last five lines			10.771

Rubidium Chlorate, $RbClO_3$ (trigonal)

ASTM cards. None.

Additional published patterns

Source	Radaition
Gomis and García-Blanco [1] 1951	Copper $K\alpha_1$

NBS sample. The sample of rubidium chlorate was prepared at NBS by reaction of solutions of rubidium sulfate and barium chlorate. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of potassium; 0.01 to 0.1 percent each of barium, calcium, cesium, sodium, nickel, strontium, and thallium; and 0.001 to 0.01 percent each of aluminum, chromium, magnesium, and silicon. The sample was colorless and optically negative. The refractive indices are $N_o=1.572$ and $N_e=1.484$.

Interplanar spacings and intensity measurements. The *d*-values of the Gomis and García-Blanco pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Gomis and García-Blanco	012	110	214
National Bureau of Standards	012	110	202

Structural data. Gomis and García-Blanco [1] in 1951 determined that rubidium chlorate has potassium bromate-type structure, the space group R3m (No. 160), and $1(RbClO_3)$ per unit rhombohedral cell or $3(RbClO_3)$ per unit hexagonal cell.

The unit-cell measurements reported by Gomis and García-Blanco in rhombohedral kX units were converted to hexagonal values in angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1951	Gomis and García-Blanco [1]	6.102	8.149
1958	National Bureau of Standards	6.089	8.174 at 25°C

The density of rubidium chlorate calculated from the NBS lattice constants is 3.206 g/cm³ at 25°C.

hkl hex.	1951 Gomis and García-Blanco Cu, 1.5405 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
101	4.37	w	4.43	13
012	3.19	vs	3.23	100
110	3.01	vs-s	3.042	68
003	2.702	vw	2.725	14
021	2.489	m	2.509	22
202	2.199	s	2.216	44
113	2.016	m	2.030	13
211	1.931	m-w	1.9355	7
104	1.897	s-m	1.9049	13
122	1.785	s-m	1.7911	16
300	1.754	m	1.7571	8
024	1.606	m-w	1.6145	7
015	1.553	w-vw	1.5608	4
220	1.519	m	1.5217	6
303	1.473	w-vw	1.4765	2
131	1.437	vw	1.4393	3
214	1.424	vs-s	1.4263	9
205	1.389	vw	1.3895	2
312	1.377	s-m	1.3769	9
006	1.354	vw	1.3620	2
223	1.326	w	1.3290	3
401	1.311	vw	1.3017	2
125	1.265	w	1.2634	4
042	1.256	w	1.2546	3
116	1.244	s-m	1.2433	4
321	1.199	vw	1.1968	<1
134	1.189	s-m	1.1894	4
232	1.160	s-m	1.1599	4
410	1.151	s-m	1.1507	3
107	1.140	w-vw	1.1405	1
404	1.109	w	1.1075	2
315	1.090	w	1.0902	1
306	-----	-----	1.0768	3
027	-----	-----	1.0679	1
413	-----	-----	1.0599	2
324	-----	-----	1.0411	2
045	-----	-----	1.0263	<1
502	-----	-----	1.0213	1

References

[1] V. Gomis and S. García-Blanco, La estructura del clorato de rubidio, Anales real soc. españ. fís y quím. (Madrid). Ser. A **47**, 95–100 (1951).

Rubidium Chlorotellurate, Rb_2TeCl_6 (cubic)

ASTM cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium chlorotellurate was prepared at NBS from chlorotelluric acid and rubidium sulfate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of cesium and potassium; and 0.001 to 0.01 percent each of silver, aluminum, silicon, and thallium.

The color of the sample was chrome yellow. The index of refraction was 1.867.

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

Pattern	1	2	3
National Bureau of Standards	220	400	111

Structural data. Engel [1] in 1933 determined that rubidium chlorotellurate has potassium chloroplatinate-type structure, the space group Fm3m (No. 225), and 4(Rb_2TeCl_6) per unit cell.

The unit-cell measurement reported by Engel [2] has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1935	Engel [2]	10.254
1958	National Bureau of Standards	10.257 at 25°C

The density of rubidium chlorotellurate calculated from the NBS lattice constant is 3.086 g/cm^3 at 25°C.

References

[1] G. Engel, Die Kristallstrukturen einiger Verbindungen vom K_2PtCl_6-Typ, Naturwiss. **21,** 704 (1933).

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

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 26°C		
	d	*I*	*a*
	A		A
111	5.92	70	10.25
220	3.627	100	10.26
311	3.091	42	10.25
222	2.961	56	10.25
400	2.5643	84	10.256
331	2.3521	17	10.253
422	2.0929	37	10.253
511	1.9733	15	10.253
440	1.8127	40	10.254
531	1.7335	13	10.255
620	1.6213	10	10.254
533	1.5632	6	10.251
622	1.5456	7	10.252
444	1.4804	12	10.257
711	1.4355	7	10.252
642	1.3703	12	10.254
731	1.3347	6	10.252
822	1.2086	7	10.255
751	1.1841	3	10.255
840	1.1468	6	10.257
911	1.1259	5	10.257
664	1.0931	4	10.254
931	1.0750	4	10.255
844	1.0467	7	10.256
933	1.0310	2	10.258
10·2·0	1.0060	4	10.259
951	0.9915	2	10.256
Average value of last five lines			10.257

Rubidium Sulfate, Rb_2SO_4 (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0878	2.98 3.10 2.16	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of rubidium sulfate was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of potassium; 0.01 to 0.1 percent each of barium, calcium, cesium, and nickel; 0.001 to 0.01 percent each of sulfur, chromium, iron, sodium, silicon, and strontium; and 0.0001 to 0.001 percent each of silver, copper, magnesium, and manganese.

The sample was colorless. The indices of refraction are too close to one another to be determined by the usual liquid grain immersion method. They are in the range of 1.52.

Interplanar spacings and intensity measurements. The d-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	013, 020	211	204, 222
National Bureau of Standards	211	013	020

Structural data. Ogg [2] in 1928 determined that rubidium sulfate has the space group Pnma (No. 62), potassium sulfate-type structure, and $4(Rb_2SO_4)$ 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 [3]	7.796	5.961	10.415
1930	Tutton [4]	7.83	5.92	10.45
1958	National Bureau of Standards	7.801	5.965	10.416 at 25°C

The density of rubidium sulfate calculated from the NBS lattice constants is 3.657 g/cm³ 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] A. Ogg, The crystal structure of the isomorphous sulfates of potassium, ammonium, rubidium, and cesium, Phil. Mag. **5**, 354–367 (1928).

[3] A. Ogg and F. L. Hopwood, A critical test of the crystallographic law of valency volumes; a note on the crystalline structure of the alkali sulphates, Phil. Mag. **32**, 518–525 (1916).

[4] A. E. H. Tutton, Note by-, Phil. Mag. **9**, 667–668 (1930).

Rubidium Sulfate, Rb_2SO_4 (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
200	----	--	3.90	6
201	----	--	3.65	9
112	3.50	20	3.51	39
210	3.27	5	3.27	15
103	----	--	3.17	13
211	3.11	75	3.117	100
013	2.99	100	3.000	97
020			2.984	66
212	----	--	2.768	9
004	2.61	10	2.603	14
203			2.595	18
301	2.52	15	2.522	36
104	2.46	10	2.470	13
122			2.457	17
221	2.29	15	2.311	17
114	----	--	2.282	14
123	----	--	2.172	5
204	2.16	50	2.165	22
222			2.156	28
303	2.07	8	2.080	11
214	----	--	2.035	8
105	2.00	5	2.013	11
223	1.95	10	1.957	12
400			1.952	13
321	1.91	8	1.926	10
124	----	--	1.903	<1
410	----	--	1.853	1
322	1.83	5	1.836	1
402	----	--	1.826	2
411				
132	----	--	1.808	1
314	1.75	15	1.758	14
412	----	--	1.746	8
231				
006	----	--	1.736	4
033	----	--	1.725	8
323	----	--	1.706	<1
403	----	--	1.701	3
133	----	--	1.684	<1
125	1.66	5	1.669	4
413	1.63	5	1.635	7
116			1.630	6
421	----	--	1.612	<1
422	1.58	5	1.556	<1
134	----	--	1.547	<1
332	----	--	1.510	<1
414				
	([a])			

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[a] Four additional lines were omitted.

Scandium Phosphate, $ScPO_4$ (tetragonal)

ASTM cards. None.

Additional published patterns. A calculated powder pattern with observed intensities has been published by Mooney [1].

NBS sample. The scandium phosphate was prepared at NBS by Alvin Perloff. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, iron, magnesium, manganese, molybdenum, lead, and silicon.

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

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

Pattern	1	2	3
National Bureau of Standards	200	112	312

Structural data. Mooney [1] in 1956 determined that scandium phosphate has a zircon-type structure, the space group $I4_1/amd$ (No. 141), and $4(ScPO_4)$ per unit cell.

Lattice constants

		a	c
		A	A
1956	Mooney [1]	6.578	5.796
1958	National Bureau of Standards	6.5772	5.7937 at 25°C

The density of scandium phosphate calculated from the NBS lattice constants is 3.707 g/cm³ at 25°C.

hkl	1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*
	A	
101	4.022	5
200	3.287	100
211	2.624	6
112	2.4590	41
220	2.3252	7
202	2.1746	17
301	2.0517	18
103	1.8538	8
321	1.7403	12
312	1.6888	36
400	1.6445	12
420	1.4708	3
004 303	1.4497	4
402	1.4300	2
332	1.3668	10
323 204	1.3260	5
501	1.2816	3
413 224	1.2299	9
521 314	1.1953	2
512	1.1783	6
440	1.1628	2
600	1.0963	3
503 404	1.0869	3
215	1.0782	2
532	1.0511	6
620	1.0398	5
523 424	1.0312	7
622 325	0.9785	<1
631	.9668	2
116 613	.9455	5
640	.9122	5
543 444	.9067	3
721 534	.8900	<1
712	.8857	7
316	.8758	5
633 604	.8739	4
703 624	.8449	4
732	.8277	7

References

[1] R. C. L. Mooney, The structure of anhydrous scandium phosphate, Acta Cryst. **9,** 677 (1956).

Silver Iodide (iodyrite), AgI (hexagonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–0502	3.74 2.29 1.96	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
3–0851	2.57 1.98 3.79	Copper	Aminoff [2] 1922.
3–0940	2.29 3.98 3.72	Molybdenum	Dow Chemical Co.

Card number 1–0502 gives a pattern which is a mixture of the hexagonal and cubic forms of AgI. The *d*-values on card number 3–0851 were apparently miscalculated since they do not agree with the data reported in the literature. This pattern was not included for comparison purposes since another more complete pattern was also prepared by Aminoff using iron radiation.

Additional published patterns

Source	Radiation
Aminoff [3] 1922	Iron
Wilsey [4] 1923	Molybdenum, Kα
Barth and Lunde [5] 1926[a]	Copper
Bloch and Möller [6] 1931	Copper
Wilman [7] 1940	Electron diffraction

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[a] No intensity data given.

NBS sample. The sample of silver iodide was prepared at NBS by precipitation from a silver nitrate solution with addition of an excess of sodium iodide. Care was necessary to prevent conversion of the hexagonal form to the cubic form through heating or abrasion. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of silicon; 0.001 to 0.01 percent each of aluminum, barium, calcium, copper, iron, magnesium, and sodium; and 0.0001 to 0.001 percent of manganese. The color of the sample was yellow. The indices of refraction were not determined because the sample was too fine-grained.

Interplanar spacings and intensity measurements. The *d*-values reported by the Dow Chemical Co., and Wilman were converted from kX to angstrom units, and the *d*-values of the Aminoff [3], Wilsey, and Bloch and Möller patterns were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Dow Chemical Co.	110	100	002
Aminoff [3]	002	110	112
Wilsey	110	112	100
Bloch and Möller	110	103	112
Wilman	002	110	100
National Bureau of Standards	002	110	100

Structural data. Aminoff [3] in 1922 determined that hexagonal silver chloride has wurtzite-type structure, the space group $P6_3mc$ (No. 186) and 2(AgI) per unit cell. Bloch and Möller [6] stated in 1931 that there are two other forms of silver iodide; a cubic form, alpha-AgI, having zincblende structure, usually in combination with the hexagonal form at room temperature, and a body centered cubic form which exists above 146°C.

