NBS MONOGRAPH 25 – SECTION 12

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Standard X-ray Diffraction Powder Patterns

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Standard X-ray Diffraction Powder Patterns

Section 12—Data for 57 Substances

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 12. --- Data for 57 Substances

by

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Standard x-ray diffraction patterns are presented for 57 substances. Twenty-five of these patterns represent experimental data and 32 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

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

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the Joint Committee on Powder Diffraction Standards,[1] the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 57 compounds (25 experimental and 32 calculated patterns), and is the twenty-second of the series of "Standard X-ray Diffraction Powder Patterns."[2]

EXPERIMENTAL POWDER PATTERNS

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the sample improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern. Unless otherwise noted, the spectrographic analyses were done at NBS after preparation of the sample was completed; the limit of detection for the alkali elements was 0.05 weight percent.

Optical data, color. A microscopic inspection for phase purity was also made on the non-opaque materials during the refractive index determination. The latter was done by grain-immersion methods in white light, using oils standardized in sodium light, in the refractive index range 1.40 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard (approximately 5 wt. percent tungsten powder). If tungsten lines were found to interfere with sample lines, silver or silicon was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid errors associated with aberrations at the very top of peaks, the readings of 2θ were taken at positions about 20 percent of the way down from the top, and in the center of the peak width. The internal standard correction for each region was then applied to the measured value of 2θ. We have reported all data as $K\alpha_1$ peaks because the internal standard corrections for all regions were established in terms of the $K\alpha_1$ wavelength.

[1] Joint Committee on Powder Diffraction Standards, 1601 Park Lane, Swarthmore, PA. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

[2] See previous page for other published volumes.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in the table below; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Calculated 2θ Angles, $CuK\alpha_1$ λ = 1.540598Å

hkℓ	W a=3.16524Å ±.00004	Ag a=4.08651Å ±.00002	Si a=5.43088Å ±.00004
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.303
310	100.632		
311		77.390	56.123
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.131
331		110.499	76.377
420		114.914	
422		134.871	88.032
511/333		156.737	94.954
440			106.710
531			114.094
620			127.547
533			136.897
444			158.638

The new internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Cell parameter data were also collected for a single crystal from the boules ground to prepare the powder. The lattice parameters from the two methods agreed within 3 parts in 10^5 [Hubbard et al.]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation: $\lambda(CuK\alpha_1, peak)$= 1.540598Å [Deslattes and Henins, 1973].

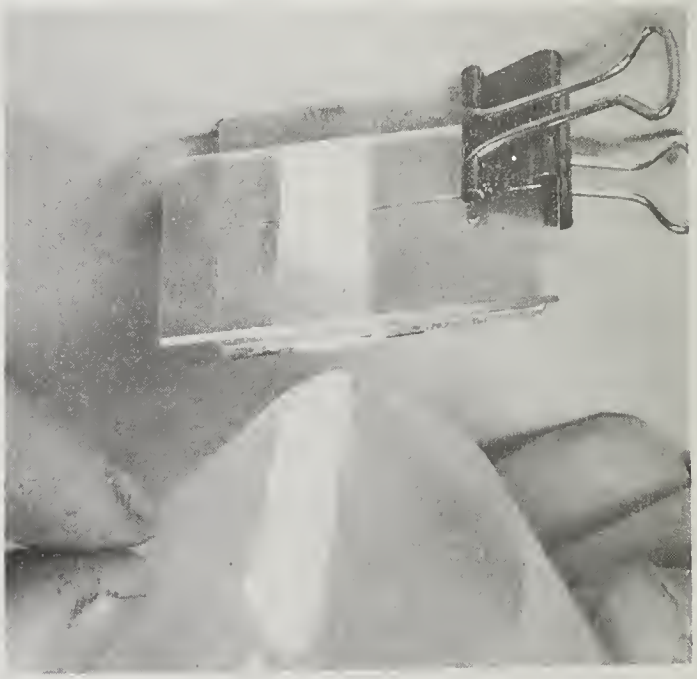
Structure, lattice constants. The space groups were listed with short Hermann-Maugin symbols as well as the space group numbers given in the *International Tables for X-ray Crystallography, Vol. I* [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of *Crystal Data* [1973]. For primitive cells, the transformed cell axes are an alternate labelling of the reduced cell axes. For centered monoclinic cells, the transformed cell is the centered cell with the three shortest non-coplanar vectors.

A computer program [Evans et al., 1963] assigned hkℓ's and refined the lattice constants. Cell refinement was based only upon $2\theta_{obs}$ values which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{obs}-\theta_{calc})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. In indexing cubic patterns, multiple hkℓ's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and atomic weights based on carbon 12 [International Union, 1961].

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical



position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (as shown in Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. At least three patterns for intensity measurements were prepared for each sample to check reproducibility.

Reference intensity, $I/I_{corundum}$. For reference intensity measurements, α-Al_2O_3 (corundum) was chosen as an internal standard to be mixed 1:1 by weight with the sample. This mixture of two components was mounted in our regular intensity sample holder (see Figures 1 and 2), and the pattern was taken. The reference intensity was then calculated as the direct ratio of the strongest line of the sample to the strongest line of corundum (hexagonal reflection (113)). In a few instances, the strongest line of one of the components coincided with a line of the other. In that case, the second strongest line was measured, and the value for the strongest line was then calculated.

CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Smith [1967] and modified at NBS.

Lattice parameters. Before the computations of the patterns, any necessary changes were made in the lattice constants in order to make them consistent with the revised value of the copper wavelength [Deslattes and Henins, 1973]. Both the altered and the original published values are given. Monoclinic and triclinic lattice constants were transformed if necessary, to follow the convention of *Crystal Data* [1973]. For primitive cells, the transformed cell axes are an alternate labelling of the reduced cell axes. For centered monoclinic cells, the transformed cell is the centered cell with the three shortest non-coplanar vectors.

Scattering factors. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, the factors were taken directly from the *International Tables for X-ray Crystallography, Vol. III,* [1962]. The factors were corrected for dispersion if the author had done so.

Thermal parameters. The computer program used thermal parameter data of only two forms, the isotropic B's or the anisotropic β_{ij}'s in the following expressions:

$$e^{(-B \sin^2\theta)/\lambda^2}$$

or

$$e^{-(h^2\beta_{11}+k^2\beta_{22}+\ell^2\beta_{33}+2hk\beta_{12}+2h\ell\beta_{13}+2k\ell\beta_{23})}.$$

Other thermal parameters were converted to one of these two forms. The isotropic parameters were used directly, if given by the structure reference. In a few of our patterns, anisotropic parameters were also used directly as given by the structure reference; in other work, instead of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined by:

$$B = 4 \left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a^{*2}\, b^{*2}\, c^{*2}} \right]^{\frac{1}{3}}$$

Integrated intensities. Intensity calculations were based on the copper $K\alpha_1$ wavelength, 1.540598Å, determined by Deslattes and Henins [1973]. The integrated intensities were computed from formula (1):

$$(1) \qquad I = F^2 \, (Lp) \, (FAC)$$

where F is the standard structure factor

FAC is the powder multiplicity

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

The intensities were scaled to the strongest line which was assigned a value of 100. Reflections were not reported which had scaled intensities of 0.1 or less.

Scale factor. For each compound, this factor multiplied by the reported integrated intensities will reproduce the unscaled intensities which were calculated from equation (1).

Peak intensities. The integrated intensities can be transformed to a Cauchy profile with an appropriate variable half-width designated to simulate a diffractometer tracing [Smith, 1967]. The term half-width as used here is defined as the full width at half maximum and was assigned a value of 0.075° at 40° (2θ, $CuK\alpha_1$). Then the intensities were summed for the overlapping peak profiles, and the resulting new peak intensities were scaled to the strongest peak height which was assigned a value of 100. Reflections were not reported which had scaled peak heights of 0.1 or less. Adjacent peaks with nearly equal 2θ values usually cannot be experimentally resolved; therefore one composite peak was calculated in such instances. The 2θ angle of this peak was assigned the hkℓ of the reflection having the greatest integrated intensity; a plus sign (+) was used to indicate additional hkℓ's.

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Aluminum nitride AlN

Sample

The sample was obtained from Cerac/Pure, Inc., Menomonee Falls, Wis. A small amount of metallic aluminum was sieved out.

Major impurities

0.001-0.01% each Ca, Ni
0.003-0.03% each Co, Cr, Cu, Sr, Ti
0.01-0.1% each Fe, Mg, Si

Color

Very pale gray

Optical data

Uniaxial, (+), N_o = 2.13, N_e = 2.20 [Kohn et al., 1956].

Structure

Hexagonal, $P6_3mc$ (186), Z=2, isostructural with wurtzite, ZnS, [Ott, 1924]. The structure of AlN was refined by Jeffrey et al. [1956].

NBS lattice constants of this sample:

a = 3.1114(1) Å
c = 4.9792(2)

Density

(calculated) 3.261 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.6

Additional patterns

1. PDF card 8-262 [Paretzkin, B., Polytechnic Inst. of Brooklyn].

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
2.695	100	100	33.21
2.490	60	002	36.04
2.371	80	101	37.92
1.829	25	102	49.80
1.5559	40	110	59.35
1.4133	30	103	66.05
1.3475	5	200	69.73
1.3194	25	112	71.44
1.3007	10	201	72.63
1.2450	1	004	76.44
1.1850	4	202	81.09
1.1301	1	104	85.94
1.0461	9	203	94.84
1.0184	3	210	98.29
0.9978	7	211	101.06
.9720	2	114	104.84
.9425	3	212	109.62
.9340	6	105	111.12
.9142	<1	204	114.82
.8982	4	300	118.10
.8680	10	213	125.11
.8448	5	302	131.51
.8298	1	006	136.33
.8008	5	205	148.28
.7931	1	106	152.44
.7882	<1	214	155.49

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Ott, Z. (1924). Z. Physik 22, 201.

Ammonium copper chloride hydrate, $(NH_4)_2CuCl_4 \cdot 2H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of a 2:1 aqueous solution of NH_4Cl and $CuCl_2$.

Major impurities:

0.001-0.01% each: Al and Mg.

Color
Brilliant greenish blue

Optical data
uniaxial (-), N_o=1.668, N_e=1.640

Structure
Tetragonal, $P4_2/mnm$ (136), Z=2. [Hendricks and Dickinson, 1927]. The structure was refined by Chrobak [1934].

NBS lattice constants of this sample:

a = 7.594(1) Å
c = 7.967(1)

Density
(calculated) 2.005 g/cm^3 at 25 °C.

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

Additional patterns
1. PDF card 1-211 [Hanawalt et al., 1938].
2. Greenberg and Walden [1940].
3. Chrobak [1934].
4. PDF card 23-1010 [Swanson et al., 1971].
5. PDF card 25-262[Technisch Physische Dienst].

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.49	100	101	16.12
5.37	50	110	16.48
3.982	50	002	22.31
3.395	20	210	26.23
3.200	25	112	27.86
3.124	30	211	28.55
2.745	70	202	32.59
2.685	90	220	33.35
2.585	17	212	34.68
2.506	12	103	35.80
2.411	8	301	37.26
2.404	8	310	37.38
2.228	20	222	40.46
2.093	9	213	43.18
2.058	6	312	43.97
2.037	12	321	44.45
1.992	20	004	45.50
1.899	14	400	47.85
1.867	9	114	48.74
1.843	8	410	49.42
1.794	8	411	50.87
1.790	7	330	50.99
1.718	5	214	53.27
1.713	8	402	53.43
1.672	8	412	54.87
1.650	4	323	55.67
1.632	5	332	56.32
1.599	18	224	57.60
1.560	5	105	59.18

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Barium aluminum oxide, $Ba_3Al_2O_6$

Sample
The sample was prepared by A. E. Moore of the Cement and Concrete Association by heating $BaCO_3$ and Al_2O_3 in a Pt crucible at 1400 °C.

Color
Colorless

Structure
Cubic, Pa3 (205), Z = 24, isostructural with $Ca_3Al_2O_6$.

NBS lattice constant of this sample:

$a = 16.4750(6)$ Å

Density
(calculated) 5.008 g/cm^3

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

Additional patterns
1. PDF card 14-106 [Planz and Müller-Hesse, 1961].
2. PDF card 15-331 [Brisi, 1962].