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

Lattice constants

		a	c
		A	A
1922	Aminoff [2]	4.58	7.52
1922	Aminoff [3]	4.60	7.55
1923	Wilsey [4]	4.602	7.515
1931	Bloch and Möller [6]	4.60	7.55
1934	Kolkmeijer and van Hengel [8]	4.59	7.51
1935	Helmholz [9]	4.60	7.54
1940	Wilman [7]	4.592	7.516
1949	Trillat and Laloeuf [10]	4.594	7.505
1956	Lieser [11]	4.584	7.489
1958	National Bureau of Standards	4.5922	7.510 at 25°C

The density of silver iodide calculated from the NBS lattice constants is 5.683 g/cm³ at 25°C.

Silver Iodide (iodyrite), AgI (hexagonal)

hkl	---- Dow Chemical Co. Mo, 0.7107 A		1922 Aminoff Fe, 1.9373 A		1923 Wilsey Mo, 0.7107 A		1931 Bloch and Möller Cu, 1.5418 A		1940 Wilman Electron Diff.		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*	
100	3.99	75	----	--	3.98	70	3.98	m	3.97	ms	3.98	61
002	3.73	62	3.74	s	3.73	70	3.75	m	3.74	s	3.75	100
101	3.51	62	3.53	w	3.51	30	3.52	m	3.52	m	3.51	38
102	2.73	25	----	--	2.73	20	2.731	w	2.733	w	2.731	16
110	2.29	100	2.29	s	2.29	100	2.298	s	2.295	s	2.296	83
103	2.11	62	2.16	w	2.11	60	2.118	s	2.121	mw	2.119	31
200	----	--	----	--	----	--	1.992	vw	1.984	mw	1.989	6
112	1.96	50	1.954	s	1.959	80	1.961	s	1.956	ms	1.959	51
201	1.92	10	-----	--	-----	--	1.924	vw	1.921	vw	1.9228	5
202	1.75	7	-----	--	-----	--	1.759	vw	1.768	vw	1.7574	7
203	1.55	17	-----	--	1.554	20	1.557	m	1.557	mw	1.5570	5
210	1.51	5	1.509	w	-----	--	1.505	vw	1.497	m	1.5031	4
211	1.47	5	-----	--	-----	--	1.475	vw	1.482	w	1.4744	3
114	----	--	-----	--	-----	--	-----	--	-----	--	1.4535	<1
105	1.40	12	-----	--	1.403	10	1.404	w	1.399	w	1.4052	4
212	1.37	3	-----	--	-----	--	1.397				1.3957	2
300	1.33	10	1.326	w	1.321	10	1.327	m	1.326	m	1.3258	9
213	1.29	17	1.292	w	1.285	10	1.289	m	1.290	w	1.2888	4
006	1.25	7	1.254	ms	1.246	10	1.251	m	1.250	m	1.2515	3
302											1.2500	4
205	1.20	5	1.208	vw	1.192	7	1.199	w	-----	--	1.1987	2
106	1.17	3	-----	--	-----	--	-----	--	-----	--	1.1943	1
220	----	--	1.145	w	1.145	4	1.149	w	1.152	mw	1.1480	2
310	----	--	-----	--	-----	--	-----	--	-----	--	1.1029	1
116	----	--	1.097	ms	1.095	1	1.098	m	1.099	m	1.0989	2
222												
311	----	--	-----	--	-----	--	-----	--	-----	--	1.0916	<1
304	----	--	-----	--	-----	--	-----	--	-----	--	1.0831	<1
215	----	--	-----	--	-----	--	1.062	w	-----	--	1.0626	2
206	----	--	-----	--	1.059	5	1.059	w	-----	--	1.0589	1
312												
313	----	--	-----	--	-----	--	1.010	w	-----	--	1.0093	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] G. Aminoff, Über die Kristallstruktur von AgJ, Z. Krist. **57**, 180–185 (1922).

[3] G. Aminoff, Über die Kristallstruktur von Jodsilber, Marshit (CuJ) und Miersit (4AgJ·CuJ), Geol. Fören. i Stockholm Förh. **44**, 444–481 (1922).

[4] R. B. Wilsey, The crystalline structures of silver iodide, Phil. Mag. **46**, 487–496 (1923).

[5] T. Barth and G. Lunde, Beiträge zur Kenntnis der Mischkristalle, Z. physik. Chem. **122**, 293–334 (1926).

[6] R. Bloch and H. Möller, Über die Mokifikationen des Jodsilbers, Z. physik. Chem. **152**, 245–268 (1931).

[7] H. Wilman, The structure and orientation of silver halides, Proc. Phys. Soc. London **52**, 323–347 (1940).

[8] N. H. Kolkmeijer and J. W. A. van Hengel, Über das reguläre und das hexagonale Silberjodid, Z. Krist. **88**, 317–322 (1934).

[9] L. Helmholz, The crystal structure of hexagonal silver iodide, J. Chem. Physics **3**, 740–747 (1935).

[10] J. J. Trillat and A. Laloeuf, Étude, par diffraction électronique, de la structure des fumées d'iodure d'argent et de chlorure d'ammonium, J. chim. phys. **46**, 168–173 (1949).

[11] K. H. Lieser, Über einige Untersuchunger am Silberjodid im Hinblick auf die Fehlordnung, Z. physik. Chem. **5**, 125–153 (1956).

Silver Perrhenate, $AgReO_4$ (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
4–0565	3.20 1.63 1.29	Copper	Buschendorf [1] 1933.

Additional published patterns. None.

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

The color of the sample was light tan and it was optically positive. The indices of refraction could not be determined by the usual liquid grain immersion method because the sample reacted with the higher index liquids.

Interplanar spacings and intensity measurements. The *d*-values of the Buschendorf pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Buschendorf	112	312	316
National Bureau of Standards	112	200	204

Structural data. Buschendorf [1] in 1933 determined that silver perrhenate has scheelite-type structure, the space group $I4_1/a$ (No. 88), and $4(AgReO_4)$ per unit cell.

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

Lattice constants

		a	*c*
		A	*A*
1933	Buschendorf [1]	5.360	11.940
1958	National Bureau of Standards	5.378	11.805 at 25°C

The density of silver perrhenate calculated from the NBS lattice constants is 6.964 g/cm³ at 25°C.

hkl	1933 Buschendorf Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
101	----	--	4.89	12
112	3.19	vvs	3.20	100
004	2.96	m	2.953	15
200	2.67	s	2.689	31
202	----	--	2.449	1
211	2.36	vw	2.358	4
114	----	--	2.332	1
213	----	--	2.053	<1
204	1.987	vs	1.987	25
220	1.893	m	1.901	9
116	1.747	vs	1.747	12
215	1.682	vw	1.685	1
312	1.629	vvs	1.634	16
224	1.598	s	1.598	8
008	1.478	w	1.476	<1
305	1.426	vw	1.428	<1
323	1.389	vw	1.3952	<1
400	1.342	w	1.3462	2
208	1.291	w	1.2934	4
316	1.286	vvs	1.2862	5
325	-----	--	1.2612	<1
332	-----	--	1.2400	1
413	1.235	m	1.2394	3
404	-----	--	1.2240	3
420	1.204	m	1.2031	2
---	1.201	m	------	--
228	1.164	m	1.1666	3
334			1.1652	2
1·1·10	1.125	w	1.1277	1
424	1.111	vs	1.1140	2
336	1.064	m	1.0655	1
512	1.036	vs	1.0383	<1
514	0.9925	w	0.9933	<1
505	-----	--	.9788	<1
3·1·10	.9670	s	.9696	1
440	-----	--	.9509	<1
428	-----	--	.9322	1
516	.9296	vs	.9292	1
2·0·12	-----	--	.9240	<1
532	-----	--	.9112	1
507	-----	--	.9067	<1
444	-----	--	.9047	<1
600	-----	--	.8962	<1
1·0·13				
2·2·12	-----	--	.8737	1
3·3·10	-----	--	.8638	<1
604	-----	--	.8579	<1
620	-----	--	.8502	<1
536	-----	--	.8350	<1
624	-----	--	.8169	1
448	-----	--	.7990	<1
5·1·10	-----	--	.7863	1

References

[1] F. Buschendorf, Die Kristallstruktur des Silberperrhenats, Z. physik. Chem. **20**, 237–244 (1933).

Sodium Carbonate Monohydrate (thermonatrite), $Na_2CO_3 \cdot H_2O$ (orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
1–1015	2.76 2.37 2.67	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.
2–0878 2–0879	2.73 2.82 2.63	Copper	British Museum.

Additional published patterns. None.

NBS sample. The sample of sodium carbonate was obtained from the J. T. Baker Chemical Co., Phillipsburg, N. J. The monohydrate was obtained by crystallizing from solution and dehydrating at 40°C for 20 hr. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, magnesium, and silicon; and 0.0001- to 0.001-percent iron.

The sample was colorless and optically negative. The indices of refraction are $N\alpha=1.421$, $N\beta=1.505$, and $N\gamma=1.524$. 2V could not be determined because the particle size of the sample was too small.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel and by the British Museum were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	202, 012	410, 121	311, 400, 112
British Museum	202, 012	---	020
National Bureau of Standards	202	121	012

Structural data. Harper [2] in 1936 determined that sodium carbonate monohydrate has the space group $Pca2_1$ (No. 29) and $4(Na_2CO_3 \cdot H_2O)$ per unit cell. Sodium carbonate monohydrate is used as a structure-type.

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

Lattice constants

		a	b	c
		A	A	A
1936	Harper [2]	10.743	5.254	6.453
1958	National Bureau of Standards	10.72	5.249	6.469 at 25°C

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		---- British Museum Cu, --------		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I	d	I
	A		A		A	
200	5.3	31	5.30	60	5.35	20
010					5.24	22
110	---	--	4.63	40	4.72	2
201	4.16	8	4.08	40	4.12	9
211	----	--	3.15	40	3.24	3
---	----	--	3.02	60	----	--
---	----	--	2.96	40	----	--
---	----	--	2.82	80	----	--
202	2.77	100	2.74	100	2.768	100
012					2.753	61
311	2.68	44	----	--	2.684	50
400					2.678	53
112					2.667	8
020	----	--	2.64	80	2.622	8
120	2.56	3	----	--	2.550	2
401	2.47	25	2.47	70	2.475	30
212					2.448	22
410	2.37	63	2.40	70	2.386	10
121			2.33	80	2.372	62
220	----	--	----	--	2.356	<1
---	----	--	2.28	40	-----	--
411	2.24	20	2.21	60	2.238	20
312	2.18	15	2.14	40	2.181	15
320	2.12	3	2.09	20	2.114	<1
402	2.06	18			2.065	17
022	----	--	2.04	60	2.036	1
321	2.00	31	----	--	2.010	26
122					2.004	20
510	----	--	1.98	70	1.985	4
113	----	--	----	--	1.961	3
412	1.91	8	----	--	1.920	7
222					1.905	3
511	----	--	1.90	40	1.898	4
420	----	--	----	--	1.875	3
213	----	--	----	--	1.869	2
600	1.78	8	1.80	20	1.787	7
322			1.76	60	1.770	5
030	----	--	----	--	1.750	4
313	1.74	8	1.73	40	1.741	7
130					1.7262	2
601	----	--	----	--	1.7220	1
512	----	--	----	--	1.6926	3
610						
403	----	--	----	--	1.6802	6
230	1.67	8B	1.67	50	1.6639	8
123	1.65	8	----	--	1.6466	9
422	----	--	1.63	50	1.6226	5
004	1.61	25			1.6174	14
231			1.60	80		
413					1.6083	13
	(a)		(b)			

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[a] Six additional lines were omitted.
[b] Twenty-two additional lines were omitted.

The density of sodium carbonate monohydrate calculated from the NBS lattice constants is 2.262 g/cm³ 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] J. P. Harper, Crystal structure of sodium carbonate monohydrate, $Na_2CO_3 \cdot H_2O$, Z. Krist. **95,** 266–273 (1936).

Strontium Formate, $Sr(HCO_2)_2$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0221	5.4 3.30 3.01	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of strontium formate was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of barium and sodium; 0.001 to 0.01 percent each of calcium, iron, magnesium, and silicon; and 0.0001 to 0.001 percent each of aluminum, cesium, copper, potassium, and manganese.

The sample was colorless and optically positive with the indices of refraction of $N\alpha = 1.552$, $N\beta = 1.556$, and $N\gamma = 1.571$. $2V \cong 60°$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	110	121	031
National Bureau of Standards	110	121	112

Structural data. Nitta [2] in 1928 determined that strontium formate has the space group $P2_12_12_1$ (No. 19) and $4[Sr(HCO_2)_2]$ per unit cell.

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

Lattice constants

		a	b	c
		A	A	A
1928	Nitta [2]	6.87	8.73	7.25
1958	National Bureau of Standards	6.872	8.754	7.264 at 25°C

The density of strontium formate calculated from the NBS lattice constants is 2.700 g/cm³ at 25°C.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
---	15.3	20	----	--
---	10.8	40	----	--
---	6.4	40	----	--
011	----	--	5.60	33
110	5.5	100	5.42	100
---	4.61	10	----	--
020	----	--	4.38	10
111	4.32	10	4.33	5
---	3.92	10	----	--
120	----	--	3.69	4
002	3.66	20	3.63	14
200	----	--	3.438	8
121	3.31	50	3.293	65
102	----	--	3.212	4
210	----	--	3.200	6
112	----	--	3.015	63
211	2.91	20	2.928	42
022	----	--	2.796	<1
031	2.71	50	2.708	48
220	----	--	2.704	5
202	2.51	40	2.497	32
013	2.35	30	2.334	15
310	2.22	30	2.215	10
040	----	--	2.189	4
222	----	--	2.169	14
231	2.12	40	2.127	25
123	2.02	50	2.026	28
141	----	--	2.004	18
321	1.95	30	1.955	23
213	----	--	1.930	2
312	1.88	20	1.8915	15
042	----	--	1.8746	4
033	----	--	1.8638	8
240	----	--	1.8468	4
004	----	--	1.8164	1
104	----	--	1.7558	<1
114	----	--	1.7217	11
400	----	--	1.7175	1
150	----	--	1.6966	3
024	----	--	1.6777	3
242	----	--	1.6450	4
233	1.64	10	1.6377	11
204	----	--	1.6050	6
420	----	--	1.5999	4
143	----	--	1.5810	7
402	----	--	1.5524	6
341	1.54	10	1.5461	5
152	----	--	1.5374	4
251	----	--	1.5253	2
224	----	--	1.5078	1

Strontium Formate, $Sr(HCO_2)_2$ (orthorhombic) —Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
243	----	--	1.4675	1
422	----	--	1.4636	1
060	----	--	1.4590	1
431	1.460	15	1.4503	8
342				
252	-----	--	1.4332	1
015				
314	1.403	10	1.4042	7
350	-----	--	1.3906	4
510	-----	--	1.3571	2
324	1.357	15	1.3536	6

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] I. Nitta, The crystal structure of some rhombic formates, Sci. Papers Inst. Phys. Chem. Research Tokyo **9,** 151–163 (1928).

Strontium Formate Dihydrate, $Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
7–756[a]	6.3 3.15 2.85	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

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[a] This ASTM card is not listed in the alphabetical section of the index.

Additional published patterns. None.

NBS sample. The sample of strontium formate was obtained from the City Chemical Corp., New York. The dihydrate was formed by recrystallization from a water solution. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of barium and sodium; 0.001 to 0.01 percent each of calcium, iron, magnesium, and silicon; and 0.0001 to 0.001 percent each of aluminum, cesium, copper, potassium, and manganese. The sample was colorless and optically negative with the indices of refraction of $N\alpha = 1.483$, $N\beta = 1.521$, and $N\gamma = 1.536$. $2V \cong 60°$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	110	131	221, 122
National Bureau of Standards	110	122	021

Structural data. Nitta [2] in 1928 determined that strontium formate dihydrate has the space group $P2_12_12_1$ (No. 19) and $4[Sr(CHO_2)_2 \cdot 2H_2O]$ per unit cell. The unit-cell measurements reported by Nitta have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1928	Nitta [2]	7.31	12.02	7.14
1958	National Bureau of Standards	7.327	12.06	7.154 at 25°C

The density of strontium formate dihydrate calculated from the NBS lattice constants is 2.245 g/cm³ at 25°C.

Strontium Formate Dihydrate, $Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
110	6.3	100	6.28	100
011	---	--	6.16	14
020	---	--	6.02	40
---	5.6	13	----	--
111	4.69	47	4.72	21
021			4.61	50
---	4.26	13	----	--
121	3.92	13	3.90	23
200	3.68	13	3.66	4
002	3.57	13	3.58	16
210	----	--	3.50	1
031				
012	----	--	3.44	2
201	----	--	3.26	6
102	----	--	3.215	38
131	3.16	83	3.160	43
220	----	--	3.129	44
112	----	--	3.106	46
221	2.86	67	2.868	48
122			2.836	53
041	----	--	2.779	30
230	----	--	2.708	<1
141	2.62	7	2.598	9
202	----	--	2.560	7
231	2.52	13	2.533	9
212			2.504	11
310	----	--	2.394	4
222	2.35	13	2.355	27
013			2.340	11
240	----	--	2.327	6
150	2.27	7	2.294	11
051			2.289	16
311			2.270	6
113	----	--	2.223	6
241	2.20	47	2.214	34
151	----	--	2.182	28
321	----	--	2.158	9
123	2.12	27	2.122	21
033	----	--	2.050	5
302	----	--	2.017	11
331	1.99	53	2.004	14
312			1.989	13
133	----	--	1.975	8
242	----	--	1.952	1
061	----	--	1.935	4
152	----	--	1.930	4
322	1.91	20	1.912	5
223	----	--	1.897	1
043	----	--	1.871	6
341	1.83	27	1.834	9
400			1.832	9
143	----	--	1.812	10
410				
004	1.79	7	1.789	10

Strontium Formate Dihydrate, $Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic)—Continued

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
014	----	--	1.768	5
260	----	--	1.762	11
420	1.75	7	1.752	6
062				
104	----	--	1.737	12
024	----	--	1.715	3
261	----	--	1.711	5
421	1.70	13	1.703	12
342	----	--	1.676	5
124	1.67	13	1.669	5
351				
153	----	--	1.652	3
402	----	--	1.640	5
412	----	--	1.616	2
214	----	--	1.593	5
262	1.58	7	1.580	6
072	----	--	1.5518	2
360				
352	----	--	1.5470	3
253	----	--	1.5384	1
044				
441	1.52	7	1.5288	6
361	----	--	1.5176	3
144	----	--	1.5060	2
163	----	--	1.5038	2
343	----	--	1.4844	3
510	----	--	1.4542	3
304	----	--	1.4423	9
413				
520	----	--	1.4244	1
362				
324	----	--	1.4031	1
353	----	--	1.3930	3

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] I. Nitta, The crystal structure of some rhombic formates, Sci. Papers Inst. Phys. Chem. Research Tokyo **9**, 151–163 (1928).

Strontium Iodide Hexahydrate, $SrI_2 \cdot 6H_2O$ (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
2–0269	4.21 3.71 2.79	Copper	Herrmann [1] 1931.
1–0369	4.34 3.85 2.38	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns. None.

NBS sample. The sample of strontium iodide was obtained from the City Chemical Corp., New York. The hexahydrate was prepared by crystallization from a water solution. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of barium, calcium, and sodium; 0.001 to 0.01 percent each of aluminum, iron, potassium, and lithium; and 0.0001 to 0.001 percent each of silver, copper, magnesium, manganese, and silicon. The sample was colorless and optically negative. The indices of refraction are $N_o = 1.649$ and $N_e = 1.632$.

Interplanar spacings and intensity measurements. The *d*-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units and the *d*-values of the Herrmann pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Herrmann	110, 001	101	210, 201
Hanawalt, Rinn, and Frevel	110, 001	101	211
National Bureau of Standards	110	101	211

Structural data. Strontium iodide hexahydrate was found to be isostructural with strontium chloride hexahydrate by Herrmann [1] in 1931. The structure of strontium chloride-type substances was determined by Jensen [3] in 1940. Strontium iodide-hexahydrate has the space group P321 (No. 150) with $1(SrI_2 \cdot 6H_2O)$ per unit cell.

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

Lattice constants

		a	c
		A	*A*
1931	Herrmann [1]	8.52	4.29
1958	National Bureau of Standards	8.604	4.268 at 25°C

The density of strontium iodide hexahydrate calculated from the NBS lattice constants is 2.727 g/cm³ at 25°C.

hkl. hex.	1931 Herrmann Cu, 1.5418 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
110	4.21	s	4.35	100	4.30	100
001					4.27	14
101	3.71	s	3.86	86	3.70	52
111	3.03	m	3.11	34	3.032	26
210	2.79	s	2.87	56	2.818	5
201					2.808	25
300	2.44	m	2.49	57	2.486	27
211	2.33	s	2.38	71	2.351	42
220	----	--	2.23	11	2.153	8
301	2.14	m	2.15	23	2.147	10
002	----	--	----	--	2.136	6
---	2.05	w	----	--	-----	--
221	1.93	s	1.98	29	1.922	2
112	----	--	1.88	6	1.912	10
311	1.83	m	1.83	11	1.861	13
401	1.70	m	1.73	11	1.708	4
---	----	--	1.66	11	-----	--
410	1.61	s	1.63	17	1.626	7
302			1.60	6	1.618	7
321	1.58	m	1.56	6	1.586	3
411	1.51	w	1.54	6	1.519	2
222					1.515	4
330	1.48	w	----	--	1.434	7
420	1.40	m			1.408	<1
501			----	--		
103					1.397	1
113	----	--	----	--	1.350	<1
510	----	--			1.337	<1
421			----	--		
203	1.33	m	1.321	6	1.3287	3
412	1.29	m	-----	--	1.2934	4
511	1.27	m	-----	--	1.2768	<1
213	----	--	-----	--	1.2699	2
600	----	--	-----	--	1.2424	<1
520	----	--	-----	--	1.1933	1
332	----	--	-----	--	1.1905	<1
431	----	--	-----	--	1.1778	<1
313	----	--	-----	--	1.1719	1
403	----	--	-----	--	1.1309	<1
611	----	--	-----	--	1.0981	<1
323	----	--	-----	--	1.0936	<1
440	----	--	-----	--	1.0751	<1
602	----	--	-----	--	1.0736	<1
004	----	--	-----	--	1.0673	<1
441	----	--	-----	--	1.0419	<1
522	----	--	-----	--	1.0355	<1
114						
620	----	--	-----	--	1.0331	<1
701						

References

[1] Z. Herrman, Über die Strukturen de Strontiumjodid-, Calciumchlorid-, und Calciumbromid-hexahydrate, Z. anorg. allgem. Chem. **197**, 212–218 (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] A. T. Jensen, On the structure of $SrCl_2 \cdot 6H_2O$, Kgl. Danske Videnskab. selskab., Mat. fys Medd. **17**, No. 9 (1940).

Tantalum Silicide, $TaSi_2$ (hexagonal)

ASTM cards. None.

Additional published patterns

Source	Radiation
Wallbaum [1] 1941	Cobalt, Kα

NBS sample. The sample of tantalum silicide was prepared at NBS by Raymond F. Walker and Sylvanus F. Holley [2] by solid-state reaction of the elements at 1,300°C for 3 hr. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, chromium, copper, iron, magnesium, nickel, and titanium; and 0.0001 to 0.001 percent each of silver, calcium, and manganese. The sample was a dark gray metallic powder.

Interplanar spacings and intensity measurements. The *d*-values reported by Wallbaum have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Wallbaum [1]	111	301	223
National Bureau of Standards	101	111	112

Structural data. Borén [3] in 1933 determined the structure of chromium silicide. Wallbaum [1] in 1941 found that tantalum silicide has chromium silicide-type structure, the space group $P6_222$ (No. 180), and $3(TaSi_2)$ per unit cell.

The unit-cell measurements reported by Wallbaum have been converted from *kX* to angstrom units.

Lattice constants

		a	c
		A	A
1941	Wallbaum [1]	4.783	6.565
1958	National Bureau of Standards	4.7821	6.5695 at 25°C

The density of tantalum silicide calculated from the NBS lattice constants is 9.072 g/cm³ at 25°C.

hkl	1941 Wallbaum Co, 1.7902 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
100	----	--	4.13	22
101	3.52	m	3.50	100
102	2.58	mw	2.57	58
110	2.39	w	2.389	17
111	2.24	s	2.246	94
003	2.185	w+	2.187	32
200	2.066	m−	2.070	36
112	1.926	mw	1.932	63
113	1.612	w	1.615	10
210	1.564	vw	1.565	6
104	-----	--	1.525	21
211	1.521	ms	1.523	27
203	1.502	m	1.505	24
212	1.410	m	1.413	17
300	1.380	vw	1.380	4
114	-----	--	1.353	21
301	1.350	s	1.351	25
213	1.272	m+	1.2726	17
302				
105	1.251	w	1.2519	6
220	1.194	m	1.1956	13
303	1.167	vw	1.1680	4
115	1.151	m	1.1513	10
214	1.131	s−	1.1330	9
311			1.1316	11
006	1.095	w−	1.0947	5
312	1.083	m−	1.0846	7
304	1.057	m−	1.0569	8
223	1.048	s	1.0493	17
400	1.0352	w+	1.0357	3
313	------	--	1.0172	1
215	------	--	1.0064	6
116	------	--	0.9975	1
206	------	--	.9679	6
305	------	--	.9518	6
314	------	--	.9412	9
321	------	--	.9404	9
403	------	--	.9360	3
107	------	--	.9152	2
322	------	--	.9129	7
410	------	--	.9038	2
117	------	--	.8735	13
323	------	--	.8716	6
315	------	--	.8648	7
306	------	--	.8579	2
413	------	--	.8356	4
501	------	--	.8223	6
226	------	--	.8074	10
108	------	--	.8051	10
217				
502	------	--	.8033	5
420	------	--	.7829	6

References

[1] H. J. Wallbaum, Disilizide des Niobs, Tantals, Vanadiums und Rheniums, Z. Metallkunde **33**, 378–381 (1941).