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$CuK\alpha_1$ $\lambda = 1.540598$ Å; temp. 25±1 °C

Internal standard W, $a = 3.16524$ Å

d(Å)	I	hkℓ	2θ(°)
5.82	3	220	15.21
4.965	3	311	17.85
4.407	1	321	20.13
4.120	35	400	21.55
3.994	1	410	22.24
3.778	9	331	23.53
3.594	2	421	24.75
3.513	2	332	25.33
3.362	3	422	26.49
3.169	13	511	28.14
3.057	6	432	29.19
3.007	14	521	29.69
2.911	100	440	30.69
2.870	3	522	31.14
2.784	2	531	32.13
2.673	2	611	33.50
2.574	1	621	34.82
2.543	2	541	35.27
2.512	2	533	35.71
2.457	2	630	36.54
2.377	20	444	37.82
2.306	7	551	39.02
2.286	1	640	39.38
2.263	4	641	39.81
2.201	5	642	40.97
2.145	5	731	42.09
2.110	1	650	42.83
2.059	30	800	43.94
2.028	1	811	44.64
2.012	6	733	45.02
1.982	1	821	45.73
1.969	2	653	46.05
1.941	5	822	46.76
1.916	2	831	47.41
1.902	3	751	47.77
1.878	3	832	48.44
1.842	15	840	49.43
1.808	5	753	50.42
1.788	2	670	51.05
1.776	2	921	51.40
1.746	1	922	52.36
1.727	3	931	52.97
1.708	1	852	53.62
1.681	20	844	54.56
1.6638	2	941	55.16
1.6557	4	933	55.45
1.6397	4	10·1·0	56.04
1.6151	2	10·2·0	56.97
1.5926	6	951	57.85
1.5706	3	10·3·1	58.74

Barium aluminum oxide, $Ba_3Al_2O_6$ (continued)

d(Å)	I	hkℓ	2θ(°)
1.5367	2	953	60.17
1.5234	3	10·4·1	60.75
1.5039	2	10·4·2	61.62
1.4855	2	11·1·1	62.47
1.4736	2	10·5·0	63.03
1.4680	2	11·2·1	63.30
1.4561	9	880	63.88
1.4392	4	11·3·1	64.72
1.4239	2	11·3·2	65.50
1.4128	3	10·6·0	66.08
1.4075	3	11·4·1	66.36
1.3977	2	11·3·3	66.89
1.3878	2	11·4·2	67.43
1.3825	3	965	67.72
1.3731	4	12·0·0	68.25
1.3591	4	11·5·1	69.05
1.3497	3	12·2·1	69.60
1.3362	4	12·2·2	70.41
1.3233	2	11·5·3	71.20
1.3105	3	11·6·1	72.00
1.3025	6	12·4·0	72.51
1.2906	4	991	73.29
1.2825	3	10·8·1	73.83
1.2598	6	13·1·1	75.39
1.2524	4	12·5·2	75.91
1.2491	4	13·2·1	76.15
1.2418	5	12·4·4	76.68
1.2315	4	13·3·1	77.44
1.2246	4	12·6·1	77.96
1.2146	3	12·6·2	78.72
1.2049	5	13·3·3	79.48
1.1890	4	888	80.76
1.1798	4	13·5·1	81.52
1.1706	3	14·1·1	82.30

Barium chloride hydrate, $BaCl_2 \cdot 2H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of an aqueous solution of $BaCl_2$.

Major impurities:

0.001 to 0.1% each Al, Ca, Si, Sr
0.0003 to 0.003% Mg

Color
Colorless.

Optical data
Biaxial (+), $N_\alpha = 1.631$, $N_\beta = 1.639$, $N_\gamma = 1.658$.

Structure
Monoclinic $P2_1/n$ (14), Z=4 [Naray-Szabo and Sasvari, 1937]. The structure was determined by Jensen [1946] and refined by electron diffraction by Padmanabhan et al. [1963].

NBS lattice constants of this sample:

$a = 6.720(1)$ Å
$b = 10.907(2)$
$c = 7.135(1)$
$\beta = 91.10(2)°$

Density
(calculated) 3.103 g/cm^3

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

Additional patterns
1. Jensen [1946].
2. PDF card 11-137 [Amendola, Polytech. Inst. of Brooklyn].
3. PDF card 1-0342 [Hanawalt et al., 1938].

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Jensen, A. T. (1946). Kgl. Danske Videnskab. Selskab Mat. fys. Medd. 22, No. 3.
Naray-Szabo, S. V., and Sasvari, K. (1937). Z. Krist. 97A, 255.
Padmanabhan, V.M., Jakkal, V.S., and Shankar, J. (1963). Indian J. Pure Appl. Phys. 1, 293.

CuKα_1 $\lambda = 1.540598$ Å; temp. 25±1 °C
Internal standard W, $a = 3.16524$ Å

d(Å)	I	hkℓ	2Θ(°)
5.96	7	011	14.84
5.72	12	110	15.49
5.45	85	020	16.26
4.94	60	$\bar{1}01$	17.95
4.84	20	101	18.30
4.50	55	$\bar{1}11$	19.72
4.42	100	111	20.05
4.33	17	021	20.49
4.23	2	$\bar{1}20$	20.99
3.661	45	$\bar{1}21$	24.29
3.622	17	121	24.56
3.569	15	002	24.93
3.390	55	012	26.27
3.359	25	200	26.51
3.240	12	031	27.51
3.213	30	210	27.74
3.200	25	$\bar{1}30$	27.86
3.048	3	$\bar{1}12$	29.28
3.003	10	$\bar{1}12$	29.73
2.948	50	$\bar{2}11$	30.29
2.928	65	$\bar{1}31$	30.51
2.908	90	131,211	30.72
2.861	45	220	31.24
2.712	50	$\bar{1}22$	33.00
2.671	15	$\bar{2}21$	33.52
2.547	75	041,032	35.21
2.527	18	$\bar{1}40$	35.49
2.469	10	$\bar{2}02$,230	36.36
2.423	18	$\bar{2}02$	37.08
2.409	42	$\bar{2}12$	37.29
2.388	18	$\bar{1}41$	37.64
2.365	19	$\bar{2}12$	38.01
2.343	20	$\bar{2}31$	38.39
2.324	3	013,231	38.72
2.256	25	$\bar{1}03$	39.93
2.229	25	103	40.44
2.214	20	$\bar{2}22$	40.72
2.209	30	$\bar{1}13$	40.82
2.148	13	$\bar{3}01$	42.02
2.116	13	240	42.68
2.085	50	311,$\bar{1}23$	43.37
2.073	30	150,320	43.62
2.068	35	$\bar{1}42$	43.74
2.061	25	123,142	43.90
2.042	13	$\bar{2}32$	44.33
2.0226	12	$\bar{2}41$	44.77
1.9985	19	$\bar{3}21$	45.34
1.9886	12	033,151	45.58
1.9069	4	330	47.65
1.8610	4	052	48.90
1.8343	3	331	49.66
1.8182	4	060	50.13
1.7834	3	004	51.18

Barium molybdenum oxide, Ba_2MoO_5

Sample

The sample was prepared at NBS by T. Negas by heating $BaCO_3$ and MoO_3 in stoichiometric proportions at 900 °C in a gold envelope for 4 days. Fine grained material was unstable when exposed to air.

Color

Colorless

Structure

Orthorhombic, Pnam(62), Z=4, isostructural with $K_2VO_2F_3$. The structure of Ba_2MoO_5 was determined by Negas and Roth [1974].

NBS lattice constants of this sample:

a = 7.4097(7) Å
b = 11.3906(8)
c = 5.7603(6)

Density

(calculated) 6.156 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.4

Additional patterns

1. Yanushkevich and Zhukovskii [1972].

References

Negas, T. and Roth, R.S. (1974). (Private communication, to be published.)
Yanushkevich, T. M. and Zhukovskii, V. M. (1972). Inorg. Materials 8, 1794.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.21	6	110	14.26
5.69	3	020	15.57
5.142	2	011	17.23
4.516	2	120	19.64
4.227	2	111	21.00
3.703	2	200	24.01
3.556	16	121	25.02
3.521	19	210	25.27
3.378	7	130	26.36
3.168	100	031	28.14
3.114	45	201	28.64
3.105	65	220	28.73
3.005	60	211	29.71
2.914	4	131	30.66
2.880	45	002	31.03
2.847	1	040	31.39
2.731	20	221	32.76
2.652	13	230	33.77
2.428	7	122	36.99
2.413	18	310,141	37.23
2.258	17	240	39.90
2.230	15	212	40.42
2.191	11	132	41.16
2.176	17	150	41.46
2.111	40	222	42.80
2.101	9	241	43.01
2.070	6	330	43.70
1.950	13	232	46.53
1.941	7	250	46.77
1.898	8	060	47.88
1.866	1	340	48.76
1.852	3	400	49.15
1.839	10	251,160	49.52
1.777	9	242	51.38
1.764	16	401	51.78
1.752	6	161	52.15
1.7428	7	411	52.46
1.7373	6	152	52.64
1.7134	15	033	53.43
1.7049	4	203	53.72
1.6895	10	260	54.25
1.6860	15	213	54.37
1.6809	6	332	54.55
1.6654	12	430	55.10
1.6335	4	223	56.27
1.6214	6	261	56.73
1.6094	4	252	57.19
1.5997	1	431	57.57
1.5891	4	170	57.99
1.5848	10	062	58.16

Barium molybdenum oxide, Ba_2MoO_5 (continued)

d(Å)	I	hkℓ	2θ(°)
1.5660	1	342,071	58.93
1.5578	4	402	59.27
1.5559	4	143,233	59.35
1.5495	3	162	59.62
1.5028	4	422	61.67
1.4686	2	053	63.27
1.4626	2	243	63.56
1.4572	8	262,361	63.82
1.4476	3	352	64.29
1.4417	19	432	64.59
1.4372	4	450	64.82
1.4239	2	511,080	65.50
1.3984	2	180	66.85
1.3943	2	451	67.07
1.3917	5	521,172	67.21
1.3653	3	253	68.69
1.3589	5	370,181	69.06
1.3424	1	531,204	70.03
1.3384	2	343	70.27
1.3338	6	362,403	70.55
1.3283	1	163	70.89
1.3244	3	413,272	71.13
1.3144	1	540	71.75
1.3064	4	224	72.26
1.2980	1	423	72.80
1.2947	2	281	73.02
1.2919	7	461	73.20
1.2860	2	452	73.59
1.2764	3	082	74.24
1.2684	3	263	74.79
1.2656	3	234	74.98
1.2582	2	433,182	75.50
1.2474	1	190	76.27
1.2423	2	550	76.64
1.2363	3	314,091	77.08
1.2348	3	600	77.19
1.2280	4	610	77.70
1.2227	1	470	78.10
1.2194	1	191	78.35
1.2143	3	551,244	78.74
1.2069	1	620,282	79.32
1.2013	3	154,611	79.76
1.1976	3	290	80.06
1.1960	2	542,471	80.19
1.1850	2	363	81.09
1.1817	4	334,621	81.36
1.1726	4	291	82.13

Barium phosphate, $Ba_3(PO_4)_2$

Sample
The sample was prepared at NBS by heating a 3:2 molar mixture of $BaCO_3$ and $(NH_4)_2HPO_4$ at 950 °C for one hour; after regrinding it was heated overnight at 800 °C.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m$ (166), Z=3. The structure of $Ba_3(PO_4)_2$ was determined by Zachariasen [1948].

NBS lattice constants of this sample:

a = 5.6033(1)Å
c = 20.9951(7)

Density
(calculated) 5.253 g/cm^3

Reference intensity
$I/I_{corundum}$ = 5.0

Additional patterns
1. PDF card 4-582 [Zachariasen, 1948].

References
Zachariasen, W. H. (1948). Acta Cryst. 1, 263.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
7.00	2	003	12.63
4.726	15	101	18.76
4.403	4	012	20.15
3.565	20	104	24.96
3.177	100	015	28.06
2.801	75	110	31.92
2.552	2	107	35.14
2.411	5	021	37.26
2.364	7	202	38.03
2.334	13	009	38.55
2.309	1	018	38.98
2.202	16	024	40.95
2.187	6	116	41.24
2.1008	35	205	43.02
1.9268	18	1·0·10	47.13
1.8865	4	027	48.20
1.8271	4	211	49.87
1.8071	1	122	50.46
1.7929	16	119	50.89
1.7318	4	214	52.82
1.6806	24	125	54.56
1.6175	13	300	56.88
1.5876	8	0·2·10	58.05
1.5645	1	217	58.99
1.5000	<1	2·0·11	61.80
1.4840	1	1·1·12	62.54
1.4682	1	306	63.29
1.4327	5	0·1·14	65.05
1.4006	12	220	66.73
1.3811	12	2·1·10	67.80
1.3431	1	131	69.99
1.3348	1	312	70.49
1.3293	5	309	70.83
1.3038	2	134	72.43
1.2814	11	315	73.90
1.2755	4	2·0·14	74.30
1.2520	8	1·1·15	75.94
1.2281	<1	137	77.69
1.2113	1	401	78.98
1.2050	1	042	79.47
1.2008	6	229	79.81
1.1878	<1	3·0·12	80.86
1.1820	1	404	81.34
1.1655	5	045	82.74
1.1610	5	1·2·14	83.13
1.1329	5	1·3·10	85.68
1.1117	<1	321	87.72
1.0891	2	324	90.03
1.0774	4	1·0·19	91.28
1.0762	8	235	91.41

Barium phosphate, $Ba_3(PO_4)_2$ (continued)

d(Å)	I	hkℓ	2θ(°)
1.0673	<1	2·1·16	92.40
1.0589	10	410	93.35
1.0505	3	4·0·10	94.32
1.0261	2	0·1·20	97.30
1.0136	2	416	98.92
1.0056	3	0·2·19	99.99
1.0017	4	3·1·14	100.53
0.9902	5	2·2·15	102.14
.9836	4	3·2·10	103.10
.9698	2	4·0·13	105.17
.9642	5	419	106.05
.9544	2	054	107.63
.9464	7	2·1·19	108.96
.9457	3	505	109.09
.9432	4	0·4·14	109.51
.9339	3	330	111.14
.9163	2	241	114.43
.9136	2	422	114.95
.9111	3	1·2·20	115.45
.9060	<1	4·1·12	116.48
.9034	2	244	117.00
.8959	4	425	118.58
.8938	5	2·3·14	119.05
.8810	4	0·5·10	121.94
.8770	1	247	122.89
.8749	1	0·0·24	123.40
.8709	<1	511	124.39
.8685	2	152	124.98
.8670	3	339	125.36
.8597	1	514	127.27
.8540	5	1·3·19	128.84
.8533	6	155	129.03
.8444	5	4·1·15	131.63
.8404	4	2·4·10	132.88

Barium tungsten oxide, Ba_2WO_5

Sample

The sample was prepared at NBS by T. Negas by heating $BaCO_3$ and WO_3 in stoichiometric proportions at 900 °C in a gold envelope for 4 days.

Major impurities

0.01-0.1% Ca, Si, Sr
0.001-0.01% Cr, Mg

Color

Colorless

Structure

Orthorhombic, Pnam(62), Z=4, isostructural with $K_2VO_2F_3$. The structure of Ba_2WO_5 was determined by Negas and Roth [1974].

NBS lattice constants of this sample

a = 7.4066(6)A°
b = 11.4785(8)
c = 5.7313(4)

Density

(calculated) 7.341 g/cm^3

Reference intensity

$I/I_{corundum}$ = 4.0

Additional patterns

1. PDF card 15-176 [Zhmud' and Ostapchenko, 1961].

References

Negas, T. and Roth, R.S. (1974) (private communication, to be published).
Zhmud', S. and Ostapchenko, E. P. (1961). J. Struct. Chem. (Eng. Transl.) 2, 27.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.223	9	110	14.22
5.738	7	020	15.43
4.535	2	120	19.56
4.219	8	111	21.04
3.702	3	200	24.02
3.557	5	121	25.01
3.523	16	210	25.26
3.401	3	130	26.18
3.184	100	031	28.00
3.111	65	220,201	28.67
3.002	45	211	29.74
2.924	4	131	30.55
2.864	45	002	31.20
2.735	25	221	32.72
2.661	17	230	33.65
2.603	2	112	34.42
2.565	<1	022	34.95
2.426	10	141	37.03
2.414	6	231	37.22
2.268	11	240,202	39.70
2.223	15	311,212	40.54
2.193	12	150,132	41.13
2.131	6	051	42.37
2.107	35	241,222	42.88
2.074	5	330	43.61
1.950	25	250,232	46.54
1.913	7	060	47.48
1.852	3	160,400	49.15
1.847	11	251	49.29
1.827	1	113	49.88
1.779	4	242	51.32
1.762	18	161,401	51.84
1.742	8	411,152	52.49
1.709	16	033	53.59
1.699	6	260	53.91
1.698	7	203	53.96
1.684	5	421	54.45
1.6795	12	332,213	54.60
1.6668	12	430	55.05
1.6290	10	261	56.44
1.6277	9	223	56.49
1.6128	5	252	57.06
1.6012	2	170,431	57.51
1.5913	8	062	57.90
1.5669	<1	342	58.89
1.5554	6	162,402+	59.37
1.5415	1	171,412	59.96
1.5008	4	441,422	61.76
1.4686	2	510,053	63.27
1.4620	9	361,262+	63.59

Barium tungsten oxide, Ba_2WO_5 (continued)

d(Å)	I	hkℓ	2θ(°)
1.4501	2	271,352	64.17
1.4407	17	450,432	64.64
1.4346	4	080	64.95
1.4328	8	004	65.04
1.3976	5	172	66.89
1.3676	3	181	68.56
1.3650	5	253	68.71
1.3376	1	280,362	70.32
1.3296	5	403	70.81
1.3207	1	413,134	71.36
1.3028	4	281	72.49
1.3014	4	224	72.58
1.2962	7	461	72.92
1.2877	2	452	73.48
1.2832	5	082,541	73.78
1.2700	3	263	74.68
1.2615	3	234	75.27
1.2449	2	091	76.45
1.2345	3	600	77.21
1.2278	2	191,610	77.71
1.2164	<1	551	78.58
1.2114	2	244	78.97
1.2059	1	290	79.40
1.1995	1	154	79.91
1.1961	1	542	80.18
1.1857	2	363	81.03

Calcium chloride hydrate (antarcticite), $CaCl_2 \cdot 6H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of an aqueous solution of $CaCl_2$. Because the sample was somewhat unstable and hygroscopic, the intensity measurements varied up to 15% in reproducibility.

Color
Colorless

Optical data
Uniaxial (-), $N_o = 1.550$, $N_e = 1.492$.

Structure
Hexagonal, P321(150), Z = 1, isostructural with $SrCl_2 \cdot 6H_2O$, and other hexahydrates of alkaline earth halides. The structure of $SrCl_2 \cdot 6H_2O$ was determined by Jensen [1940].

NBS lattice constants of this sample:

$a = 7.876(1)$ Å
$c = 3.9555(6)$

Density
(calculated) 1.712 g/cm^3

Additional patterns
1. Herrmann [1931].
2. PDF card 1-1220 [Hanawalt et al., 1938].
3. Torii and Ossaka [1965].

References

Hanawalt, J. D., Rinn, H. W. and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Herrmann, Z. (1931). Z. anorg. u. allgem. Chem. 197, 212.
Jensen, A. T. (1940). Kgl. Danske Videnskab. Selskab Mat. Fys. Medd. 17, No. 9.
Torii, T. and Ossaka, J. (1965). Science 149, 975.

CuKα_1 $\lambda = 1.540598$ Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.80	35	100	13.00
3.93	90	110	22.60
3.420	65	101	26.03
2.792	75	111	32.03
2.582	60	201	34.71
2.273	60	300	39.61
2.159	100	211	41.81
1.977	20	002	45.86
1.899	12	102	47.87
1.767	8	112	51.68
1.711	10	202	53.53
1.706	25	311,400	53.68
1.569	12	212	58.81
1.566	12	401,320	58.95
1.492	20	302	62.18
1.488	25	410	62.34
1.455	10	321	63.93
1.396	9	222	66.99
1.3929	9	411	67.15
1.3675	5	312	68.57
1.3129	3	330	71.85
1.2946	5	103	73.03
1.2915	4	402	73.23
1.2505	2	113	76.05
1.2295	7	203	77.59
1.2256	5	421,510	77.88
1.1895	5	412	80.71
1.1743	4	213	81.99

Calcium oxide phosphate, $Ca_4O(PO_4)_2$

Sample

The sample was prepared at NBS by E. Carlson by heating an equimolar mixture of $CaHPO_4$ and $CaCO_3$ at 1500 °C for 24 hours in platinum foil.

Major impurities

0.003 to 0.03% each Mg, Sr
0.001 to 0.1% each Ba, Fe, Pt

Color

Colorless

Structure

Monoclinic, $P2_1$ (4), Z=4, [Brown and Epstein, 1965]. The structure was determined by Dickens et al. [1973]. Earlier work by Trömel and Zaminer [1959] reported this phase to be orthorhombic in space group $P2_122$ (17).

NBS lattice constants of this sample:

$a = 7.018(1)$ Å
$b = 11.980(2)$
$c = 9.469(2)$
$\beta = 90.88(2)°$

Density

(calculated) 3.056 g/cm^3

Reference intensity

$I/I_{corundum} = 7.3$

Additional patterns

1. PDF card 11-232 [Sarver, J.F., Penn. State Univ., University Park, Pa.]
2. Bauer and Balz [1965].

References

Bauer, H., and Balz, W. (1965). Z. Anorg. u. allgem. Chem., 340, 225.

Brown, W.E., and Epstein, E.F. (1965). J. Res. NBS 69A, 547.

Dickens, B., Brown, W. E., Kruger, G. J., and Stewart, J.M. (1973). Acta Cryst. B29, 2046.

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CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.06	4	110	14.61
5.99	5	020	14.77
5.69	4	$\bar{1}01$	15.57
4.739	3	002	18.71
4.558	5	120	19.46
4.405	2	$0\bar{1}2$	20.14
4.122	14	$\bar{1}21$	21.54
4.092	20	$1\bar{2}1$	21.70
3.959	2	$\bar{1}02$	22.44
3.897	3	102	22.80
3.754	4	$\bar{1}12$	23.68
3.711	8	022,112	23.96
3.684	10	031	24.14
3.511	45	200	25.35
3.473	20	130	25.63
3.366	3	210	26.46
3.302	7	$\bar{2}01$,$\bar{1}22$	26.98
3.268	16	$\bar{1}31$,122	27.27
3.190	30	$\bar{2}11$	27.95
3.160	20	211,003	28.22
3.053	80	032,013	29.23
2.995	100	$0\bar{4}0$	29.80
2.895	30	$\bar{1}03$,$\bar{2}21$	30.86
2.872	45	$2\bar{2}1$	31.11
2.811	25	$\bar{1}13$,$\bar{1}32$	31.81
2.789	35	023,132	32.06
2.784	35	$1\bar{1}3$	32.12
2.763	50	$\bar{2}12$	32.38
2.724	40	$2\bar{1}2$	32.85
2.649	14	$\bar{1}41$	33.81
2.642	18	$1\bar{4}1$	33.90
2.607	12	$\bar{1}23$	34.37
2.583	6	$1\bar{2}3$	34.70
2.567	5	$\bar{2}22$	34.93
2.545	9	$\bar{2}31$	35.23
2.534	16	222,231+	35.39
2.476	16	$0\bar{3}3$	36.25
2.387	2	$\bar{1}42$	37.66
2.367	7	004,$\bar{2}03$	37.99
2.322	15	051,014+	38.75
2.314	12	$\bar{2}32$	38.88
2.292	12	232	39.28
2.268	5	$1\bar{5}0$	39.71
2.237	7	$\bar{3}11$	40.29
2.207	12	$\bar{1}51$	40.85

Calcium oxide phosphate $Ca_4O(PO_4)_2$ (continued)

d(Å)	I	hkℓ	2θ(°)
2.204	9	151,024	40.92
2.173	9	043	41.53
2.137	5	052	42.26
2.130	6	$\bar{3}21$	42.40
2.109	4	$\bar{3}02,\bar{1}24$	42.84
2.092	3	124	43.22
2.082	4	$\bar{1}43$	43.42
2.077	10	$\bar{3}12$	43.53
2.061	3	$\bar{2}42$	43.90
2.050	9	$\bar{1}52$	44.15
2.035	3	034,$\bar{2}33$	44.49
2.018	6	330	44.88
2.012	6	233	45.03
1.990	4	$\bar{3}22$	45.55
1.976	25	$\bar{2}04$	45.88
1.963	3	$\bar{1}34$	46.22
1.948	19	134,204	46.58
1.934	6	251	46.93
1.922	4	214	47.24
1.908	20	053	47.62
1.881	6	161	48.36
1.869	11	015,$\bar{3}13$	48.67
1.865	15	303,$\bar{3}32$	48.79
1.846	8	$\bar{1}53$	49.32
1.842	10	340,313	49.43
1.837	9	243,153	49.57
1.831	13	$\bar{2}52$	49.76
1.820	12	252	50.09
1.804	13	$\bar{3}23$	50.55
1.780	4	323	51.28
1.753	25	400	52.13
1.735	8	410,260	52.72
1.724	3	$\bar{3}42$	53.07
1.708	15	$\bar{2}61$	53.59
1.7046	17	261	53.73
1.6877	5	063	54.31
1.6837	8	054,420+	54.45
1.6696	3	253	54.95
1.6624	2	170,$\bar{4}21$	55.21
1.6497	7	$\bar{2}44$	55.67
1.6327	6	$\bar{2}62$,244+	56.30
1.6221	1	412	56.70

Cobalt acetate hydrate, $Co(C_2H_3O_2)_2 \cdot 4H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of an aqueous solution of $Co(C_2H_3O_2)_2$.

Color
Deep red

Structure
Monoclinic, $P2_1/c$, (14), Z = 2, isostructural with $Ni(C_2H_3O_2)_2 \cdot 4H_2O$. The structure of $Ni(C_2H_3O_2)_2 \cdot 4H_2O$ was determined by van Niekerk and Schoening [1953].

NBS lattice constants of this sample:

a = 4.8084(9) Å
b = 11.924(2)
c = 8.464(1)
β = 94.33(1)°

Density
(calculated) 1.709 g/cm^3

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

Additional pattern
1. PDF card 14-718 [Hanawalt et al., 1938].

References
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
van Niekerk, J. N. and Schoening, F. R. (1953). Acta. Cryst. 6, 609.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.89	100	011	12.84
5.97	1	020	14.82
4.870	1	021	18.20
4.795	9	100	18.49
4.451	1	110	19.93
4.221	9	002	21.03
4.055	5	$\bar{1}11$	21.90
3.978	4	012	22.33
3.828	4	111	23.22
3.599	4	031	24.72
3.446	<1	022	25.83
3.347	<1	121	26.61
3.295	<1	$\bar{1}02$	27.04
3.175	10	$\bar{1}12$	28.08
3.058	3	130,102	29.18
2.980	<1	040	29.96
2.962	<1	112	30.15
2.922	3	$\bar{1}31$	30.57
2.892	4	032	30.89
2.882	3	$\bar{1}22$	31.00
2.737	<1	013	32.69
2.721	2	122	32.89
2.543	1	023	35.26
2.532	3	140	35.43
2.456	<1	$\bar{1}13$	36.56
2.451	<1	$\bar{1}41$	36.63
2.423	1	132	37.08
2.399	1	141,200	37.46
2.306	5	$\bar{2}11$,113	39.02
2.295	2	033,051	39.23
2.210	1	$\bar{1}42$	40.79
2.187	1	123	41.25
2.156	<1	$\bar{2}02$	41.87
2.135	1	150,142	42.30
2.122	<1	$\bar{1}33$,$\bar{2}12$	42.58
2.111	<1	004	42.81
2.087	1	$\bar{1}51$	43.32
2.076	<1	014,052	43.55
2.053	<1	151,230	44.07
2.047	<1	043	44.21
2.026	2	$\bar{2}22$,$\bar{2}31$	44.69
1.989	<1	024	45.57
1.965	<1	231	46.15
1.961	<1	$\bar{1}14$	46.26
1.934	<1	061	46.94
1.912	1	222	47.51
1.885	1	$\bar{1}24$	48.23
1.880	1	152,104	48.38
1.873	1	$\bar{2}13$	48.57
1.868	2	240	48.71
1.819	<1	053	50.12
1.798	1	062	50.74
1.747	1	$\bar{2}42$	52.34
1.741	1	213	52.51
1.729	<1	$\bar{1}53$	52.91
1.722	<1	044	53.15
1.712	1	$\bar{2}33$	53.49
1.701	1	$\bar{1}62$	53.84
1.670	2	015,071	54.92
1.6408	<1	251	56.00
1.6232	<1	025,063	56.66
1.6162	<1	$\bar{1}15$	56.93
1.6100	1	233	57.17
1.5787	1	072,$\bar{3}11$	58.41
1.5699	<1	171	58.77
1.5533	<1	035	59.46
1.5425	<1	115	59.92

Cobalt borate, $Co_3(BO_3)_2$

Sample
Cobalt oxide (CoO) and B_2O_3 in a 3:1 molar ratio were melted together and quenched.