[2] R. F. Walker and S. F. Holley, NBS Report **3252**, (March 31, 1954).

[3] B. Borén, Röntgenuntersuchung der Leigierungen von Silicium mit Chrom, Mangan, Kobalt und Nickel, Arkiv Kemi, Mineral., Geol., **11A**, No. 10, 1–28 (1933).

Thallium(I) Bromate, $TlBrO_3$ (trigonal)

ASTM cards. None.

Additional published patterns

Source	Radiation
Rivoir and Abbad [1] 1948	Copper, $K\alpha_1$

NBS sample. The sample of thallium bromate was precipitated at NBS from a solution of thallium hydroxide with a solution of hydrogen bromate. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of calcium, magnesium, and silicon.

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

Interplanar spacings and intensity measurements. The *d*-values reported in the Rivoir and Abbad pattern were converted from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Rivoir and Abbad	012	110	202
National Bureau of Standards	012	110	202

hkl hex.	1948 Rivoir and Abbad Cu, 1.5405 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
101	4.35	m	4.46	32
012	3.20	vs	3.222	100
110	3.04	vs	3.086	67
003	2.68	w	2.696	11
021	2.52	m	2.539	23
202	2.220	vs	2.231	50
113	2.030	w	2.030	10
211	1.955	w	1.960	7
104	1.886	s	1.891	29
122	1.802	vs	1.808	31
300	1.773	m	1.783	13
024	1.608	m	1.613	12
015	-----	--	1.585	14
220	1.538	s	1.544	16
303	1.484	vw	1.487	5
131	1.452	w	1.458	5
214	1.426	s	1.430	19
312	-----	--	1.393	11
205	1.381	s	1.384	7
006	1.341	vw	1.349	14
223	-----	--	1.340	4
401	-----	--	1.319	3
042	1.262	w	1.270	7
125	1.258	vw	1.263	5
116	1.231	m	1.236	8
321	1.208	vw	1.2126	2
134	1.192	m	1.1968	6
232	-----	--	1.1742	1
410	1.166	vs	1.1674	7
107	1.129	vw	1.1299	1
404	1.111	w	1.1159	4
315	1.090	vw	1.0937	1
306	-----	--	1.0757	3
413	1.069	vs	1.0716	3
027 051	1.057	vw	1.0609	1
324	1.046	w	1.0492	3
502	1.033	vw	1.0343	3
045	1.028	vw	1.0308	2
226	1.013	w	1.0157	1
217 241	1.000	w	1.0033	1
018	0.9911	vw	0.9936	2
422	------	--	.9807	3
235	.9771	m	.9784	3
333	-----	--	.9622	1
511	-----	--	.9540	<1
208 054	.9461	w	.9458	<1
152	.9322	w	.9348	2
137	.9099	vw	.9116	<1
128 244	-----	--	.9044	4
009	-----	--	.8988	<1
505	-----	--	.8925	1
600	-----	--	.8916	<1
416	-----	--	.8824	2
431 407	-----	--	.8742	<1
514	-----	--	.8678	1
119	-----	--	.8629	1
342	-----	--	.8593	2
425	-----	--	.8572	1
520	-----	--	.8566	<1
603	-----	--	.8465	<1
327	-----	--	.8414	<1
318	-----	--	.8359	<1
155	-----	--	.8258	1
336	-----	--	.8182	2
523	-----	--	.8164	3
048 434	-----	--	.8065	2
309	-----	--	.8026	1
1·0·10 612	-----	--	.7998	3
057	-----	--	.7850	1
238	-----	--	.7803	3

Structural data. Rivoir and Abbad [1] in 1948 determined that thallium bromate has potassium bromate-type structure, the space group R3m (No. 160), 1($TlBrO_3$) per unit rhombohedral cell, or 3($TlBrO_3$) per unit hexagonal cell.

The rhombohedral unit cell measurements reported by Rivoir and Abbad in kX units were converted to hexagonal values in angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1948	Rivoir and Abbad [1]	6.16	8.09
1958	National Bureau of Standards	6.179	8.089 at 25°C

The density of thallium bromate calculated from the NBS lattice constants is 6.188 g/cm³ at 25°C.

References

[1] L. Rivoir and M. Abbad, La estructura del bromato talioso, Anales real soc. españ. fís. y quím. (Madrid). Ser. A 44, 5–15 (1948).

Thallium(I) Chlorate, $TlClO_3$ (trigonal)

ASTM cards. None.

Additional published patterns

Source	Radiation
Smith and Carrera [1] 1951	Copper $K\alpha_1$

NBS sample. The sample of thallous chlorate was made at NBS by reaction of solutions of thallous sulfate and barium chlorate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of silicon and sodium; and 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, and barium.

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

Interplanar spacings and intensity measurements. The *d*-values of the Smith and Carrera pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Smith and Carrera [1]	101	012	110
National Bureau of Standards	012	110	101

Structural data. Smith and Carrera [1] in 1951 determined that thallous chlorate has potassium bromate-type structure, the space group R3m (No. 160), and 1($TlClO_3$) per unit rhombohedral cell, or 3($TlClO_3$) per unit hexagonal cell.

The rhombohedral unit cell measurements reported by Smith and Carrera have been converted to hexagonal values for comparison with the NBS values.

hkl hex.	1951 Smith and Carrera Cu, 1.5405 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
101	4.43	vs	4.42	74
012	3.23	vs	3.21	100
110	3.06	vs	3.05	83
003	2.71	w	2.701	15
021	2.52	s	2.509	40
202	2.217	vs	2.211	41
113	2.021	s	2.021	26
211	1.940	ms	1.9371	22
104	1.893	ms	1.8904	16
122	1.793	s	1.7889	24
300	1.758	m	1.7583	14
024	1.611	m	1.6060	9
015	1.556	w	1.5482	6
220	1.522	m	1.5230	10
303	1.474	m	1.4733	6
131	1.437	mw	1.4399	7
214	1.425	s	1.4205	12
205	1.381	s	1.3798	6
312			1.3762	11
006	1.354	vvw	1.3498	2
223	1.326	w	1.3266	4
401	1.304	vw	1.3017	2
125	1.259	m	1.2575	5
042	-----	--	1.2545	4
116	1.238	m	1.2334	5
321	-----	--	1.1969	2
134	1.189	m	1.1857	4
232	1.162	ms	1.1591	4
410	1.149	ms	1.1513	4
107	-----	--	1.1301	2
404	1.104	w	1.1051	1
315	1.089	m	1.0858	2
306	1.075	m	1.0708	2
027	1.062	vw	1.0591	3
413				

hkl hex.	1951 Smith and Carrera Cu, 1.5405 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
051	-----	--	1.0462	1
324	1.041	m	1.0388	3
045	-----	--	1.0231	2
502	-----	--	1.0211	1
330	-----	--	1.0153	2
226	-----	--	1.0102	2
217	-----	--	1.0008	<1
018	-----	--	0.9942	1
241	-----	--	.9899	2
235	-----	--	.9693	2
422	-----	--	.9681	2
333	-----	--	.9502	<1
208	-----	--	.9449	<1
511	-----	--	.9411	<1
054	-----	--	.9356	2
152	-----	--	.9226	1

Lattice constants

		a	c
		A	A
1951	Smith and Carrera [1]-----	6.059	8.153
1958	National Bureau of Standards--------------	6.092	8.098 at 25°C

The density of thallous chlorate calculated from the NBS lattice constants is 5.508 g/cm³ at 25°C.

References

[1] P. Smith and S. Martínez Carrera, La estructura del clorato talioso, Anales real soc. españ. fís y quím., (Madrid) Ser. A **47**, 89–94 (1951).

Thallium(I) Iodate, $TlIO_3$ (trigonal)

ASTM cards. None.

Additional published patterns

Source	Radiation
Rivoir and Abbad [1] 1947------------	Copper, Kα

NBS sample. The sample of thallous iodate was made at NBS by precipitation. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, barium, iron, magnesium, sodium, lead, and silicon; and 0.0001 to 0.001 percent each of calcium and manganese.

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

Interplanar spacings and intensity measurements. The *d*-values of the Rivoir and Abbad pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Rivoir and Abbad [1]---------	110	122, 300	202
National Bureau of Standards-	012	110	202

Structural data. Wyckoff [2] in 1951 determined that thallous iodate has the potassium bromate-type structure, the space group R3m (No. 160) with 1($TlIO_3$) per unit rhombohedral cell and 3($TlIO_3$) per hexagonal cell.

hkl hex.	1947 Rivoir and Abbad Cu, 1.5405 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
101	----	--	4.52	6
012	----	--	3.21	100
110	3.14	vs	3.17	94
003	----	--	2.644	2
021	2.579	vw	2.598	7
202	2.251	s	2.259	54
113	2.023	vw	2.029	1
211	-----	--	2.011	2
104	1.853	m	1.8635	18
122	1.826	vs	1.8384	40
300			1.8335	30
024	1.597	m	1.6065	12
220	1.578	m	1.5860	14
303	-----	--	1.5049	<1
214	1.421	s	1.4330	16
312			1.4221	16
223	-----	--	1.3585	<1
006	1.317	vw	1.3211	2
042	1.294	w	1.2977	4
116	1.214	m	1.2190	7
134	-----	--	1.2078	7
232	1.198	s	1.2013	10
410			1.1995	10
404	1.125	w	1.1287	4
107	-----	--	1.1094	<1
315	-----	--	1.0992	<1
413	-----	--	1.0918	<1
051	-----	--	1.0880	1
306	1.070	m	1.0709	6
324	-----	--	1.0632	3

hkl hex.	1947 Rivoir and Abbad Cu, 1.5405 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
502	1.055	s	1.0588	3
330			1.0575	3
226	1.011	m	1.0148	2
422	1.002	m	1.0045	3
217	-----	--	0.9943	<1
511	-----	--	.9789	<1
018	0.973	w	.9745	1
054	-----	--	.9610	2
152	.956	m	.9576	3
208	.930	w	.9321	1
244	.916	m	.9196	3
600	.910	w	.9155	<1

The rhombohedral unit-cell measurements reported by Rivoir and Abbad in kX units were converted to hexagonal values in angstrom units for comparison with the NBS values.

Lattice constants

		a	c
		A	A
1947	Rivoir and Abbad [1]	6.24	7.83
1958	National Bureau of Standards	6.344	7.925 at 25°C

The density of thallous iodate calculated from the NBS lattice constants is 6.839 g/cm³ at 25°C.

References

[1] L. Rivoir and M. Abbad, La estructura del yodato talioso, Anales real soc. españ. fís. y quím. (Madrid) **43**, 1051–1060 (1947).

[2] R. W. G. Wyckoff, Crystal Structures **I**, chap. VII 17a (1951).

Thallium(I) Thiocyanate, TlCNS (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
2–0773	2.87 1.82 1.18	Chromium	Strada [1] 1933.

Card number 2–0773 gives a pattern based on a tetragonal structure which is presumably wrong [2]. It is included for comparison to show a possible relation to the orthorhombic pattern.

Additional published patterns

Source	Radiation
Büssem, Günther, and Tubin [3] 1934	Copper, Kα

NBS sample. The sample of thallous thiocyanate was prepared at NBS by precipitation from solutions of thallium sulfate and potassium thiocyanate. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of silver, silicon, and tin; 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, nickel, and sodium; and 0.0001 to 0.001 percent each of barium, chromium, copper, lead, and manganese.