Major impurities:

0.1 to 1.0% each Fe, Ni
0.01 to 0.1% each Ca, Cu

Color
Strong purple

Structure
Orthorhombic, Pnmn (58), Z=2. The structure was determined by Berger [1949].

NBS lattice constants of this sample:

a = 5.465(1) Å
b = 8.442(1)
c = 4.531(1)

Density
(calculated) 4.678 g/cm^3

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

Additional Patterns
1. PDF card 5-647 [Berger, 1949]

References
Berger, S. V. (1949). Acta. Chem. Scand. 3, 660.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.223	4	020	21.02
3.994	40	011	22.24
3.489	25	101	25.51
3.226	3	111	27.63
2.734	9	200	32.73
2.689	100	121	33.29
2.503	40	130	35.85
2.391	6	031	37.58
2.341	8	201	38.42
2.295	6	220	39.23
2.255	50	211	39.95
2.190	16	131	41.19
2.093	4	102	43.19
1.805	7	141	50.52
1.800	8	321	50.68
1.744	30	202	52.43
1.678	35	132	54.64
1.613	5	150	57.04
1.582	12	051	58.26
1.569	13	321	58.81
1.544	4	042	59.85
1.529	18	330	60.52
1.4863	6	013,142	62.43
1.4068	7	060	66.40
1.3759	10	123	68.09
1.3689	14	251	68.49
1.3661	12	400	68.65
1.3311	3	033	70.72
1.3058	5	213	72.30
1.2927	4	133,411	73.15
1.2677	5	332	74.84

Cobalt bromide hydrate, $CoBr_2 \cdot 6H_2O$

Sample
The sample was prepared by adding HBr to $CoCO_3$ in water, and evaporating the solution slowly at room temperature.

Major impurities:

0.01 to 0.1% each Ca, Fe, Mg
0.003 to 0.03% Cu
0.001 to 0.01% each Al, Mn, Ni

Color
Very dark purplish red

Structure
Monoclinic, $P2_1$ (4), Z=2. The structure was determined by Stroganov et al. [1961].

NBS lattice constants of this sample:

a = 9.074(2)Å
b = 7.173(1)
c = 6.905(2)
β = 94.11(2)°

Density
(calculated) 2.421 g/cm^3

Additional patterns
1. PDF card 23-184 [Mauret and Girou, 1969].

References
Mauret, P., and Girou, A. (1969). Bull. Soc. Chim. France 1969, 2238.
Stroganov, E. V., Andreev, S. N., Kozhina, I. I., and Solov'ev, V. E. (1961). Vestn. Leningr. Univ. Ser. Fiz. i Khim. 16, No. 3, 114.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
5.679	100	$\bar{1}01$	15.59
4.971	40	011	17.83
4.525	4	200	19.60
3.589	7	020	24.79
3.436	7	$\bar{2}11$	25.91
3.031	6	$\bar{1}21$	29.44
2.997	50	$\bar{1}12$	29.79
2.881	14	112	31.02
2.840	35	$\bar{2}02,\bar{3}01$	31.47
2.810	11	220	31.82
2.781	18	310	32.16
2.693	10	301	33.24
2.485	9	212,022	36.11
2.262	15	$\bar{1}03,400$	39.81
2.238	4	$\bar{3}12$	40.27
2.225	2	$\bar{3}21$	40.51
2.191	2	302	41.16
2.154	3	321	41.91
2.132	2	222	42.35
2.098	19	312	43.09
2.025	2	$\bar{2}13$	44.72
2.021	3	411	44.82
1.956	8	$\bar{4}02$	46.38
1.936	7	$\bar{1}32$	46.90
1.914	11	$\bar{1}23,420$	47.46
1.893	2	$\bar{3}03$	48.01
1.873	2	$\bar{4}21$	48.57
1.793	2	040	50.88
1.755	1	510	52.06
1.716	10	313	53.33
1.667	6	$\bar{1}14,240$	55.05
1.649	5	$\bar{2}04$	55.71
1.628	3	$\bar{4}13$	56.47
1.616	5	332	56.93

Cobalt nitrate hydrate, α-$Co(NO_3)_2 \cdot 6H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of an aqueous solution of $Co(NO_3)_2$ over concentrated H_2SO_4 in a desiccator.

Color
Strong reddish brown

Optical data
Biaxial (-) N_α = 1.40, N_γ = 1.549. 2 V is medium. N_β could not be determined.

Structure
Monoclinic, I2/a(15), Z=4 [Jayaraman, 1958].

NBS lattice constants of this sample:

a = 14.295(5) Å
b = 6.139(2)
c = 12.661(2)
β = 112.79°(3)

Density
(calculated) 1.887 g/cm^3

Reference intensity
$I/I_{corundum}$ = 0.7

Polymorphism
Pouillen et al. [1965] report that three forms of $Co(NO_3)_2 \cdot 6H_2O$ exist. The form reported here is stable above -18 °C; the β form, stable between -18 °C and -34 °C is isostructural with the room temperature form of $Zn(NO_3)_2 \cdot 6H_2O$. The γ form is stable below -34 °C.

Additional patterns
1. PDF card 1-317 [Hanawalt et al.].
2. PDF card 12-572 [University of Cardiff].
3. PDF card 19-357 [Weigel et al., 1964].
4. PDF card 24-335 [Weigel et al., 1964]. (Partially indexed by NBS).
5. Pouillen et al. [1965].

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
5.84	30	002	15.17
5.57	19	$\bar{2}02$	15.90
5.44	11	011	16.28
4.621	100	$\bar{2}11$	19.19
3.864	15	211	23.00
3.712	10	$\bar{2}02$	23.95
3.509	10	$\bar{4}02$	25.36
3.424	2	$\bar{2}13$	26.00
3.285	60	013	27.12
3.160	30	$\bar{2}04$	28.22
3.067	5	020	29.09
2.918	20	004	30.61
2.837	5	121	31.51
2.781	10	220	32.16
2.716	12	022	32.95
2.688	14	$\bar{2}22$	33.30
2.615	6	$\bar{4}11$	34.26
2.341	3	$\bar{2}15$	38.42
2.310	5	$\bar{4}22$	38.95
2.228	7	$\bar{4}15$	40.46
2.202	16	$\bar{2}24$	40.96
2.196	30	600	41.06
2.183	8	015	41.33
2.112	5	024	42.75
2.099	2	$\bar{2}06$	43.05
2.058	3	$\bar{4}06$	43.93
2.042	2	$\bar{5}23$	44.32
1.945	3	006	46.66
1.879	5	215	48.40
1.867	3	224	48.73
1.834	3	$\bar{6}02$	49.67
1.721	8	$\bar{4}17$	53.19
1.5796	4	$\bar{4}08$	58.37
1.4589	2	008	63.74

References

Hanawalt, J. D., Rinn, H. W. and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Jayaraman, A. (1958). Proc. Indian Acad. Sci. A47, 147.

Pouillen, P., Bernard, M. J. and Massaux, M. (1965). Compt. Rend. 260, 6861.

Weigel, D., Imelik, B. and Prettre, M. (1964). Bull. Soc. Chim. France 1964, 836.

Lead chloride (cotunnite), $PbCl_2$

Sample
The sample was obtained from the National Lead Co.

Major impurities:

<0.01% each Bi and Fe
traces of Ag, Al, Ca, Cu, Mg, and Si

Structure
Orthorhombic, Pnam(62), Z=4, isostructural with $PbBr_2$. The structure of $PbCl_2$ was determined by Bräkken and Harang [1928], and refined by Sahl and Zemann [1961].

NBS lattice constants of this sample:

a = 7.6222(5)Å
b = 9.0448(7)
c = 4.5348(4)

Density
(calculated) 5.908 g/cm^3

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

Additional patterns
1. Bräkken and Harang [1928].
2. Döll and Klemm [1939].
3. PDF card 5-0416 [Swanson et al., 1953].

References
Bräkken, H., and Harang, L. (1928). Z. Krist. 68, 123.
Döll, W., and Klemm, W. (1939). Z. anorg. u. allgem. Chem. 241, 239.
Sahl,K., and Zemann,J.(1961). Naturwissenschaften 48, 641.
Swanson, H. E., and Fuyat, R. K. (1953). Nat'l Bur. Std., U. S. Circ. 539, Vol. II, 45.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
5.84	1	110	15.17
4.523	14	020	19.61
4.057	35	011	21.89
3.890	75	120	22.84
3.810	40	200	23.33
3.579	100	111	24.86
3.512	2	210	25.34
2.953	6	121	30.24
2.915	20	201,220	30.64
2.802	5	130	31.91
2.776	55	211	32.22
2.510	45	031	35.74
2.453	2	221	36.61
2.446	2	310	36.71
2.385	5	131	37.69
2.364	4	230	38.03
2.267	25	002	39.73
2.261	25	040	39.84
2.214	25	320	40.72
2.168	8	140	41.63
2.152	35	311	41.95
2.096	40	231	43.12
2.027	2	022	44.67
1.992	2	321	45.51
1.959	18	122	46.31
1.948	14	202	46.58
1.944	13	240,330	46.69
1.905	6	400,212	47.69
1.865	1	410	48.80
1.789	5	222	51.01
1.7629	1	132	51.82
1.7566	1	401,420	52.02
1.7243	2	411	53.07
1.6889	3	340	54.27
1.6806	2	051	54.56
1.6405	12	151	56.01
1.6365	8	232	56.16
1.6105	1	430	57.15
1.6010	6	042	57.52
1.5844	13	322	58.18
1.5667	4	142	58.90
1.5179	5	431	60.99
1.5077	3	060	61.45
1.5035	2	510	61.64
1.4911	1	013	62.21
1.4787	2	160	62.79
1.4759	4	242,332	62.92
1.4634	4	113	63.52
1.4591	6	402	63.73
1.4573	4	440	63.82

Lead chloride (cotunnite), $PbCl_2$ - continued

d(Å)	I	hkℓ	2θ(°)
1.4450	3	520	64.43
1.4272	7	511	65.33
1.4017	11	260,351	66.67
1.3889	3	213,422	67.37
1.3545	4	342	69.32
1.3514	4	033	69.50
1.3395	1	261	70.21
1.3304	1	133	70.76
1.3130	1	432	71.84
1.3027	1	531	72.50
1.2964	1	360	72.91
1.2858	3	313	73.61
1.2736	4	170,233	74.43
1.2703	3	600	74.66
1.2641	2	540	75.09
1.2554	2	062	75.70
1.2529	2	512	75.88
1.2427	2	071	76.61
1.2386	2	162	76.91
1.2261	2	171,442	77.84
1.2232	2	601,620	78.06
1.2184	4	522	78.43
1.2123	2	611	78.90

Magnesium titanium oxide, Mg_2TiO_4

Sample
The sample was prepared by heating together TiO_2 and $MgCO_3$ at 1380 °C, grinding and reheating.

Color
Colorless

Optical data
Isotropic, N = 1.95

Structure
Cubic, Fd3m (227), Z=8, inverse spinel type [Barth and Posnjak, 1932].

NBS lattice constants of this sample:

$a = 8.4409(3)$ Å

Density
(calculated) 3.546 g/cm^3

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

Additional patterns
1. PDF card 3-858 [Hanawalt et al., 1938].
2. Holgersson and Herrlin [1931].
3. Barth and Posnjak [1932].

References

Barth, T.F.W. and Posnjak, E. (1932). Z. Krist. 82, 325.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem., Anal. Ed. 10, 457.
Holgersson, S. and Herrlin, A. (1931). Z. anorg. u. allgem. Chem. 198, 69.

CuKα_1 $\lambda = 1.540598$ Å; temp. 25±1 °C

Internal standard W, $a = 3.16524$ Å

d(Å)	I	hkℓ	2θ(°)
4.876	45	111	18.18
2.986	20	220	29.90
2.544	100	311	35.25
2.435	2	222	36.88
2.110	60	400	42.82
1.936	<1	331	46.88
1.722	6	422	53.13
1.624	30	511	56.62
1.492	50	440	62.18
1.4268	3	531	65.35
1.3346	1	620	70.50
1.2874	6	533	73.50
1.2724	2	622	74.51
1.2185	5	444	78.42
1.1820	2	551	81.34
1.1280	1	642	86.14
1.0989	9	731	89.01
1.0551	5	800	93.78
0.9948	1	822	101.49
.9747	6	751	104.43
.9682	1	662	105.42
.9438	3	840	109.41
.9265	1	911	112.48
.8997	1	664	117.77

Nickel nitrate hydrate, $Ni(NO_3)_2 \cdot 6H_2O$

Sample
The sample was prepared by slow evaporation of an aqueous solution of $Ni(NO_3)_2$.

Color
strong brilliant green

Structure
Triclinic, Z = 2 [Weigel et al., 1962].

NBS lattice constants of this sample:

a = 7.699(4) Å
b = 11.677(2)
c = 5.799(2)
α = 98.56(3)°
β = 102.22(3)
γ = 105.80(2)

Density
(calculated) 2.019 g/cm^3

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

Additional pattern
1. PDF card 14-452 [Weigel et al., 1962].

Reference
Weigel, D.A., Imelick, B. and Lafitte, P. (1962). Bull. Soc. Chim. France 1962, 544.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
10.93	7	010	8.08
7.11	2	$\bar{1}10$	12.44
5.48	100	020	16.16
5.27	6	110	16.81
5.07	20	$\bar{1}01$	17.48
4.65	2	$\bar{1}11$	19.09
4.56	1	$\bar{1}\bar{1}1$,011	19.47
4.405	6	$02\bar{1}$	20.14
4.124	6	$1\bar{1}1$	21.53
3.901	3	101	22.78
3.808	12	$\bar{1}20$	23.34
3.761	25	$\bar{1}21$,210	23.64
3.652	4	030	24.35
3.546	1	$\bar{2}20$	25.09
3.526	1	021	25.24
3.413	16	$03\bar{1}$	26.09
3.348	4	$\bar{1}11$	26.60
3.141	3	$2\bar{1}1$	28.39
3.084	3	$\bar{2}30$	28.93
2.931	2	$\bar{1}31$	30.47
2.905	14	$\bar{1}30$	30.75
2.882	5	$\bar{1}40$	31.01
2.832	5	$2\bar{2}1$,$01\bar{2}$	31.57
2.741	65	040	32.64
2.691	4	201	33.27
2.606	2	$\bar{2}40$	34.39
2.552	13	$01\bar{2}$	35.14
2.483	2	$03\bar{2}$,$\bar{2}12$	36.14
2.455	1	$1\bar{2}2$	36.57
2.435	<1	$\bar{3}21$	36.88
2.430	1	211,$\bar{1}22$	36.96
2.390	3	$\bar{1}41$	37.61
2.375	4	$\bar{1}02$	37.85
2.322	2	$\bar{2}31$	38.75
2.319	2	$\bar{2}22$,131	38.80
2.282	5	$\bar{2}\bar{2}2$	39.46
2.212	3	$0\bar{5}1$	40.75
2.200	2	$04\bar{2}$,$\bar{2}50$	40.99
2.166	4	$\bar{3}40$	41.66
2.146	2	221,$\bar{1}32$	42.08
2.063	3	$\bar{3}41$,$2\bar{2}2$	43.84
2.030	1	$\bar{1}51$	44.60
2.006	2	$\bar{2}51$	45.16
1.996	2	$1\bar{5}1$	45.40
1.991	2	$\bar{2}41$	45.52
1.980	4	$12\bar{2}$	45.78
1.931	1	150,$\bar{1}\bar{1}3$	47.01
1.912	3	$16\bar{1}$,$\bar{1}03$	47.52
1.903	2	240,$\bar{4}11$ +	47.76
1.884	3	$\bar{2}60$	48.27
1.863	1	$0\bar{6}1$,311	48.86
1.843	5	$\bar{3}\bar{3}1$,003 +	49.41
1.828	2	$1\bar{5}\bar{2}$,060	49.85
1.807	<1	$\bar{2}13$	50.46
1.736	<1	$\bar{3}60$	52.67
1.733	<1	$1\bar{1}3$	52.79
1.714	2	$04\bar{3}$	53.42
1.708	4	$\bar{1}6\bar{1}$,$06\bar{2}$	53.62

Potassium chromium oxide sulfate, $K_2(CrO_4)_{.67}(SO_4)_{.33}$

Sample
The sample was prepared by melting together a 1:2 molar mixture of K_2SO_4 and K_2CrO_4 and annealing at about 600 °C for 18 hours.

Major impurities

0.001-0.01% each Al,Ba
0.003-0.03% Si
0.01-0.1% Ca

Color
Brilliant yellow

Structure
Orthorhombic, Pnam(62), Z=4. There is a complete solid solution series between K_2SO_4 and K_2CrO_4 [Groschuff, 1908], isostructural with low K_2SO_4. The structure of low K_2SO_4 was determined by Ehrenberg and Hermann [1929].

NBS lattice constants of this sample

a = 7.6095(9) Å
b = 10.300(1)
c = 5.8737(8)

Density
(calculated) 2.707 g/cm^3

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

Polymorphism
This composition inverts at about 650 °C to a hexagonal form [Groschuff, 1908].

References
Ehrenberg, W. and Hermann, C. (1929). Z. Krist. 70, 163.
Groschuff, E. (1908). Z. anorg. Chem. 58, 107.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.116	1	110	14.47
5.148	10	020	17.21
5.098	5	011	17.38
4.265	30	120	20.81
4.237	35	111	20.95
3.805	20	200	23.36
3.569	5	210	24.93
3.452	8	121	25.79
3.194	9	201	27.91
3.127	5	130	28.52
3.060	55	220	29.16
3.050	70	211	29.26
2.963	100	031	30.14
2.937	60	002	30.41
2.763	1	131	32.38
2.714	6	221	32.98
2.647	2	112	33.83
2.575	14	040	34.81
2.549	18	022,230	35.18
2.462	20	310	36.46
2.440	4	140	36.80
2.419	6	122	37.14
2.339	2	231	38.46
2.268	25	212	39.70
2.253	12	141	39.99
2.141	9	132	42.17
2.133	10	240	42.34
2.120	20	321,222	42.61
2.040	6	330	44.37
2.004	2	241	45.20
1.988	3	150	45.59
1.944	2	051	46.68
1.925	9	232	47.17
1.903	8	400	47.75
1.888	5	312	48.16
1.865	<1	113	48.80
1.810	5	250,401	50.37
1.808	4	340	50.45
1.783	2	411	51.20
1.779	1	123	51.32
1.741	2	203	52.53
1.7272	6	341	52.97
1.7170	8	060,213	53.31
1.7008	10	033	53.86
1.6646	4	430	55.13
1.6601	3	133	55.29
1.6470	2	152	55.77
1.6099	2	161	57.17
1.6004	5	431	57.54
1.5966	6	402	57.69
1.5779	2	412	58.44
1.5643	2	260	59.00
1.5530	<1	233	59.47
1.5391	3	342	60.06
1.5327	2	313	60.34
1.5270	2	143	60.59
1.5119	2	261	61.26
1.4820	7	062	62.63
1.4682	7	004	63.29
1.4593	8	520	63.72

Potassium chromium oxide sulfate, $K_2(CrO_4)_{.33}(SO_4)_{.67}$

Sample
The sample was prepared by melting together a 2:1 molar mixture of K_2SO_4 and K_2CrO_4, and annealing at 600 °C for 18 hours.

Color
Brilliant yellow

Major impurities

0.001-0.01% each Al, Ba
0.003-0.03% Si
0.01-0.1% Ca

Structure
Orthorhombic, Pnam (62), Z=4. There is a complete solid solution series between K_2SO_4 and K_2CrO_4 [Groschuff, 1908], isostructural with low K_2SO_4. The structure of low K_2SO_4 was determined by Ehrenberg and Hermann [1929].

NBS lattice constants of this sample:

a = 7.551(2)Å
b = 10.195(2)
c = 5.825(1)

Density
(calculated) 2.679 g/cm^3

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

Polymorphism
This composition inverts at about 620 °C to a hexagonal form. [Groschuff, 1908].

References
Ehrenberg, W. and Hermann, C. (1929). Z. Krist. 70, 163.
Groschuff, E. (1908). Z. anorg. Chem. 58, 107.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
5.10	10	020	17.38
5.06	5	011	17.50
4.221	30	120	21.03
4.203	30	111	21.12
3.778	25	200	23.53
3.538	6	210	25.15
3.420	10	121	26.03
3.168	8	201	28.14
3.099	5	130	28.78
3.027	75	211	29.48
2.935	100	031	30.43
2.912	60	002	30.68
2.691	6	221	33.27
2.626	2	112	34.11
2.548	13	040	35.19
2.527	15	022,230	35.49
2.443	30	310	36.76
2.413	4	140	37.23
2.398	8	122	37.48
2.249	18	212	40.05
2.230	12	141	40.42
2.122	8	132	42.57
2.112	10	240	42.78
2.100	20	222	43.03
2.022	5	330	44.79
1.986	2	241	45.64
1.969	3	150	46.07
1.908	9	232	47.61
1.888	6	400	48.15
1.871	4	312	48.61
1.794	4	250	50.84
1.769	2	411	51.64
1.727	2	203	52.98
1.710	5	242	53.53
1.700	6	060	53.89
1.685	10	033	54.39

Potassium rubidium chromium oxide, $KRbCrO_4$

Sample
The sample was prepared by melting together a 1:1 molar mixture of K_2CrO_4 and Rb_2CrO_4 and annealing the product at 600 °C for 18 hours.

Major impurities

0.001-0.01% Ag
0.003-0.03% Mg
0.01-0.1% each Al, Ba, Ca
0.03-0.3% Si

Color
Brilliant yellow

Structure
Orthorhombic, Pnam(62), Z=4, isostructural with low K_2SO_4. The structure of low K_2SO_4 was determined by Glossner [1928]. $KRbCrO_4$ is the midpoint in the complete solid solution series between K_2CrO_4 and Rb_2CrO_4 [Samuseva et al. 1967].

NBS lattice constants of this sample:

a = 7.853(1)Å
b = 10.517(1)
c = 5.9969(9)

Density
(calculated) 3.226 g/cm^3

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

Polymorphism
This composition inverts at about 630 °C to a high temperature crystal modification, presumably isostructural with high K_2SO_4 [Samuseva et al. 1967].

References
Glossner, B. (1928). Neues Jahrb. Mineral. Geol. Beilage B. 57A, 89.
Samuseva, R.G., Okunev, Y.A.,and Plyushchev, V.E. (1967). Russ. J. Inorg. Chem.(English Transl.), 12, 1489.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.25	6	020	16.87
5.211	4	011	17.00
4.371	3	120	20.30
4.341	4	111	20.44
3.926	13	200	22.63
3.676	10	210	24.19
3.530	25	121	25.21
3.285	19	201	27.12
3.202	7	130	27.84
3.145	65	220	28.36
3.136	85	211	28.44
3.026	100	031	29.49
2.997	70	002	29.79
2.785	10	221	32.11
2.706	1	112	33.08
2.629	13	040	34.08
2.614	20	230	34.27
2.539	30	310	35.32
2.493	4	140	36.00
2.472	11	122	36.31
2.396	4	231	37.51
2.339	14	311	38.45
2.324	18	212	38.71
2.302	9	141	39.09
2.184	14	240,321	41.30
2.171	25	222	41.57
2.098	6	330	43.09
2.053	4	241	44.07
2.031	5	150	44.57
1.984	2	051	45.68
1.971	18	232	46.02
1.938	9	312	46.83
1.866	6	401	48.75
1.854	4	340,250	49.09
1.837	4	411	49.59
1.818	2	123	50.15
1.781	4	203	51.26
1.772	10	341,251	51.52
1.756	9	213	52.03
1.753	7	060	52.14
1.737	14	033	52.66
1.713	5	430	53.46
1.696	1	133	54.02
1.682	5	152	54.52
1.646	4	431,161	55.80
1.643	4	402	55.93
1.623	3	412	56.68
1.600	3	260	57.54
1.578	3	342,252	58.43
1.5713	2	313	58.71
1.5466	4	261	59.74
1.5132	6	062	61.20
1.5041	10	511	61.61
1.4995	10	004	61.82
1.4874	8	432	62.38
1.4753	2	170,243	62.95
1.4581	3	114,071	63.78
1.4356	1	450	64.90
1.4126	7	262	66.09
1.4010	3	403,204	66.71
1.3886	2	413,214	67.38

Silver chromium oxide, Ag_2CrO_4

Sample
The sample was prepared at NBS by adding $AgNO_3$ in aqueous solution to one of K_2CrO_4. The precipitate was washed and dried.

Color
Dark grayish brown

Optical data
Opaque

Structure
Orthorhombic, Pmnb(62), Z = 4. The structure of Ag_2CrO_4 was determined by Hackert and Jacobson [1971].

NBS lattice constants of this sample:

a = 7.0220(9)Å
b = 10.065(2)
c = 5.5380(7)

Density
(calculated) 5.629 g/cm^3

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

Polymorphism
Pistorius [1967] reports that Ag_2CrO_4 inverts to a hexagonal form above 479 °C.

Additional pattern
1. PDF card 20-1055 [Kloberstein and Backmann, Degussa Forschung Chemie,Frankfurt-am-Main, Germany, 1967].

References
Hackert, M.L. and Jacobson, R.A. (1971). J. Solid State Chem. 3, 364.
Pistorius, C. W. F. T. (1967). J. Chem. Phys. 46, 2167.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.03	8	020	17.62
4.86	1	011	18.24
4.087	12	120	21.73
3.994	3	111	22.24
3.512	5	200	25.34
2.879	75	220	31.04
2.870	100	031	31.14
2.844	90	211	31.43
2.769	40	002	32.30
2.671	4	021	33.53
2.657	11	131	33.70
2.557	3	221	35.07
2.516	2	040	35.65
2.426	3	022	37.02
2.369	1	140	37.95
2.293	13	122	39.26
2.174	1	202	41.51
2.157	1	301	41.85
2.136	1	032	42.28
2.122	5	320	42.56
2.109	1	311	42.85
2.045	19	240,132	44.26
1.996	19	222	45.41
1.892	5	051	48.06
1.827	1	151	49.86
1.814	5	331	50.25
1.785	1	103	51.12
1.755	11	400	52.06
1.684	3	322	54.43
1.677	5	060	54.69
1.665	5	251	55.10
1.645	16	242	55.86
1.631	4	160	56.37
1.6172	11	033	56.89
1.6125	20	213	57.07
1.5757	2	133	58.53
1.4971	12	431	61.93
1.4827	8	402	62.60
1.4348	3	062	64.94
1.4218	<1	422	65.61
1.4053	3	162	66.48
1.3847	3	004	67.60
1.3639	2	360	68.77
1.3607	2	053	68.96
1.3311	1	333	70.72
1.2938	3	271	73.08
1.2878	2	204	73.48
1.2690	1	253	74.75
1.2581	1	080	75.50
1.2477	2	224	76.25
1.2226	1	163	78.11
1.2124	2	460	78.89
1.1952	<1	144	80.25
1.1895	1	433	80.72
1.1463	4	244	84.44
1.1376	3	611	85.24
1.1107	2	513	87.82

Strontium nitrate, $Sr(NO_3)_2$

Sample
The sample was specially purified material from the Mallinckrodt Chemical Works, New York.

Color
Colorless

Optical data
Isotropic N = 1.587

Structure
Cubic, $P2_13$ (198), Z = 4, isostructural with $Ba(NO_3)_2$. The structure of $Ba(NO_3)_2$ was determined by Birnstock [1967]. Previously the space group for $Sr(NO_3)_2$ was considered to be Pa3(205).