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

Interplanar spacings and intensity measurements. The *d*-values of the Büssem, Günther, and Tubin and the M. Strada patterns were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

hkl	1934 M. Strada Cr, 2.2909 A		1934 Büssem, Günther, and Tubin Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I	d	I
	A		A		A	
100	----	--	----	--	6.78	5
110	4.48	70	----	--	4.80	84
002	----	--	3.80	20	3.81	22
020	3.26	80	3.41	57	3.40	45
200					3.39	48
102	----	--	----	--	3.32	7
210	----	--	----	--	3.04	13
112	2.88	100	2.96	100	2.983	100
121	----	--	2.81	7	2.823	8
211						
022	2.45	80	2.52	33	2.538	42
202					2.531	44
220	2.33	70	2.39	16	2.404	25
212					2.377	6
122						
300	----	--	2.27	3	2.2596	4
130	2.08	60	2.14	21	2.1532	27
310					2.1464	24
311	----	--	----	--	2.0655	1
222	----	--	2.02	11	2.0316	21
302	----	--	----	--	1.9434	5
004	----	--	----	--	1.8993	9
320	----	--	----	--	1.8827	6
132	1.82	100	1.87	16	1.8743	21
312					1.8696	20
114	----	--	1.76	7	1.7672	12
040	----	--	1.68	5	1.7030	3
400					1.6949	3
232					1.6903	6
204	----	--	1.65	6	1.6584	10
410					1.6450	3

hkl	1934 M. Strada Cr, 2.2909 A		1934 Büssem, Günther, and Tubin Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
214	----	--	----	--	1.6122	2
330	----	--	----	--	1.6024	3
042	1.51	80	----	--	1.5546	7
402	----	--	----	--	1.5487	6
240	----	--	----	--	1.5221	5
420	----	--	----	--	1.5181	6
412	----	--	----	--	1.5100	5
224	1.47	70	----	--	1.4910	8
332	1.46	50	----	--	1.4767	8
304	----	--	----	--	1.4549	1
134	1.44	60	----	--	1.4250	8
314	----	--	----	--	1.4230	8
242	----	--	----	--	1.4129	4
422 403	1.38	80	----	--	1.4097	5
430	----	--	----	--	1.3578	3
500	----	--	----	--	1.3563	3

References

[1] M. Strada, Ricerche sulla struttura dei pseudo-alogeni e dei loro compotti. I. Tiocianato di tallio, Gazz. chim. ital. **64**, 400–429, 526 (1934).

[2] R. W. G. Wyckoff, The structure of crystals, Supp. to 2d Ed., p. 43 (1935).

[3] W. Büssem, P. Günther, and R. Tubin, Die Struktur des Thallorhodanids und des Kaliumrhodanids, Z. phys. Chem. **24B**, 1–21 (1934).

Pattern	1	2	3
M. Strada	112	132, 312	020, 200
Büssem, Günther, and Tubin	112	020, 200	202, 022
National Bureau of Standards	112	110	200

Structural data. Büssem, Günther, and Tubin [3] in 1934 determined that thallous thiocyanate has potassium thiocyanate-type structure, the space group Pbcm (No. 57), and 4(TlCNS) per unit cell.

The unit-cell measurements reported by Büssem, Günther, and Tubin [3] have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1934	Büssem, Günther, and Tubin [3]	6.79	6.81	7.54
1958	National Bureau of Standards	6.782	6.814	7.603 at 25°C

The density of thallous thiocyanate calculated from the NBS lattice constants is 4.961 g/cm³ at 25°C.

Titanium Silicide, Ti_5Si_3 (hexagonal)

ASTM cards. None.

Additional published patterns

Source	Radiation
Hansen, Kessler, and McPherson [1] 1952	Copper, Kα

NBS sample. The sample of titanium silicide was prepared at NBS by Ramond F. Walker and Sylvanus F. Holley by solid-state reaction of the elements at 1,300°C for 3 hr [2]. Spectrographic analysis showed the following impurities: 0.1 to 1.0-percent aluminum; 0.01 to 0.1 percent each of calcium, chromium, iron, and zirconium; and 0.001 to 0.01 percent each of cobalt, copper, magnesium, manganese, nickel, antimony, and tin. The sample was a dark gray metallic powder.

Interplanar spacings and intensity measurements. The *d*-values reported by Hansen, Kessler, and McPherson are, as published, in angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Hansen, Kessler, and McPherson [1]	211	112	300
National Bureau of Standards	211	112	210

hkl	1952 Hansen, Kessler, and McPherson Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
200	----	--	3.220	7
111	----	--	3.010	6
002	2.54	vvw	2.569	14
210	2.41	vvw	2.412	47
102	2.37	vw	2.385	30
211	2.19	mw	2.198	100
300	2.14	w	2.145	38
112	2.11	mw	2.113	98
202	----	--	2.007	6
220	----	--	1.857	6
221	----	--	1.745	10
311	1.675	<vvw	1.685	9
400	-----	--	1.6075	9
222	1.506	vw	1.5056	18
312	1.470	<vvw	1.4656	8
321	1.421	w	1.4180	10
410	-----	--	1.4039	15
213	-----	--	1.4003	29
402	1.367	vw	1.3637	12
500	1.285	w	1.2867	15
004			1.2846	21

hkl	1952 Hansen, Kessler, and McPherson Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
104 223	-----	--	1.2597	3
313	1.238	vvw	1.2360	6
420	1.221	<vvw	1.2156	7
331	1.208	<vvw	1.2040	9
421	-----	--	1.1825	2
502	1.163	<vvw	1.1502	14
214	1.136	<vvw	1.1360	11
511	1.120	<vvw	1.1275	3
323	-----	--	1.1180	4
332	-----	--	1.1151	10
304	1.105	w	1.1021	11
521	1.012	<vvw	1.0101	7
333 404	0.995	<vvw	1.0030	9
602	-----	--	0.9897	5
610	-----	--	.9813	6
432	-----	--	.9785	4
513	.962	--	.9578	2
522	----	--	.9560	2
215	.951	vw	.9469	11
440	.932	<vvw	.9283	7
504	----	--	.9094	6
523 424	.886	vvw	.8830	8
621	.870	vw	.8791	8
532 702	-----	--	.8654	7
514	.856	<vvw	.8590	5
710	----	--	.8522	4
325	.844	<vvw	.8438	4
116	.838	vvw	.8344	8
206	----	--	.8277	5
524 800	.806	<vvw	.8039	4
631	----	--	.8008	3
623	.782	vvw	.7913	3
---	.778	mw	-----	---

Structural data. Pietrokowsky and Duwez [3] in 1951 determined that titanium silicide has manganese silicide-type structure, space group $P6_3/mcm$ (No. 193), and $16(Ti_5Si_3)$ per unit cell. Unit-cell measurements compare as follows:

Lattice constants

		a	*c*
		A	*A*
1951	Pietrokowsky and Duwez [3]	7.465	5.162
1958	National Bureau of Standards	7.429	5.1392 at 25°C

The density of titanium silicide calculated from the NBS lattice constants is 3.501 g/cm³ at 25°C.

References

[1] M. Hansen, H. D. Kessler, and J. D. McPherson, The titanium-silicon system, Trans. A. S. M. **44,** 518-38 (1952).

[2] R. F. Walker and S. F. Holley, NBS Report **3252,** (March 31, 1954).

[3] P. Pietrokowsky and P. Duwez, Crystal structure of Ti_5Si_3, Ti_5Ge_3 and Ti_5Sn_3, J. Metals **3,** 772–773 (1951).

Tungsten Sulfide (tungstenite), WS_2 (hexagonal)

ASTM cards

Card number	Index lines	Radiation	Source
2-0131	6.2 2.68 2.28	Copper	Harcourt [1] 1938.

Additional published patterns

Source	Radiation
van Arkel [2] 1926	Copper, K_α

NBS sample. The sample of tungsten sulfide was made at NBS by direct combination of the elements in a sealed fused silica tube at 900°C. Ehrlich [3] determined that the homogeneity range of tungsten sulfide is from $WS_{1.95}$ to $WS_{2.00}$. A pattern from a second NBS sample which contained excess sulfur showed no apparent change in lattice constants; hence it is assumed that the ratio of tungsten to sulfur in each sample of WS_2 is 1:2. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of magnesium and silicon; 0.001 to 0.01 percent each of chromium, copper, manganese, and lead. The same a, was black metallic powder.

Interplanar spacings and intensity measurements. The *d*-values reported by Harcourt have been converted from kX to angstrom units. The *d*-

Tungsten Sulfide (tungstenite), WS_2 (hexagonal)

hkl	1926 van Arkel Cu, 1.5418 A		1942 Harcourt Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
002	6.10	---	6.2	100	6.18	100
004	3.10	---	---	--	3.089	13
100	----	---	---	--	2.731	24
101	2.68	---	2.69	66	2.667	27
102	----	---	----	--	2.498	7
103	2.30	---	2.28	22	2.277	36
006	2.09	---	2.05	11	2.061	12
105	1.86	---	1.88	11	1.834	17
106	1.66	---	----	--	1.6455	2
110	1.60	---	1.58	22	1.5783	16
008	1.56	---	----	--	1.5458	8
112	1.50	---	1.52	20	1.5288	14
107	----	---	----	--	1.4832	3
114	1.42	---	1.40	3	1.4052	5
200	1.38	---	----	--	1.3658	3
201	1.36	---	1.35	6	1.3575	3
108	1.32	---	1.31	3	1.3449	4
116	1.26	---	1.25	6	1.2524	7
0·0·10	1.24	---	----	--	1.2362	1
109	1.21	---	----	--	1.2274	1
205	1.14	---	----	--	1.1954	4
1·0·10	1.12	---	----	--	1.1271	<1
118	1.10	---	1.10	11	1.1037	8
---	1.06	---	----	--	------	--
1·0·11	1.05	---	----	--	1.0392	2
0·0·12	1.02	---	1.027	11	1.0300	4
213	----	---	1.002	11	1.0012	4
1·1·10	0.989	---	0.962	6	0.9726	3
215	----	---	----	--	.9524	4
300	----	---	----	--	.9117	1
302	----	---	----	--	.9021	1
1·0·13	----	---	----	--	.8981	3
0·0·14	----	---	----	--	.8830	<1
2·0·11	----	---	----	--	.8630	1
1·1·12	----	---	----	--	.8626	1

values of the van Arkel pattern were calculated from Bragg angle data. The van Arkel pattern did not include intensity measurements. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Harcourt	002	101	103
National Bureau of Standards	002	103	101

Structural data. Van Arkel [2] in 1926 determined that tungsten sulfide has molybdenum sulfide-type structure, space group $P6_3/mmc$ (No. 194), and $2(WS_2)$ 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	van Arkel [2]	3.19	12.5
1948	Ehrlich [3]	3.15	12.3
1948	Glemser, Sauer, and König [4]	3.18	12.5
1958	National Bureau of Standards	3.154	12.362 at 25°C

The density of tungsten sulfide calculated from the NBS lattice constants is 7.732g/cm³ at 25°C.

References

[1] G. A. Harcourt, Tables for the identification of ore minerals by X-ray powder patterns, Am. Mineralogist **27**, 63–113 (1942).

[2] A. E. van Arkel, Über die Kristallstruktur der Verbindungen Manganfluorid, Bleijodid und Wolframsulfid, Rev. trav. chim. **45**, 437–444 (1926).

[3] P. Ehrlich, Untersuchungen an Wolframsulfiden, Z. anorg. u. allgem. Chem. **257**, 247–253 (1948).

[4] O. Glemser, H. Sauer and P. König, Über Wolframsulfide und Wolframselenide, Z. anorg. u. allgem. Chem. **257**, 241–246 (1948).

Vanadium(V) Oxide, V_2O_5 (orthorhombic)

ASTM cards

Card numbers	Index lines	Radiation	Source
3–0206 and 3–0207	4.40 2.90 3.41	Chromium	Ketelaar [1] 1936.
1–0359	4.38 3.39 2.87	Molybdenum	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns. None.

NBS sample. The sample of vanadium pentoxide was obtained from the Vanadium Corp. of America, New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of aluminum; 0.001 to 0.01 percent each of iron and silicon; and 0.0001 to 0.001 percent each of chromium, copper, magnesium, manganese, and tin.

The color of the sample was dull orange. The indices of refraction were not determined by the usual liquid grain immersion method because the sample was too fine-grained.

Interplanar spacings and intensity measurements. The d-values reported by Hanawalt, Rinn, and Frevel were converted from kX to angstrom units and the d-values of the Ketelaar pattern were calculated from reported Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Ketelaar	001	400	110
Hanawalt, Rinn, and Frevel	001	110	400
National Bureau of Standards	001	110	400

Structural data. Byström, Wilhelmi, and Brotzen [3] in 1950 determined that vanadium pentoxide has the space group Pmmn (No. 59) and $2(V_2O_5)$ per unit cell. Vanadium pentoxide is used as a structure type.

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

Lattice constants

		a	*b*	*c*
		A	*A*	*A*
1936	Ketelaar [1]	11.50	3.56	4.37
1950	Byström, Wilhelmi, and Brotzen[3]	11.519	3.564	4.373
1958	National Bureau of Standards	11.51	3.559	4.371 at 25°C

The density of vanadium pentoxide calculated from the NBS lattice constants is 3.372 g/cm³ at 25°C.

References

[1] J. A. A. Ketelaar, Die Kristallstruktur des Vanadinpentoxyds, Z. Krist. **95,** 9–27 (1936).

[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] A. Byström, K. A. Wilhelmi, and O. Brotzen, Vanadium pentoxide–a compound with five-coordinated vanadium atoms, Acta Chem. Scand. **4,** 1119–1130 (1950).

Vanadium(V) Oxide, V_2O_5 (orthorhombic)

hkl	1936 Ketelaar Cr, 2.291 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
200	5.77	mw	5.8	33	5.76	42
001	4.39	vvs	4.39	100	4.38	100
101	4.09	m	----	--	4.09	36
201	3.49	vvw	----	--	3.48	7
110	3.42	s	3.40	83	3.40	91
400	2.90	s+	2.88	53	2.88	65
011	2.77	mw+	2.77	13	2.76	35
111	2.69	vw	2.69	7	2.687	14
310	2.61	mw	2.62	13	2.610	39
211	2.51	vvw	----	--	2.492	6
401	----	---	----	--	2.405	6
---	2.24	w	----	--	-----	--
002	2.18	s	2.18	7	2.185	17
102	2.14	m	----	--	2.147	10
202	2.04	vw	----	--	2.042	2
411	1.99	vw	1.99	7	1.992	16
600	1.92	m	1.92	13	1.919	26
302	1.89	w+	----	--	1.900	16
012	1.86	mw	1.86	7	1.864	12
112	1.84	w−	----	--	1.840	4
020	1.78	mw	----	--	1.778	2
601	1.76	mw	1.77	10	1.757	28
402	1.73	vvw	----	--	1.740	13
---	1.70	vw	----	--	-----	--
021	1.65	mw+	1.65	7	1.648	11
---	1.63	vw	----	--	1.632	6
611	1.57	w	----	--	1.5764	9
412	1.56	mw	1.56	7	1.5640	11
701	1.54	w	----	--	1.5396	3
321	----	--	1.51	7	1.5149	16
420	----	--	----	--	1.5124	10
710	1.49	m	1.493	7	1.4925	16
103	1.44	s	1.455	7	1.4447	6
602	1.43	mw	-----	--	1.4421	4
711	1.41	vw	-----	--	1.4123	6
022	1.38	mw	-----	--	1.3801	5
---	1.37	w	-----	--	------	--
303	1.36	vw	1.305	7	1.3625	4

Yttrium Phosphate (xenotime), YPO_4 (tetragonal)

ASTM cards

Card number	Index lines	Radiation	Source
5-0454	3.43 1.76 2.55	Copper	Horne, Geological Museum, London

Additional published patterns

Source	Radiation
Vegard [1] 1927	Chromium K_α
Strada and Schwendimann [2] 1934	Chromium K_α

NBS sample. The sample of yttrium phosphate was prepared in a hydrothermal bomb at 375°C at

Yttrium Phosphate (xenotime), YPO_4 (tetragonal)

hkl	---- Horne Cu, 1.5418 A		1927 Vegard Cr, 2.2909 A		1934 Strada and Schwendimann Cr, 2.2909 A		1958 National Bureau of Standards Cu, 1.5405 A at 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*	
101	4.53	30	4.57	15	----	--	4.54	24
200	3.43	100	3.45	90	3.35	s	3.443	100
211	2.73	20	2.73	5	----	--	2.744	9
112	2.55	60	2.56	60	2.52	m	2.558	58
220	2.43	40	2.44	15	----	--	2.434	19
202	2.26	10	2.27	10	2.25	w	2.265	9
301	2.14	50	2.15	30	2.12	m	2.145	23
103	1.925	20	1.93	30	----	--	1.927	13
321	1.820	50	1.82	25	1.80	m	1.820	16
312	1.763	70	1.77	100	1.75	vs	1.762	47
400	1.719	50	1.72	40	1.71	m	1.721	17
213	1.681	10	1.69	5	----	--	1.681	7
411	1.609	10	1.61	5	----	--	1.608	5
420	1.539	40	1.54	15	1.53	m	1.540	10
303	1.511	10	1.52	10	1.50	w	1.505	4
332	1.428	30	1.43	50	1.42	s	1.428	13
323	1.379	30	1.38	30	----	--	1.379	10
431	1.343	30	1.34	15	1.34	m	1.342	7
413	1.281	30	1.28	60	1.29	m	1.280	11
314	1.232	40	1.24	90	1.24	s	1.232	11
440	1.218	10	1.22	20	1.22	m	1.2171	<1
600	1.149	30	----	--	----	--	1.1475	6
503	1.135	20	----	--	----	--	1.1331	6
611	-----	--	----	--	----	--	1.1118	1
532	1.100	30	----	--	----	--	1.0991	6
620	1.090	30	----	--	----	--	1.0885	6
523	1.077	30	----	--	----	--	1.0762	10
631	1.013	10	----	--	----	--	1.0114	4
613	0.985	10	----	--	----	--	0.9826	6
116	-----	--	----	--	----	--	.9765	2
640	.957	20	----	--	----	--	.9547	4
543	.949	10	----	--	----	--	.9464	6
721	----	--	----	--	----	--	.9340	3
534	.928	40	----	--	----	--	.9262	8
712								
633	.914	20	----	--	----	--	.9111	6
604								
703	.885	20	----	--	----	--	.8819	5
732	.868	20	----	--	----	--	.8656	6
800	----	--	----	--	----	--	.8604	<1
723	----	--	----	--	----	--	.8533	2
820	----	--	----	--	----	--	.8347	3
802	----	--	----	--	----	--	.8282	3
660	----	--	----	--	----	--	.8112	2
644	----	--	----	--	----	--	.8053	7
813	----	--	----	--	----	--	.7857	2

the NBS by Alvin Perloff using yttrium oxide and an excess of 1:1 phosphoric acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, dysprosium, platinum, and silicon; 0.001 to 0.01 percent each of erbium, iron, magnesium, and ytterbium; and 0.001 to 0.001 percent of lead. The sample was colorless. The particle size was too small to determine the refractive indices.

Interplanar spacings and intensity measurements. The *d*-values reported by Horne and by Strada and Schwendimann have been converted from kX to angstrom units. The *d*-values of the Vegard pattern were calculated from Bragg angle data. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
Horne	200	312	112
Vegard	312	200	314
Strada and Schwendimann	312	200	114
National Bureau of Standards	200	112	312

Structural data. Vegard [1] in 1923 determined that yttrium phosphate has a zircon-type structure, the space group being $I4_1/amd$ (No. 141), and $4(YPO_4)$ per unit cell. Two unit-cell measurements have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	*c*
		A	*A*
1927	Vegard [1]	6.90	6.03
1934	Strada and Schwendimann [2]	6.88	6.19
1958	National Bureau of Standards	6.885	5.982 at 26°C

The density of yttrium phosphate calculated from the NBS lattice constants is 4.306 g/cm³ at 26°C.

References

[1] L. Vegard, The structure of xenotime and the relation between chemical constitution and crystal structure, Phil. Mag. **4**, 511 (1927).

[2] M. Strada and G. Schwendimann, La struttura cristallina di alcuni forfati des metalli trivalenti. II. Arseniato e fosfato di ittrio, Gazz. Chim. Ital. **64**, 662–674 (1934).

Zinc Carbonate (smithsonite), $ZnCO_3$ (trigonal)

ASTM cards

Card numbers	Index lines	Radiation	Source
3–0774	2.75 1.71 3.56	Molybdenum	The Dow Chemical Co.
3–1336	No powder data		Brentano and Adamson [1] 1929.

Additional published patterns

Source	Radiation
Levi and Ferrari [2] 1924	Copper, K_α

NBS sample. The zinc carbonate used was the Natural Museum sample No. 96155 from Broken Hill, Rhodesia. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of cadmium, iron, magnesium, and lead; 0.001 to 0.01 percent each of calcium, manganese, and silicon; and 0.0001 to 0.001 percent of copper. The sample was colorless and optically negative. The indices of refraction are $N_o=1.841$ and $N_e=1.630$.

Interplanar spacings and intensity measurements. The *d*-values reported by Levi and Ferrari have been converted from kX to angstrom units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
The Dow Chemical Co.	104	116,018	012
Levi and Ferrari	104	116,018	3·0·12
National Bureau of Standards	104	012	116,018

hkl hex.	---- The Dow Chemical Co. Mo, 0.7107 A		1924 Levi and Ferrari Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*	
012	3.56	32	3.33	m	3.55	49
104	2.75	100	2.63	vs	2.750	100
110	2.33	16	2.26	ms	2.327	25
113	2.11	10	2.05	ms	2.110	18
202	1.95	20	1.90	s	1.946	26
024	1.78	8	1.74	m	1.776	11
116 018	1.71	48	1.67	vs	1.703	44
211	----	--	1.47	s	1.515	13
122	1.49	10	1.39	s	1.493	13
214	1.41	11	----	--	1.411	9
1·0·10	----	--	----	--	1.408	2
208	1.38	3	----	--	1.374	3
119	----	--	----	--	1.357	2
300	1.34	8	1.33	ms	1.343	9
0·0·12	1.26	2	1.24	m	1.2524	6
217	----	--	----	--	1.2423	1
0·2·10	1.21	2	1.20	w	1.2048	3
306 128	1.18	5	1.17	s	1.1833	8
220	1.16	2	1.16	w	1.1632	1
312	----	--	----	--	1.1057	2
1·1·12	----	--	----	--	1.1028	2
134	----	--	1.06	s	1.0710	6
2·1·10	----	--	----	--	1.0699	3
226	----	--	----	--	1.0552	2
0·1·14	----	--	----	--	1.0371	<1
404	----	--	----	--	0.9730	5
318	----	--	0.956	m	.9606	8
2·0·14	----	--	.946	w	.9473	1

hkl hex.	---- The Dow Chemical Co. Mo, 0.7107 A		1924 Levi and Ferrari Cu, 1.5418 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
1·1·15	----	--	----	--	.9201	3
232	----	--	----	--	.9174	3
3·0·12	----	--	.915	vs	.9160	8
324	----	--	.897	m	.8977	<1
1·3·10	----	--	----	--	.8967	<1
048	----	--	.888	m	.8878	<1
410	----	--	.878	ms	.8793	1
1·2·14	----	--	----	--	.8775	<1
2·2·12	----	--	.855	ms	.8523	1
0·2·16	----	--	----	--	.8514	<1
4·0·10	----	--	----	--	.8370	<1
416 238	----	--	.832	s	.8295	2
502	----	--	.802	ms	.8013	<1
2·1·16	----	--	----	--	.7994	3
054	----	--	----	--	.7878	1
3·2·10	----	--	.790	s	.7873	2
1·1·18	----	--	----	--	.7857	2

Structural data. Wyckoff [3] in 1920 determined the structure of calcite. Levi and Ferrari [2] showed in 1924 that zinc carbonate has calcite-type structure, the space group $\mathrm{R}\bar{3}\mathrm{c}$ (No. 167), and 2($ZnCO_3$) per unit rhombohedral cell or 6($ZnCO_3$) per unit hexagonal cell.

The unit-cell measurements reported by Goldschmidt have been converted from kX to angstrom units for comparison with the NBS values. Cell measurements were reported by Brentano and Adamson [1] and by Levi and Ferrari [2] but were not included as they were given as large pseudo-cubic values.

Lattice constants

		a	*c*
		A	A
1932	Goldschmidt and Hauptmann [4]	4.6612	15.007
1958	National Bureau of Standards	4.6533	15.028 at 25°C

The density of zinc carbonate calculated from the NBS lattice constants is 4.333 g/cm³ at 25°C.

References

[1] J. Brentano and J. Adamson, Precision measurements of X-ray reflections from crystal powders. The lattice constants of zinc carbonate, manganese carbonate and cadmium oxide, Phil. Mag. **7,** 507–517 (1929).

[2] G. R. Levi and A. Ferrari, I reticoli crystallini dei carbonati romboedrici di metalli bivalenti, Rend. Accad. Lincei **33,** 516–521 (1924).

[3] R. W. G. Wyckoff, The crystal structures of some carbonates of the calcite group, Am. J. Sci. **50,** 317–360 (1920).

[4] V. M. Goldschmidt and H. Hauptmann, Isomorphie von Boraten und Karbonaten, Nachr. Ges. Wiss. Göttingen, Mathphysik Kl. **1932–1933,** 53–72 (1932–1933).