NBS lattice constants of this sample:

$a = 7.7813(2)$ Å

Density
(calculated) 2.984 g/cm^3

Reference intensity
$I/I_{corundum} = 3.5$

Additional patterns
1. Vegard [1922].
2. PDF card 4-310 [Swanson and Tatge, 1953].

References
Birnstock, R., (1967). Z. Krist. 124, 310.
Swanson, H. E. and Tatge, E. (1953). Natl. Bur. Std. U. S. Circ. 539, 1, 80.
Vegard, L. (1922). Z. Phys. 9, 395.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
4.494	100	111	19.74
3.890	15	200	22.84
3.480	25	210	25.58
3.177	16	211	28.06
2.753	20	220	32.50
2.595	1	221	34.54
2.346	65	311	38.33
2.245	55	222	40.13
2.081	1	321	43.46
1.947	14	400	46.62
1.887	1	410	48.18
1.834	1	411	49.68
1.786	12	331	51.10
1.740	10	420	52.54
1.698	<1	421	53.94
1.660	<1	332	55.31
1.588	6	422	58.02
1.556	<1	430	59.34
1.527	1	510	60.61
1.497	9	511	61.92
1.445	1	520	64.44
1.421	<1	521	65.64
1.3752	6	440	68.13
1.3342	1	530	70.53
1.3156	10	531	71.68
1.2968	4	600	72.88
1.2792	1	610	74.05
1.2625	<1	611	75.20
1.2303	2	620	77.53
1.2155	<1	621	78.65
1.1866	3	533	80.96
1.1731	4	622	82.09
1.1599	1	630	83.23
1.1473	<1	631	84.35
1.1232	1	444	86.60
1.0896	2	711	89.98
1.0791	1	640	91.10
1.0688	<1	720	92.23
1.0588	<1	721	93.36
1.0398	2	642	95.60
1.0307	<1	722	96.72
1.0131	4	731	98.99
0.9962	<1	650	101.29
.9884	<1	732	102.40
.9728	<1	800	104.72
.9652	<1	810	105.90
.9506	<1	733	108.25
.9437	2	820	109.43
.9368	<1	821	110.63
.9170	2	822	114.29
.9044	1	831	116.79
.8985	2	751	118.03
.8925	1	662	119.32
.8867	<1	832	120.62
.8700	1	840	124.61
.8541	3	911	128.81
.8490	1	842	130.28

Strontium tungsten oxide, Sr_2WO_5

Sample
The sample was prepared at NBS by T. Negas by heating $SrCO_3$ and WO_3 in stoichiometric proportions at 950° C in a gold envelope for 2 weeks.

Color
Colorless

Structure
Orthorhombic, Pnam (62), Z = 4, isostructural with $K_2VO_2F_3$. The structure of Sr_2WO_5 was determined by Negas and Roth [1974].

NBS lattice constants of this sample:

a = 7.2506(4) Å
b = 10.8963(7)
c = 5.5480(4)

Density
(calculated) 6.654 g/cm^3

Reference intensity
$I/I_{corundum}$ = 5.7

Reference
Negas, T. and Roth, R. S. (1974). Private communication (to be published).

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.04	11	110	14.66
5.45	13	020	16.26
4.95	3	011	17.91
4.356	9	120	20.37
4.085	30	111	21.74
3.626	5	200	24.53
3.440	10	210	25.88
3.037	100	031,201	29.39
3.020	30	220	29.56
2.923	30	211	30.56
2.804	4	131	31.89
2.774	35	002	32.24
2.652	17	221	33.77
2.567	11	230	34.93
2.551	4	140	35.15
2.521	2	112	35.58
2.473	1	022	36.30
2.329	7	231	38.63
2.318	6	141	38.82
2.204	4	202	40.92
2.178	7	240	41.42
2.172	6	311	41.55
2.159	11	212	41.80
2.109	2	132	42.84
2.088	4	150	43.30
2.052	5	321	44.09
2.043	25	222	44.31
2.028	7	051,241	44.64
2.013	3	330	45.00
1.954	<1	151	46.43
1.884	14	232	48.28
1.868	4	250	48.71
1.817	6	060	50.18
1.812	4	400	50.31
1.798	3	312	50.74
1.789	1	410	51.02
1.7699	12	251	51.60
1.7616	3	160	51.86
1.7231	12	401	53.11
1.7135	3	242	53.43
1.7023	2	123,411	53.81
1.6680	1	152	55.01
1.6473	16	033,203	55.76
1.6429	12	421	55.92
1.6285	8	213,332	56.46
1.6227	10	260,430	56.68
1.6066	1	133	57.30
1.5767	4	223	58.49
1.5583	4	261	59.25
1.5493	4	252	59.63
1.5191	8	062	60.94
1.5026	2	412	61.68
1.4998	3	233	61.81
1.4971	3	143	61.93
1.4870	3	162	62.40
1.4676	1	171	63.32
1.4618	1	422	63.60
1.4520	<1	360	64.08
1.4376	1	510	64.80
1.4181	1	323	65.80
1.4101	2	053,243	66.22
1.4047	5	361	66.51
1.3999	14	432	66.77
1.3973	7	352	66.91
1.3869	5	004	67.48

Strontium tungsten oxide, Sr_2WO_5 - continued

d(Å)	I	hkℓ	2θ(°)
1.3621	1	080,333	68.88
1.3586	1	521	69.08
1.3516	1	114,451	69.49
1.3442	1	024	69.93
1.3343	2	172	70.52
1.3220	1	124	71.28
1.3143	3	253	71.76
1.3013	1	181	72.59
1.2946	4	403	73.03
1.2859	1	214,362	73.60
1.2760	1	512,163	74.27
1.2751	1	134,280	74.33
1.2598	5	224,423	75.39
1.2506	4	552	76.04
1.2474	4	541	76.27
1.2458	4	452	76.39
1.2426	3	281	76.62
1.2224	3	082	78.12
1.2198	5	263,234	78.32
1.2082	1	600	79.22
1.2009	<1	610	79.80
1.1827	1	091	81.28
1.1801	1	620,551	81.50
1.1752	1	173	81.91
1.1698	1	244	82.37
1.1672	2	191	82.59
1.1623	1	542	83.02
1.1585	1	282	83.35
1.1553	2	154,471	83.63
1.1542	1	621	83.73
1.1483	1	290	84.26
1.1464	1	630	84.43
1.1422	2	363,334	84.82
1.1248	1	291	86.45
1.1230	3	631	86.62
1.1135	1	254	87.54
1.1079	1	602	88.10
1.1023	3	064,612	88.66
1.0962	<1	414	89.29
1.0913	1	115,382	89.80
1.0898	1	164,0•10•0	89.95
1.0832	1	641	90.66
1.0823	1	390	90.75
1.0690	1	481	92.21
1.0679	1	373	92.33
1.0610	4	292,205	93.11
1.0558	2	215	93.70
1.0541	6	463,434	93.90
1.0499	2	135,283	94.39
1.0414	1	225	95.41

Telluric Acid, H_6TeO_6

Sample
The sample was obtained from K&K Laboratories, Plainview, N.J.

Major impurities

0.01-0.1% Ca
0.001-0.01% Fe

Color
Colorless

Structure
Monoclinic, $P2_1/c$ (14), Z=4 [Gossner and Kraus, 1934]. The structure was determined by Lindqvist [1970] who confirmed this space group. Other space groups have been reported by Aviness and Petit [1968] and by Bayer [1968]. The NBS data could also be indexed on these space groups.

NBS lattice constants for this sample:

a = 6.4979(6)A°
b = 9.3223(9)
c = 8.3334(9)
β = 99.69(1)°

Density
(calculated) 3.065 g/cm^3

Reference intensity
$I/I_{corundum}$ = 5.9

Polymorphism
Three forms of H_6TeO_6 have been reported. The cubic phase transforms to either the monoclinic or tetragonal phase depending on conditions of humidity and temperature. It was not possible to convert the monoclinic phase into the cubic form in either dry or moist air; this suggests that the monoclinic phase is the stable modification [Bayer, 1968].

Additional patterns
1. PDF card 21-388 [Bayer, 1968]
2. PDF card 24-1266 [Lindqvist, 1970]
3. Aviness and Petit [1968]

References

Aviness, C. and Petit, H. (1968). Compt. Rend. 266, 981.
Bayer, G. (1968). J. Less-Common Metals 16, 215.
Gossner, B. and Kraus, O. (1934). Z. Krist. 88, 298.
Lindqvist, O. (1970). Acta Chem. Scand. 24, 3178.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.75	100	$\bar{1}11$	18.65
4.67	45	020	19.00
4.183	65	111	21.22
4.107	30	002	21.62
3.485	1	$\bar{1}12$	25.54
3.203	7	200	27.83
3.083	11	022	28.94
2.761	4	$\bar{2}02$	32.40
2.708	7	$\bar{1}31$,211	33.05
2.639	20	220	33.94
2.622	4	$\bar{2}21$	34.17
2.589	25	131	34.62
2.582	30	$\bar{1}13$	34.72
2.376	5	$\bar{2}22$	37.83
2.331	3	040	38.60
2.303	2	113	39.08
2.243	2	041	40.18
2.2361	1	132	40.30
2.1013	5	$\bar{3}11$	43.01
2.0925	8	222,231	43.20
2.0536	2	033,004	44.06
2.0475	4	$\bar{2}23$	44.20
2.0322	5	$\bar{1}33$	44.55
2.0274	4	042	44.66
1.9932	<1	$\bar{3}12$	45.47
1.9431	6	311	46.71
1.8879	13	133,142	48.16
1.8839	16	240,$\bar{1}$24	48.27
1.8791	16	024,$\bar{2}$04	48.40
1.8055	4	$\bar{3}13$	50.51
1.7808	5	223,$\bar{2}$42	51.26
1.7718	6	$\bar{3}31$	51.54
1.7667	6	$\bar{1}51$	51.70
1.7422	4	$\bar{2}24$	52.48
1.7321	3	124,151	52.81
1.6738	4	331	54.80
1.6525	4	242	55.57
1.6346	4	$\bar{1}15$	56.23
1.6133	1	152	57.04
1.6102	1	204	57.16
1.6007	1	400,$\bar{1}$34	57.53
1.5839	3	$\bar{3}33$,$\bar{3}41$	58.20
1.5535	1	060	59.45
1.5399	4	044,$\bar{3}$13	60.03
1.5320	2	$\bar{3}24$,$\bar{1}53$	60.37
1.5216	2	224	60.83
1.5146	2	420	61.14
1.5121	3	341	61.25
1.5106	3	115,160	61.32
1.5002	2	$\bar{4}22$	61.79

d(Å)	I	hkℓ	2θ(°)
1.4665	3	$1\bar{5}3$	63.37
1.4626	4	$\bar{2}44$	63.56
1.4534	1	062,035	64.01
1.4247	<1	$\bar{4}23$	65.46
1.4136	1	402	66.04
1.4102	2	$\bar{3}51$	66.22
1.4064	2	$\bar{3}15$	66.42
1.3977	1	260,412	66.89
1.3949	1	$\bar{2}61,333$	67.04
1.3800	1	$\bar{4}04,054$	67.86
1.3765	1	$\bar{3}52$	68.06
1.3731	2	135	68.25
1.3595	1	$35\bar{1}$	69.03
1.3540	3	$01\bar{6},\bar{2}62$	69.35
1.3426	<1	$\bar{2}06,045$	70.02
1.3234	2	$\bar{4}24,\bar{2}54$	71.19
1.3099	3	$\bar{3}53$	72.04
1.2946	2	$26\bar{2},\bar{1}71$	73.03
1.2868	1	$\bar{5}11,432$	73.54
1.2809	<1	500,171	73.94
1.2396	1	$\bar{1}55,\bar{5}22$	76.84
1.2325	1	$055,\bar{5}13$	77.36
1.2236	1	361,511	78.03
1.2086	<1	442	79.19
1.1973	3	$\bar{2}64,353$	80.09
1.1934	2	$52\bar{1},\bar{1}73$	80.40
1.1878	1	$\bar{5}32,\bar{4}44$	80.86
1.1808	1	$\bar{1}17,344$	81.44
1.1710	<1	404	82.27

Zinc nitrate hydrate, α-$Zn(NO_3)_2 \cdot 6H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of an aqueous solution of $Zn(NO_3)_2$. Because of instability and strong cleavage the intensities are subject to some error.

Major impurities:

0.001-0.01% each Ag, Ba, Cr, Si, Sr
0.003-0.03% Fe
0.01-0.1% Ca

Color
Colorless

Structure
Orthorhombic, $Pn2_1a$ (33), Z=4. The structure was determined by Ferrari et al. [1967]. It is isostructural with β-$Co(NO_3)_2 \cdot 6H_2O$ [Pouillen et al., 1965].

NBS lattice constants of this sample:

a = 12.372(3)Å
b = 12.902(3)
c = 6.302(2)

Density
(calculated) 1.964 g/cm^3

Polymorphism
Pouillen [1960] reports polymorphic transformations of $Zn(NO_3)_2 \cdot 6H_2O$ at + 19 ° and -13 °C; however Weigel et al [1964] did not find a transition at -13 °C.

Additional patterns
1. PDF card 19-1465 [Weigel et al., 1964].
2. Pouillen et al., [1965].