Zinc Fluosilicate Hexahydrate, $ZnSiF_6 \cdot 6H_2O$ (trigonal)

ASTM cards

Card number	Index lines	Radiation	Source
1–0298	4.72 4.17 2.59	Molybdenum	New Jersey Zinc Co.

Additional published patterns. None.

NBS sample. The sample of zinc fluosilicate hexahydrate was obtained from the City Chemical Corp., New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, iron, and magnesium; 0.001 to 0.01 percent each of aluminum, nickel, lead, and titanium; and 0.0001 to 0.001 percent each of silver, barium, copper, and manganese. The sample was colorless. The indices of refraction were too low to be determined by the liquid grain-immersion method.

Interplanar spacings and intensity measurements. The *d*-values reported by the New Jersey Zinc Co. were converted from kX to angstrom

hkl hex.	---- New Jersey Zinc Co. Mo, --------		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		A	
101	----	--	6.22	2
110	4.73	100	4.68	100
012	4.18	75	4.16	46
202	3.10	5	3.11	5
---	3.02	1	------	--
211	2.93	15	2.922	10
113	2.68	5	2.660	5
122	2.60	50	2.590	27
104	----	--	2.321	2
131	----	--	2.191	2
024	2.08	13	2.080	6
303	----	--	2.074	4
312	2.03	1	2.040	2
401	1.988	8	1.9835	4
---	1.946	3	------	--

hkl hex.	---- New Jersey Zinc Co. Mo, --------		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	*I*	*d*	*I*
	A		*A*	
214	1.901	32	1.9008	10
042	1.868	5	1.8706	5
321	1.827	3	1.8270	3
410	1.776	6	1.7694	4
232	1.741	6	1.7372	4
134	1.647	25	1.6488	7
051	-----	--	1.5999	1
330	1.556	4	1.5603	2
116	-----	--	1.5271	2
324	1.479	6	1.4754	2
422	-----	--	1.4611	1
511	-----	--	1.4403	1
333	-----	--	1.4050	<1
045	-----	--	1.4007	<1
152	-----	--	1.3946	1
306	1.395	8	1.3866	2
107	-----	--	1.3651	1
600	1.355	5	1.3510	3
226	1.331	5	1.3299	1
520	1.297	6	1.2981	2
244	-----	--	1.2950	2
342	-----	--	1.2858	<1
514	-----	--	1.2484	<1
612	1.198	9	1.1976	5
440	-----	--	1.1701	1
434	-----	--	1.1675	<1
208	-----	--	1.1604	<1
532 128	1.127	5	1.1265	2
345	-----	--	1.0988	<1
262	-----	--	1.0956	1
170	-----	--	1.0740	1
318	-----	--	1.0666	1
057	-----	--	1.0530	<1
704	-----	--	1.0451	<1
606	-----	--	1.0366	<1
247	1.023	3	1.0276	<1
526	-----	--	1.0122	1
535	-----	--	0.9942	<1
508 722	-----	--	.9706	1

units. The indices of the three strongest lines of each pattern are as follows:

Pattern	1	2	3
New Jersey Zinc Co.	110	012	122
National Bureau of Standards	110	012	122

Structural data. Hassel [1] in 1927 determined that zinc fluosilicate hexahydrate has nickel chlorostannate structure type, the space group $R\bar{3}$ (No. 148) and $1(ZnSiF_6{\cdot}6H_2O)$ per unit rhombohedral cell or $3(ZnSiF_6{\cdot}6H_2O)$ per unit hexagonal cell.

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

Lattice constants

		a	*c*
		A	*A*
1927	Hassel and Salvesen [2]	9.344	9.66
1958	National Bureau of Standards	9.362	9.695 at 25°C

The density of zinc fluosilicate hexahydrate calculated from the NBS lattice constants is 2.135 g/cm^3 at 25°C.

References

[1] O. Hassel, Vorläufige Notiz über die Kristallstruktur einiger Verbindungen von der Zusammensetzung $MG_6{\cdot}LR_6$, Z. physik. Chem. **126,** 118–126 (1927).

[2] O. Hassel and J. R. Salvesen, Über den Kristallbau der trigonal kristallisierenden heteropolaren Verbindungen von der Zusammensetzung $MG_6{\cdot}LR_6$, $MG_5D{\cdot}LR_6$ und $MG_4D_2{\cdot}LR_6$, Z. physik. Chem. **128,** 345–361 (1927).

Zinc Sulfate Heptahydrate (goslarite), $ZnSO_4{\cdot}7H_2O$ (orthorhombic)

ASTM cards

Card number	Index lines	Radiation	Source
1–0402	4.20 5.3 3.44	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of zinc sulfate heptahydrate was a specially purified sample obtained from Mallinckrodt Chemical Works, New York. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent magnesium; 0.001 to 0.01 percent each of calcium and sulfur; and 0.0001 to 0.001 percent each of aluminum, barium, copper, iron, and lead. The NBS pattern was obtained at approximately 100-percent humidity. The sample was colorless and optically negative. The refractive indices are $N_\alpha=1.458$, $N_\beta=1.480$, and $N_\gamma=1.485$. The calculated value of 2V was 25°.

Interplanar spacings and intensity measurements. The *d*-values of the Hanawalt, Rinn, and

Zinc Sulfate Heptahydrate (goslarite), $ZnSO_4 \cdot 7H_2O$ (orthorhombic)

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7107 A		1958 National Bureau of Standards Cu, 1.5405 A at 25°C	
	d	I	d	I
	A		A	
110	----	--	8.43	10
020	----	--	6.02	10
101	----	--	5.91	6
120	5.3	60	5.36	78
210	----	--	5.29	37
021	4.51	16	4.52	7
201	----	--	4.46	25
121	4.21	100	4.21	100
220				
211	----	--	4.18	47
130	3.93	12	3.80	10
310	3.77	20	3.74	21
031	3.45	30	3.457	23
002	----	--	3.411	9
131	3.31	4	3.319	15
230				
112	3.15	2	3.162	4
231	3.00	12	2.985	14
202	----	--	2.953	8
212	2.88	30	2.867	33
330	----	--	2.809	22
041	2.76	10	2.754	20
141	----	--	2.682	16
240	----	--	2.680	16
222	2.67	25	2.651	29
420	----	--	2.648	15
032	----	--	2.599	3
241	2.51	12	2.497	9
421	----	--	2.469	6
340	----	--	2.394	3
232	2.37	8	2.376	8
430				
150	----	--	2.362	9
042	2.25	20	2.258	3
341			2.255	13
013	----	--	2.236	11
103	----	--	2.233	5
113	----	--	2.195	17
052				
023	2.12	20	2.127	7
242	----	--	2.109	2
123	2.08	20	2.092	11
422				
350	----	--	2.055	6
530	----	--	2.034	10
441	2.02	6	2.012	7
060	----	--	2.007	6
033	----	--	1.979	9
303	----	--	1.968	11
052				
133	1.95	12	1.950	7
512	----	--	1.914	10
161	----	--	1.902	9
601	1.87	12	1.888	11
233	----	--	1.874	7
620	----	--	1.867	8
540	----	--	1.857	5
261	----	--	1.831	8
621	1.80	10	1.801	9
143	----	--	1.795	4
630	----	--	1.761	5
352				
062	1.74	6	1.731	13
162	1.71	8	1.713	8
004	----	--	1.706	8
104	----	--	1.687	5
114	----	--	1.671	8
343	----	--	1.648	8
204	1.63	14	1.638	5
622				
153				
124	----	--	1.625	8
214	----	--	1.624	8
224	1.58	4	1.581	5
134	----	--	1.557	2
443	1.52	2	1.546	3
080	1.495	8	1.506	4
603				
272			1.487	8
740	1.468	8	1.467	6
414				
810	----	--	1.461	6
623	1.438	2	1.443	4
424			1.433	3
750	1.385	4	1.379	5
105	1.360	4	1.355	5
831				
254				
812	1.325	2	1.342	3
282				
671	----	--	1.273	3

Frevel pattern were converted from kX to angstrom units. The indices of the three strongest lines for each pattern are as follows:

Pattern	1	2	3
Hanawalt, Rinn, and Frevel	121,220	120	031
National Bureau of Standards	121,220	120	211

Structural data. Westenbrink [2] in 1926 determined that zinc sulfate heptahydrate has magnesium sulfate heptahydrate-type structure, the space group $P2_12_12_1$ (No. 19), and $4(ZnSO_4 \cdot 7H_2O)$ per unit cell.

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

Lattice constants

		a	b	c
		A	A	A
1926	Westenbrink [2]	11.87	12.11	6.84
1958	National Bureau of Standards	11.779	12.050	6.822 at 25°C

The density of zinc sulfate heptahydrate calculated from the NBS lattice constants is 1.972 g/cm^3 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. G. K. Westenbrink, The space groups of the rhombic and monoclinic heptahydrates of the sulfates of bivalent metals, Proc. Accad. Sci. Amsterdam **29**, 1223–1232 (1926).

CUMULATIVE INDEX TO VOLUMES 1, 2, 3, 4, 5, 6, 7, AND 8[6]