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.449	6	020	13.72
5.580	100	210	15.87
5.145	75	111	17.22
4.235	85	121	20.96
3.646	15	221	24.39
3.532	20	230	25.19
3.415	4	131	26.07
3.336	30	311	26.70
3.228	30	040	27.61
3.154	2	002	28.27
3.095	40	400	28.82
3.042	30	321	29.34
2.971	8	112	30.05
2.832	5	022	31.57
2.788	35	420	32.08
2.744	30	212	32.61
2.715	4	411	32.97
2.551	3	421	35.15
2.504	9	302	35.83
2.457	10	312	36.54
2.380	3	250	37.77
2.344	12	151	38.37
2.302	3	501	39.09
2.267	4	511	39.73
2.208	20	402	40.84
2.169	16	521	41.61
2.149	25	060	42.00
2.088	9	422	43.29
2.071	8	103	43.67
2.067	10	351	43.75
2.036	4	610	44.45
2.008	6	161	45.12
1.990	4	203	45.54
1.946	4	502	46.64

References

Ferrari, A., Braibanti,A., Manotti-Lanfredi, A.N. and Tirificchio,A. (1967). Acta Cryst. 22, 240.
Pouillen, P. (1960). Compt. Rend. 250, 3318.
Pouillen, P., Bernard, M. J., and Massaux, M. (1965). Compt. Rend. 260, 6861.
Weigel, D., Imelik, B., and Prettre, M. (1964). Bull. Soc. Chem. France 1964, 836.

Zinc titanium oxide, Zn_2TiO_4

Sample
The sample was prepared at NBS by heating a 2:1 mixture of ZnO and TiO_2 (anatase) at 1300 °C for 45 minutes, followed by heating at 1450 °C for 10 minutes.

Color
Colorless

Structure
Cubic, Fd3m (227), Z = 8. Verwey and Heilmann [1947] found Zn_2TiO_4 to be an inverse spinel structure. Billiet and Poix [1963] found that at high temperatures there was some randomness of the cation occupation. The structure was also studied by Bartram and Stepetys [1961] who also noted some departure from perfect inverse spinel structure.

NBS lattice constant of this sample:

$$a = 8.4602(5)\text{Å}$$

Density
(calculated) 5.323 g/cm^3

Reference intensity
$I/I_{corundum} = 4.5$

Polymorphism
Besides the order-disorder of the spinel type, Billiet and Poix [1963] reported a tetragonal, distorted spinel form below about 500 °C.

Additional patterns
1. Bartram and Stepetys [1961].
2. Dulin and Rase [1960].

References

Bartram, S. F. and Stepetys, R. A. (1961). J. Am. Cer. Soc. 44, 493.
Billiet, Y. and Poix, P. (1963). Bull. Soc. Chem. France 1963, 477.
Dulin, F. H. and Rase, D. E. (1960). J. Am. Cer. Soc. 43, 125.
Verwey, E. J. W. and Heilmann, E. L. (1947). J. Chem. Phys. 15, 174.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.89	4	111	18.11
2.993	35	220	29.83
2.552	100	311	35.13
2.444	4	222	36.74
2.115	13	400	42.72
1.727	11	422	52.98
1.627	30	511	56.50
1.4958	30	440	61.99
1.4305	<1	531	65.16
1.3377	3	620	70.32
1.2901	6	533	73.32
1.2758	2	622	74.28
1.2214	1	444	78.20
1.1306	4	642	85.89
1.1013	9	731	88.77
1.0576	2	800	93.50
0.9971	2	822	101.17
.9769	5	751	104.10
.9706	1	662	105.06
.9457	1	840	109.07
.9019	1	664	117.32
.8868	4	931	120.61
.8634	7	844	126.30

Barium calcium nitrate, $Ba(NO_3)_2$-$Ca(NO_3)_2$, calculated solid solution series

Structure

Cubic, $P2_13$ (198), Z = 4. The structure of $Ca(NO_3)_2$ was determined by Vegard and Bilberg [1931], and the space group was given as Pa3. However, later work by Birnstock [1967] on the isomorph $Ba(NO_3)_2$ indicated that the space group is $P2_13$. In the present calculated patterns, the atomic positions given by Vegard and Bilberg have been modified for the change in space group. The system $Ba(NO_3)_2$-$Ca(NO_3)_2$ forms a complete solid solution series [Protsenko and Belova, 1957].

Lattice constants

The constants were derived by interpolation on a molar ratio using the following: for $Ba(NO_3)_2$ a = 8.1148Å [Swanson et al., 1973]; for $Ca(NO_3)_2$, a=7.6005Å [Swanson et al., 1957, modified to conform to new wavelength measurements].

Thermal parameters

Isotropic: barium B = 0.93; calcium B = 1.0; nitrogen B = 1.2; oxygen B = 1.2.

Scattering factors

Ca^{2+}, N^0, O^- [International Tables, 1962].

Ba^{2+} [Cromer and Waber, 1965].

The factors used were proportional to the molar ratio, assuming random distribution of the cations.

References

Birnstock, R. (1967). Z. Krist. 124, 310.

Cromer, D. T. and Waber, J. T. (1965). Acta Cryst. 18, 104.

International Tables for X-ray Crystallography III (1962), 202, 210.

Protsenko, P. I. and Belova, Z. I. (1957). Zhur. Neorg. Khim. 2, 2619.

Swanson, H. E., Gilfrich, N. T., and Cook, M. I. (1957). Nat'l. Bur. Std. U.S. Circ. 539, VII, 14.

Swanson, H. E., McMurdie, H. F., Morris, M. C., Evans, E. H., and Paretzkin, B. (1973). Nat'l. Bur. Std. U.S. Monograph 25, 11, 14.

Vegard, L. and Bilberg, L. (1931). Avhandl. Norske Videnskaps Mat.-Nat. Kl. 1931 No. 12.

	$Ba_{.75}Ca_{.25}(NO_3)_2$			$Ba_{.5}Ca_{.5}(NO_3)_2$			$Ba_{.25}Ca_{.75}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598			λ=1.540598	
111	4.610	100	19.24	4.535	100	19.56	4.463	100	19.88
200	3.994	25	22.24	3.928	15	22.62	3.864	5	23.00
210	3.573	17	24.90	3.515	28	25.32	3.456	42	25.76
211	3.262	13	27.32	3.209	20	27.78	3.155	31	28.26
220	2.824	26	31.66	2.779	22	32.18	2.733	17	32.74
221	2.664	<1	33.62	2.620	2	34.20	2.576	5	34.80
311	2.409	75	37.30	2.370	75	37.94	2.331	71	38.60
222	2.306	44	39.02	2.268	53	39.70	2.232	64	40.38
321 +	2.135	<1	42.30	2.101	1	43.02	2.066	2	43.78
400	1.997	13	45.38	1.965	16	46.16	1.933	19	46.98
410	1.937	<1	46.86	1.906	<1	47.68	1.875	<1	48.52
411	1.883	2	48.30	1.853	3	49.14	1.822	5	50.02
331	1.833	15	49.70	1.803	14	50.58	1.773	11	51.50
024 +	1.787	14	51.08	1.757	13	52.00	1.728	11	52.94
124	1.744	1	52.44	1.715	1	53.38	1.687	1	54.34
332	1.703	<1	53.78	1.676	<1	54.74	1.648	1	55.74
422	1.631	10	56.38	1.604	8	57.40	1.5780	6	58.44
430	1.598	<1	57.64	1.5721	<1	58.68	1.5462	1	59.76
134 +	1.567	<1	58.90	1.5415	<1	59.96	1.5159	1	61.08
511 +	1.537	11	60.14	1.5123	11	61.24	1.4878	10	62.36
432	1.4836	1	62.56	1.4593	1	63.72	1.4352	2	64.92
125	1.4585	<1	63.76	1.4348	<1	64.94	1.4113	<1	66.16
440	1.4124	6	66.10	1.3894	7	67.34	1.3666	8	68.62
522 +	1.3909	--	67.26	1.3680	--	68.54	1.3457	<1	69.84
433	1.3701	<1	68.42	1.3480	<1	69.70	1.3255	1	71.06

Barium calcium nitrate, $Ba(NO_3)_2$-$Ca(NO_3)_2$, calculated solid solution series - Continued

	$Ba_{.75}Ca_{.25}(NO_3)_2$			$Ba_{.5}Ca_{.5}(NO_3)_2$			$Ba_{.25}Ca_{.75}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598			λ=1.540598	
531 +	1.3504	13	69.56	1.3284	12	70.88	1.3067	11	72.24
442 +	1.3314	6	70.70	1.3099	5	72.04	1.2883	4	73.44
610	1.3134	<1	71.82	1.2920	<1	73.20	1.2709	<1	74.62
235 +	1.2959	<1	72.94	1.2749	<1	74.34	1.2540	1	75.80
620 +	1.2631	3	75.16	1.2426	3	76.62	1.2222	2	78.14
126 +	1.2476	--	76.26	1.2275	<1	77.74	1.2072	<1	79.30
145 +	1.2328	--	77.34	1.2128	--	78.86	1.1927	<1	80.46
533	1.2182	4	78.44	1.1986	4	79.98	1.1789	3	81.60
622	1.2044	4	79.52	1.1849	5	81.10	1.1653	5	82.76
542	1.1910	<1	80.60	1.1715	<1	82.22	1.1523	<1	83.90
136 +	1.1779	<1	81.68	1.1589	<1	83.32	1.1398	<1	85.04
444	1.1532	1	83.82	1.1344	1	85.54	1.1158	1	87.32
543	1.1297	--	85.98	1.1115	<1	87.74	1.0932	<1	89.60
711 +	1.1186	4	87.04	1.1006	4	88.84	1.0824	3	90.74
640 +	1.1079	2	88.10	1.0899	2	89.94	1.0719	1	91.88
146	1.0974	<1	89.16	1.0796	<1	91.04	1.0618	<1	93.02
633	1.0871	--	90.24	1.0696	--	92.14	1.0519	<1	94.16
246 +	1.0676	4	92.36	1.0502	4	94.36	1.0330	3	96.44
544	1.0583	--	93.42	1.0410	--	95.46	1.0239	<1	97.58
137 +	1.0401	6	95.56	1.0231	5	97.68	1.0063	5	99.90
650	1.0228	<1	97.72	1.0063	<1	99.90	0.9898	<1	102.20
156 +	1.0145	<1	98.80	0.9981	<1	101.02	.9817	<1	103.38
800	0.9986	<1	100.96	.9824	<1	103.28	.9663	<1	105.72
652 +	.9909	<1	102.04	.9749	<1	104.40	.9587	1	106.92
147	.9833	--	103.14	.9675	--	105.54	.9515	<1	108.10
733	.9761	1	104.22	.9601	1	106.70	.9444	1	109.30
644 +	.9687	3	105.34	.9531	3	107.84	.9374	3	110.52
247 +	.9617	<1	106.44	.9462	<1	109.00	.9306	<1	111.74
822 +	.9415	2	109.80	.9262	2	112.54	.9110	2	115.46
831 +	.9287	<1	112.08	.9136	<1	114.94	.8986	<1	118.02
751 +	.9225	3	113.24	.9075	3	116.16	.8925	3	119.32
662	.9164	1	114.40	.9015	1	117.40	.8867	1	120.62
832 +	.9104	<1	115.58	.8957	<1	118.64	.8809	<1	121.96
048 +	.8932	1	119.18	.8787	1	122.48	.8642	1	126.08
744 +	.8877	--	120.40	.8732	--	123.80	.8589	<1	127.50
753 +	.8769	4	122.90	.8627	4	126.48	.8485	4	130.42
842 +	.8717	2	124.18	.8575	2	127.86	.8434	2	131.94
761 +	.8615	--	126.80	.8475	--	130.70	.8335	<1	135.08
664	.8516	1	129.52	.8378	1	133.68	.8240	1	138.40
922 +	.8469	--	130.90	.8331	--	135.22	.8194	<1	140.14
158	.8421	--	132.34	.8285	--	136.80	.8148	<1	141.94
931 +	.8374	2	133.80	.8239	2	138.44	.8103	2	143.84
844	.8154	1	141.72	.8021	1	147.60	.7889	1	155.04
933 +	.8029	4	147.22	.7899	4	154.42			
068 +	.7989	2	149.24	.7859	1	157.10			
249 +	.7949	<1	151.40						
862 +	.7834	4	159.04						
Lattice constant	7.9889Å			7.8594Å			7.7300Å		
Density (calc.)	3.088 g/cm^3			2.910 g/cm^3			2.709 g/cm^3		

Barium lead nitrate, $Ba(NO_3)_2$-$Pb(NO_3)_2$, calculated solid solution series

Structure

Cubic, $P2_13(198)$, Z=4. The structure of $Pb(NO_3)_2$ was determined by Hamilton [1957] and the space group given as Pa3. However, later work on the isomorph $Ba(NO_3)_2$ [Birnstock, 1967] indicated that the space group is $P2_13$. In the present calculated patterns the atom positions given by Hamilton were modified for the change in space group. The system $Ba(NO_3)_2$-$Pb(NO_3)_2$ forms a complete solid solution series [Laybourn, et al., 1934].

Lattice constants

The constants were derived by interpolation on a molar ratio using the following: for $Ba(NO_3)_2$, a=8.1148Å [Swanson et al., 1974]; for $Pb(NO_3)_2$, a = 7.8573 [Swanson et al., 1955, modified to conform to new wavelength measurements].

Thermal parameters

Isotropic: barium B = .93, lead B = 1.0, nitrogen B = 1.21, oxygen B = 1.16.

Scattering factors

N^0, O^- [International Tables, 1962].
Ba^{2+}, Pb^{2+} [Cromer and Waber, 1965].
The factors used were proportional to the molar ratio, assuming random distribution of the cations.