	Volume	Page
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Aluminum antimony, AlSb	4	72
Aluminum calcium sulfate hydrate (ettringite), $Al_2O_3\cdot 6CaO\cdot 3SO_3\cdot 31H_2O$	8	3
Aluminum chloride hexahydrate (chloraluminite), $AlCl_3\cdot 6H_2O$	7	3
Aluminum oxide, alpha (corundum), Al_2O_3	2	20
Aluminum oxide monohydrate, alpha (böhmite), $Al_2O_3\cdot H_2O$	3	38
Aluminum oxide monohydrate, beta (diaspore), $Al_2O_3\cdot H_2O$	3	41
Ammonium aluminum sulfate dodecahydrate, $NH_4Al(SO_4)_2\cdot 12H_2O$	6	3
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Ammonium bromoosmate, $(NH_4)_2OsBr_6$	3	71
Ammonium bromoselenate, $(NH_4)_2SeBr_6$	8	4
Ammonium bromotellurate, $(NH_4)_2TeBr_6$	8	5
Ammonium chloride (sal-ammoniac), NH_4Cl	1	59
Ammonium chloroiridate, $(NH_4)_2IrCl_6$	8	6
Ammonium chloropalladate, $(NH_4)_2PdCl_6$	8	7
Ammonium chloropalladite, $(NH_4)_2PdCl_4$	6	6
Ammonium chloroplatinate, $(NH_4)_2PtCl_6$	5	3
Ammonium chlorostannate $(NH_4)_2SnCl_6$	5	4
Ammonium chlortellurate, $(NH_4)_2TeCl_6$	8	8
Ammonium chromium sulfate dodecahydrate, $NH_4Cr(SO_4)_2\cdot 12H_2O$	6	7
Ammonium dihydrogen phosphate, $NH_4H_2PO_4$	4	64
Ammonium fluogermanate, $(NH_4)_2GeF_6$	6	8
Ammonium fluosilicate (cryptohalite), $(NH_4)_2SiF_6$	5	5
Ammonium gallium sulfate dodecahydrate, $NH_4Ga(SO_4)_2\cdot 12H_2O$	6	9
Ammonium iodide, NH_4I	4	56
Ammonium iron sulfate dodecahydrate, $NH_4Fe(SO_4)_2\cdot 12H_2O$	6	10
Ammonium metavanadate, NH_4VO_3	8	9
Ammonium nitrate (ammonia-niter), NH_4NO_3	7	4
Ammonium oxalate monohydrate (oxammite), $(NH_4)_2C_2O_4\cdot H_2O$	7	5
Ammonium perchlorate, NH_4ClO_4, (orthorhombic)	7	6
Ammonium phosphomolybdate tetrahydrate, $(NH_4)_3PO_4(MoO_3)_{12}\cdot 4H_2O$	8	10
Ammonium sulfate (mascagnite), $(NH_4)_2SO_4$	6	12
Ammonium zirconium fluoride $(NH_4)_3ZrF_7$	6	14
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Antimony (III) iodide, SbI_3	6	16
Antimony (III) sulfide (stibnite), Sb_2S_3	5	6
Antimony trioxide (senarmontite), Sb_2O_3	3	31
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Arsenic trioxide (arsenolite), As_2O_3	1	51
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Barium carbonate (witherite), $BaCO_3$	2	54
Barium fluoride, BaF_2	1	70
Barium molybdate, $BaMoO_4$	7	7
Barium nitrate (nitrobarite), $Ba(NO_3)_2$	1	81
Barium peroxide, BaO_2	6	18
Barium sulfate (barite), $BaSO_4$	3	65
Barium sulfide, BaS	7	8
Barium titanate, $BaTiO_3$	3	45
Barium tungstate, $BaWO_4$	7	9
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Cadmium sulfide (greenockite), CdS	4	15
tri-Calcium aluminate, $3CaO\cdot Al_2O_3$	5	10
Calcium bromide hexahydrate, $CaBr_2\cdot 6H_2O$	8	15
Calcium carbonate (aragonite), $CaCO_3$	3	53
Calcium carbonate (calcite), $CaCO_3$	2	51
Calcium chromate, $CaCrO_4$	7	13
Calcium fluoride (fluorite), CaF_2	1	69
Calcium formate, $Ca(HCO_2)_2$	8	16
Calcium hydroxide (portlandite), $Ca(OH)_2$	1	58
Calcium molybdate (powellite), $CaMoO_4$	6	22
Calcium nitrate, $Ca(NO_3)_2$	7	14
Calcium oxide, CaO	1	43
Calcium sulfate (anhydrite), $CaSO_4$	4	65
Calcium sulfide (oldhamite), CaS	7	15
Calcium tungstate (scheelite), $CaWO_4$	6	23
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Cerium (IV) oxide (cerianite) CeO_2	1	56
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Cesium bromate, $CsBrO_3$	8	18
Cesium bromide, CsBr	3	49
Cesium bromoplatinate, Cs_2PtBr_6	8	19
Cesium bromoselenate, Cs_2SeBr_6	8	20
Cesium chlorate, $CsClO_3$	8	20
Cesium chloride, CsCl	2	44
Cesium chloroplatinate, Cs_2PtCl_6	5	14
Cesium chlorostannate, Cs_2SnCl_6	5	16
Cesium chromium sulfate dodecahydrate, $CsCr(SO_4)_2\cdot 12H_2O$	8	21
Cesium dichloroiodide, $CsICl_2$	3	50
Cesium fluoborate, $CsBF_4$	8	22
Cesium fluogermanate, Cs_2GeF_6	5	17
Cesium fluoplatinate, Cs_2PtF_6	6	27
Cesium fluosilicate, Cs_2SiF_6	5	19
Cesium gallium sulfate dodecahydrate, $CsGa(SO_4)_2\cdot 12H_2O$	8	23
Cesium iodide, CsI	4	47
Cesium iron sulfate dodecahydrate, $CsFe(SO_4)_2\cdot 12H_2O$	6	28
Cesium sulfate, Cs_2SO_4	7	17
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Chromium (III) oxide, Cr_2O_3	5	22
Chromium silicide, Cr_3Si	6	29
Copper, Cu	1	15
Copper (I) bromide, CuBr	4	36
Copper (I) chloride (nantokite), CuCl	4	35
Copper (I) iodide (marshite), CuI	4	38
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Copper (II) oxide (tenorite), CuO	1	49
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Germanium dioxide, GeO_2	8	28
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Germanium oxide, GeO_2	1	51
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[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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Lead carbonate (cerussite), $PbCO_3$	2	56
Lead chloride (cotunnite), $PbCl_2$	2	45
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Lead fluoride, beta, PbF_2	5	33
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Lead monoxide (massicot), PbO (yellow)	2	32
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Lead (II, III) oxide (minium), Pb_3O_4	8	32
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Lead selenide (clausthalite), PbSe	5	38
Lead sulfate (anglesite), $PbSO_4$	3	67
Lead sulfide (galena), PbS	2	18
Lead titanate, $PbTiO_3$	5	39
Lead tungstate (stolzite), $PbWO_4$	7	24
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Lithium fluoride, LiF	1	61
Lithium iodate, $LiIO_3$	7	26
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Manganese(II) carbonate (rhodochrosite), $MnCO_3$	7	32
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Potassium bromoselenate, K_2SeBr_6	8	41
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Potassium chloroplatinate, K_2PtCl_6	5	49
Potassium chlorostannate K_2SnCl_6	6	38
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Potassium cyanide, KCN	1	77
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Potassium fluoplatinate, K_2PtF_6	6	42
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Potassium fluosilicate (hieratite), K_2SiF_6	5	50
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Potassium iodide, KI	1	68
Potassium metaperiodate, KIO_4	7	41
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Rubidium bromide, RbBr	7	43
Rubidium bromotellurate, Rb_2TeBr_6	8	46
Rubidium chlorate, $RbClO_3$	8	47
Rubidium chloride, RbCl	4	41
Rubidium chloroplatinate, Rb_2PtCl_6	5	53
Rubidium chlorostannate, Rb_2SnCl_6	6	46
Rubidium chlorotellurate, Rb_2TeCl_6	8	48
Rubidium chromium sulfate dodecahydrate, $RbCr(SO_4)_2 \cdot 12H_2O$	6	47
Rubidium fluoplatinate, Rb_2PtF_6	6	48
Rubidium fluosilicate, Rb_2SiF_6	6	49
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Silver chloride (cerargyrite), AgCl	4	44
Silver iodide (iodyrite), AgI (hexagonal)	8	51
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Silver perrhenate, $AgReO_4$	8	53
Silver phosphate, Ag_3PO_4	5	62
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Sodium fluoride (villiaumite), NaF	1	63
Sodium iodate, $NaIO_3$	7	47
Sodium iodide, NaI	4	31
Sodium metaperiodate, $NaIO_4$	7	48
Sodium nitrate (soda-niter), $NaNO_3$	6	50
Sodium nitrite, $NaNO_2$	4	62
Sodium perchlorate, $NaClO_4$, (orthorhombic)	7	49
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Strontium carbonate (strontianite) $SrCO_3$	3	56
Strontium chloride, $SrCl_2$	4	40
Strontium chloride hexahydrate, $SrCl_2 \cdot 6H_2O$	4	58
Strontium fluoride, SrF_2	5	67
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Strontium formate dihydrate, $Sr(CHO_2)_2 \cdot 2H_2O$ orthorhombic	8	56
Strontium iodide hexahydrate, $SrI_2 \cdot 6H_2O$	8	58
Strontium molybdate, $SrMoO_4$	7	50
Strontium nitrate, $Sr(NO_3)_2$	1	80
Strontium oxide, SrO	5	68
Strontium peroxide, SrO_2	6	52
Strontium sulfate (celestite), $SrSO_4$	2	61
Strontium sulfide, SrS	7	52
Strontium titanate, $SrTiO_3$	3	44
Strontium tungstate, $SrWO_4$	7	53
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Thallium bromide, $TlBr$	7	57
Thallium(I) chlorate, $TlClO_3$	8	61
Thallium(I) chloride, $TlCl$	4	51
Thallium chloroplatinate, Tl_2PtCl_6	5	70
Thallium chlorostannate, Tl_2SnCl_6	6	54
Thallium chromium sulfate dodecahydrate, $TlCr(SO_4)_2 \cdot 12H_2O$	6	55
Thallium fluosilicate, Tl_2SiF_6	6	56
Thallium gallium sulfate dodecahydrate, $TlGa(SO_4)_2 \cdot 12H_2O$	6	57
Thallium(I) iodate, $TlIO_3$	8	62
Thallium(I) iodide, TlI, (orthorhombic)	4	53
Thallium(I) nitrate, $TlNO_3$	6	58
Thallium(III) oxide, Tl_2O_3	2	28
Thallium(I) phosphate, Tl_3PO_4	7	58
Thallium(III) phosphate, $TlPO_4$	7	59
Thallium(I) sulfate, Tl_2SO_4	6	59
Thallium(I) thiocyanate, $TlCNS$	8	63
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Tin, beta, Sn	1	24
Tin (IV) iodide, SnI_4	5	71
Tin(II) oxide, SnO	4	28
Tin(IV) oxide (cassiterite), SnO_2	1	54
Tin(II) telluride, $SnTe$	7	61
Titanium, Ti	3	1
Titanium dioxide (anatase), TiO_2	1	46
Titanium dioxide (rutile), TiO_2	1	44
Titanium silicide, Ti_5Si_3	8	64
Tungsten, W	1	28
Tungsten sulfide (tungstenite), WS_2	8	65
Uranium dioxide, UO_2	2	33
Urea, $CO(NH_2)_2$	7	61
Vanadium(V) oxide, V_2O_5	8	66
Yttrium, oxide, Y_2O_3	3	28
Yttrium phosphate (xenotime), YPO_4	8	67
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Zinc aluminate (gahnite), $ZnAl_2O_4$	2	38
Zinc borate, ZnB_2O_4	1	83
Zinc carbonate (smithsonite), $ZnCO_3$	8	69
Zinc cyanide, $Zn(CN)_2$	5	73
Zinc fluoride, ZnF_2	6	60
Zinc fluosilicate hexahydrate, $ZnSiF_6 \cdot 6H_2O$	8	70
Zinc orthosilicate (willemite), Zn_2SiO_4	7	62
Zinc oxide (zincite), ZnO	2	25
Zinc pyrosilicate hydrate (hemimorphite) $Zn_4(OH)_2Si_2O_7 \cdot H_2O$	2	62
Zinc senenide, $ZnSe$	3	23
Zinc sulfate (zinkosite), $ZnSO_4$	7	64
Zinc sulfate heptahydrate (goslarite), $ZnSO_4 \cdot 7H_2O$	8	71
Zinc sulfide, alpha (wurtzite), ZnS	2	14
Zinc sulfide, beta (sphalerite), ZnS	2	16
Zirconium, alpha, Zr	2	11
Zirconium silicate (zircon), $ZrSiO_4$	4	68
Zirconium sulfate tetrahydrate, $Zr(SO_4)_2 \cdot 4H_2O$	7	66

THE NATIONAL BUREAU OF STANDARDS

The scope of activities of the National Bureau of Standards at its headquarters in Washington, D. C., and its major laboratories in Boulder, Colorado, is suggested in the following listing of the divisions and sections engaged in technical work. In general, each section carries out specialized research, development, and engineering in the field indicated by its title. A brief description of the activities, and of the resultant publications, appears on the inside front cover.

WASHINGTON, D. C.

Electricity and Electronics. Resistance and Reactance. Electron Devices. Electrical Instruments. Magnetic Measurements. Dielectrics. Engineering Electronics. Electronic Instrumentation. Electrochemistry.

Optics and Metrology. Photometry and Colorimetry. Optical Instruments. Photographic Technology. Length. Engineering Metrology.

Heat. Temperature Physics. Thermodynamics. Cryogenic Physics. Rheology. Engine Fuels. Free Radicals Research.

Atomic and Radiation Physics. Spectroscopy. Radiometry. Mass Spectrometry. Solid State Physics. Electron Physics. Atomic Physics. Neutron Physics. Radiation Theory. Radioactivity. X-rays. High Energy Radiation. Nucleonic Instrumentation. Radiological Equipment.

Chemistry. Organic Coatings. Surface Chemistry. Organic Chemistry. Analytical Chemistry. Inorganic Chemistry. Electrodeposition. Molecular Structure and Properties of Gases. Physical Chemistry. Thermochemistry. Spectrochemistry. Pure Substances.

Mechanics. Sound. Mechanical Instruments. Fluid Mechanics. Engineering Mechanics. Mass and Scale. Capacity, Density, and Fluid Meters. Combustion Controls.

Organic and Fibrous Materials. Rubber. Textiles. Paper. Leather. Testing and Specifications. Polymer Structure. Plastics. Dental Research.

Metallurgy. Thermal Metallurgy. Chemical Metallurgy. Mechanical Metallurgy. Corrosion. Metal Physics.

Mineral Products. Engineering Ceramics. Glass. Refractories. Enameled Metals. Concreting Materials. Constitution and Microstructure.

Building Technology. Structural Engineering. Fire Protection. Air Conditioning, Heating, and Refrigeration. Floor, Roof, and Wall Coverings. Codes and Safety Standards. Heat Transfer.

Applied Mathematics. Numerical Analysis. Computation. Statistical Engineering. Mathematical Physics.

Data Processing Systems. SEAC Engineering Group. Components and Techniques. Digital Circuitry. Digital Systems. Analog Systems. Application Engineering.

● Office of Basic Instrumentation. ● Office of Weights and Measures.

BOULDER, COLORADO

Cryogenic Engineering. Cryogenic Equipment. Cryogenic Processes. Properties of Materials. Gas Liquefaction.

Radio Propagation Physics. Upper Atmosphere Research. Ionospheric Research. Regular Propagation Services. Sun-Earth Relationships. VHF Research. Ionospheric Communication Systems.

Radio Propagation Engineering. Data Reduction Instrumentation. Modulation Systems. Navigation Systems. Radio Noise. Tropospheric Measurements. Tropospheric Analysis. Radio Systems Application Engineering. Radio-Meteorology.

Radio Standards. High Frequency Electrical Standards. Radio Broadcast Service. High Frequency Impedance Standards. Electronic Calibration Center. Microwave Physics. Microwave Circuit Standards.


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