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	$Ba_{.67}Pb_{.33}(NO_3)_2$			$Ba_{.33}Pb_{.67}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598	
111	4.638	100	19.12	4.586	100	19.34
200	4.015	35	22.12	3.973	35	22.36
210 +	3.593	9	24.76	3.553	6	25.04
211	3.278	6	27.18	3.243	4	27.48
220	2.840	30	31.48	2.808	30	31.84
311	2.421	67	37.10	2.395	64	37.52
222	2.319	33	38.80	2.293	30	39.26
123	2.146	<1	42.06	2.123	<1	42.54
400	2.008	11	45.12	1.986	10	45.64
410 +	1.948	<1	46.58	1.926	<1	47.14
411	1.893	1	48.02	1.873	<1	48.58
331	1.843	17	49.42	1.823	16	50.00
024 +	1.796	15	50.80	1.776	15	51.40
124	1.753	<1	52.14	1.734	<1	52.76
332	1.713	<1	53.46	1.694	<1	54.10
422	1.640	11	56.04	1.622	11	56.72
431	1.575	<1	58.56	1.558	<1	59.26
511 +	1.546	11	59.78	1.529	11	60.52
432	1.4917	<1	62.18	1.4751	<1	62.96
440	1.4201	5	65.70	1.4042	5	66.54

Barium lead nitrate, $Ba(NO_3)_2$-$Pb(NO_3)_2$, calculated solid solution series - continued

	$Ba_{.67}Pb_{.33}(NO_3)_2$			$Ba_{.33}Pb_{.67}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598	
433	1.3775	<1	68.00	1.3624	<1	68.86
531 +	1.3576	13	69.14	1.3426	12	70.02
442 +	1.3386	6	70.26	1.3239	6	71.16
610	1.3204	<1	71.38	1.3058	--	72.30
611	1.3030	<1	72.48	1.2886	--	73.42
620 +	1.2700	3	74.68	1.2559	3	75.66
533	1.2248	4	77.94	1.2113	4	78.98
622	1.2110	4	79.00	1.1976	4	80.06
444	1.1593	1	83.28	1.1465	1	84.42
711 +	1.1246	4	86.46	1.1123	4	87.66
640 +	1.1139	2	87.50	1.1015	2	88.74
146	1.1033	<1	88.56	1.0911	<1	89.82
246 +	1.0734	4	91.72	1.0614	4	93.06
553 +	1.0456	6	94.90	1.0341	5	96.30
800	1.0041	<1	100.20	0.9929	<1	101.76
733	0.9813	1	103.44	.9704	1	105.08
644 +	.9741	3	104.52	.9633	3	106.20
822 +	.9467	2	108.92	.9361	2	110.74
831	.9337	<1	111.18	.9234	--	113.06
751 +	.9275	3	112.30	.9172	3	114.24
662	.9213	1	113.46	.9112	1	115.42
840 +	.8980	1	118.14	.8881	1	120.30
753 +	.8817	4	121.78	.8719	4	124.12
842 +	.8764	2	123.04	.8667	2	125.44
664	.8562	1	128.22	.8468	1	130.92
931 +	.8420	2	132.36	.8327	2	135.36
844	.8198	1	139.98	.8107	1	143.66
933 +	.8073	4	145.18	.7983	4	149.54
068 +	.8032	2	147.08	.7944	2	151.72
862 +	.7876	4	155.92			
Lattice constant	8.0322Å			7.9435Å		
Density (calc.)	3.645 g/cm^3			4.083 g/cm^3		

Barium strontium nitrate, $Ba(NO_3)_2$-$Sr(NO_3)_2$, calculated solid solution series

Structure

Cubic, $P2_13$ (198), Z = 4. The structures of both $Ba(NO_3)_2$ and $Sr(NO_3)_2$ were originally determined by Vegard and Bilberg [1931]; they found the compounds isostructural and assigned the space group Pa3(205). Later work on $Ba(NO_3)_2$ by Birnstock [1967] indicated instead that the space group is $P2_13$(198) which is used here. The system $Ba(NO_3)_2$-$Sr(NO_3)_2$ forms a complete solid solution series [Ringdal, 1932].

Lattice constants

The constants were derived by interpolation on a molar ratio using the following; for $Ba(NO_3)_2$, a = 8.1184Å [Swanson et al., 1974] and for $Sr(NO_3)_2$, a = 7.7813Å [McMurdie et al., 1974].

Thermal parameters

Isotropic: barium B = 0.93; strontium B = 1.0; nitrogen B = 1.21; oxygen B = 1.16.

Scattering factors

N^0, O^- [International Tables, 1962].
Ba^{2+}, Sr^{2+} [Cromer and Waber, 1965].
The factors used were proportional to the molar ratio, assuming random distribution of the cations.

References

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	$Ba_{.75}Sr_{.25}(NO_3)_2$			$Ba_{.5}Sr_{.5}(NO_3)_2$			$Ba_{.25}Sr_{.75}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598			λ=1.540598	
111	4.638	100	19.12	4.590	100	19.32	4.539	100	19.54
200	4.015	26	22.12	3.973	21	22.36	3.931	17	22.60
210	3.593	16	24.76	3.556	18	25.02	3.517	22	25.30
211	3.281	10	27.16	3.246	12	27.46	3.211	14	27.76
220	2.840	26	31.48	2.810	26	31.82	2.781	25	32.16
221	2.678	<1	33.44	2.650	1	33.80	2.621	2	34.18
311	2.423	69	37.08	2.396	67	37.50	2.372	65	37.90
222	2.319	39	38.80	2.295	42	39.22	2.271	46	39.66
321 +	2.148	<1	42.04	2.124	1	42.52	2.102	1	43.00
400	2.009	12	45.10	1.988	13	45.60	1.967	14	46.12
410 +	1.948	<1	46.58	1.928	<1	47.10	1.907	<1	47.64
411	1.894	1	48.00	1.874	2	48.54	1.854	2	49.10
331	1.843	15	49.40	1.824	14	49.96	1.804	14	50.54
024 +	1.796	14	50.78	1.778	14	51.36	1.759	13	51.94
124	1.753	1	52.12	1.735	1	52.72	1.716	1	53.34
332	1.713	<1	53.46	1.695	<1	54.06	1.677	<1	54.70
422	1.640	10	56.04	1.623	9	56.68	1.606	8	57.34
430	1.607	<1	57.30	1.590	<1	57.96	1.573	<1	58.64
134 +	1.576	<1	58.54	1.559	<1	59.22	1.542	<1	59.92
511 +	1.546	11	59.76	1.530	11	60.46	1.514	11	61.18
432	1.4917	1	62.18	1.4764	1	62.90	1.4606	1	63.66
125	1.4667	<1	63.36	1.4516	<1	64.10	1.4360	<1	64.80
440	1.4201	6	65.70	1.4053	6	66.48	1.3905	6	67.28
433	1.3779	<1	67.98	1.3634	<1	68.80	1.3490	<1	69.64
531 +	1.3579	12	69.12	1.3436	12	69.96	1.3294	12	70.82

Barium strontium nitrate, $Ba(NO_3)_2$-$Sr(NO_3)_2$ - continued

	$Ba_{.75}Sr_{.25}(NO_3)_2$			$Ba_{.5}Sr_{.5}(NO_3)_2$			$Ba_{.25}Sr_{.75}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598			λ=1.540598	
442 +	1.3390	6	70.24	1.3249	5	71.10	1.3108	5	71.98
610	1.3207	<1	71.36	1.3071	<1	72.22	1.2932	<1	73.12
611 +	1.3033	<1	72.46	1.2895	<1	73.36	1.2758	<1	74.28
620 +	1.2703	3	74.66	1.2571	3	75.58	1.2437	3	76.54
621	1.2548	<1	75.74	1.2415	<1	76.70	1.2285	<1	77.66
533	1.2251	4	77.92	1.2123	4	78.90	1.1994	3	79.92
622	1.2113	4	78.98	1.1984	4	80.00	1.1858	4	81.02
542	1.1976	<1	80.06	1.1851	<1	81.08	1.1725	<1	82.14
136 +	1.1846	<1	81.12	1.1720	<1	82.18	1.1598	<1	83.24
444	1.1595	1	83.26	1.1474	1	84.34	1.1362	1	85.46
543	1.1361	--	85.38	1.1242	--	86.50	1.1123	<1	87.66
711 +	1.1251	4	86.42	1.1131	4	87.58	1.1013	4	88.76
640 +	1.1141	2	87.48	1.1025	2	88.64	1.0907	2	89.86
146	1.1035	<1	88.54	1.0920	<1	89.72	1.0804	<1	90.96
246 +	1.0736	4	91.70	1.0623	4	92.96	1.0510	4	94.26
137 +	1.0460	5	94.86	1.0349	5	96.20	1.0241	5	97.56
650	1.0287	--	96.98	1.0179	<1	98.36	1.0070	<1	99.80
651 +	1.0203	<1	98.04	1.0096	<1	99.46	0.9990	<1	100.90
800	1.0042	<1	100.18	0.9937	<1	101.64	.9832	<1	103.16
652 +	0.9966	<1	101.24	.9861	<1	102.74	.9751	<1	104.28
733	.9816	1	103.40	.9712	1	104.96	.9610	1	106.56
644 +	.9742	3	104.50	.9640	3	106.08	.9538	1	107.72
128 +	.9672	<1	105.58	.9570	<1	107.20	.9469	<1	108.88
822 +	.9468	2	108.90	.9369	2	110.60	.9270	2	112.40
831 +	.9339	<1	111.14	.9242	<1	112.92	.9144	<1	114.80
751 +	.9277	3	112.26	.9180	3	114.10	.9082	3	116.02
662	.9216	1	113.40	.9119	1	115.28	.9023	1	117.24
832 +	.9156	--	114.56	.9060	<1	116.48	.8964	<1	118.48
048 +	.8983	1	118.08	.8888	1	120.14	.8794	1	122.32
753 +	.8818	4	121.74	.8726	4	123.96	.8634	4	126.30
842 +	.8766	2	122.98	.8674	2	125.26	.8582	2	127.68
664	.8565	1	128.16	.8475	1	130.72	.8384	1	133.48
931 +	.8422	2	132.30	.8333	2	135.14	.8246	2	138.20
844	.8200	1	139.90	.8114	1	143.38	.8028	1	147.30
933 +	.8075	4	145.10	.7990	4	149.20	.7905	4	154.02
068 +	.8034	1	146.98	.7950	1	151.38	.7866	1	156.66
10·1·0 +	.7994	<1	148.98	.7910	<1	153.70	.7827	<1	159.60
862 +	.7878	4	155.80						
Lattice constant	8.0341Å			7.9498Å			7.8656Å		
Density (calc.)	3.188 g/cm³			3.126 g/cm³			3.058 g/cm³		

Calcium lead nitrate, $Ca(NO_3)_2$-$Pb(NO_3)_2$, calculated solid solution series

Structure

Cubic, $P2_13$ (198), Z = 4. The structures of $Ca(NO_3)_2$ and $Pb(NO_3)_2$ were determined respectively by Vergard and Bilberg [1931] and Hamilton [1957]. The space group was given as Pa3. However, later work by Birnstock [1967] on the isomorph $Ba(NO_3)_2$ indicated that the space group is $P2_13$. In the present calculated patterns, the atomic positions have been modified for the change in space group. The system $Ca(NO_3)_2$-$Pb(NO_3)_2$ forms a complete solid solution series [Laybourn et al., 1934].

Lattice constants

The constants were derived by interpolation on a molar ratio using the following: for $Ca(NO_3)_2$, a = 7.6005Å [Swanson et al., 1957]; for $Pb(NO_3)_2$, a = 7.8573 [Swanson et al., 1955]. Both constants were modified to conform to new wavelength measurements.

Thermal parameters

Isotropic: calcium B = 1.0; lead B = 1.0; nitrogen B = 1.2; oxygen B = 1.2.

Scattering factors

Ca^{2+}, N^0, O^- [International Tables, 1962].
Pb^{2+} [Cromer and Waber, 1965].
The factors used were proportional to the molar ratio, assuming random distribution of the cations.

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	$Ca_{.67}Pb_{.33}(NO_3)_2$			$Ca_{.33}Pb_{.67}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598	
111	4.436	100	20.00	4.485	100	19.78
200	3.841	15	23.14	3.887	31	22.86
210	3.437	19	25.90	3.477	8	25.60
211	3.138	14	28.42	3.173	6	28.10
220	2.717	23	32.94	2.748	30	32.56
221	2.561	2	35.00	2.590	<1	34.60
311	2.317	63	38.84	2.344	66	38.38
222	2.218	46	40.64	2.244	35	40.16
321 +	2.054	1	44.06	2.077	<1	43.54
400	1.921	14	47.28	1.944	11	46.70
410	1.864	<1	48.82	1.885	<1	48.24
411	1.811	2	50.34	1.832	1	49.72
331	1.763	14	51.82	1.783	16	51.18
024 +	1.718	13	53.26	1.738	15	52.62
124	1.677	<1	54.68	1.696	<1	54.02
332	1.639	<1	56.08	1.657	<1	55.40
422	1.569	8	58.82	1.586	10	58.10
430	1.537	<1	60.16	1.555	--	59.40
134 +	1.507	<1	61.48	1.524	<1	60.70
511 +	1.4789	11	62.78	1.4956	11	62.00

Calcium lead nitrate, $Ca(NO_3)_2$-$Pb(NO_3)_2$, calculated solid solution series - continued

	$Ca_{.67}Pb_{.33}(NO_3)_2$			$Ca_{.33}Pb_{.67}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598	
432	1.4270	1	65.34	1.4432	<1	64.52
125	1.4030	<1	66.60	1.4189	--	65.76
440	1.3586	6	69.08	1.3740	6	68.20
433	1.3181	<1	71.52	1.3330	<1	70.60
531 +	1.2990	11	72.74	1.3137	12	71.80
442 +	1.2808	5	73.94	1.2953	5	72.98
610	1.2633	<1	75.14	1.2779	--	74.14
235 +	1.2467	<1	76.32	1.2608	<1	75.32
620 +	1.2151	2	78.68	1.2291	3	77.62
621	1.2001	<1	79.86	1.2138	--	78.78
533	1.1720	3	82.18	1.1854	4	81.06
622	1.1586	4	83.34	1.1718	4	82.20
542	1.1457	<1	84.50	1.1586	<1	83.34
136 +	1.1331	<1	85.66	1.1461	--	84.46
444	1.1093	1	87.96	1.1219	1	86.72
543	1.0869	<1	90.26	1.0992	--	88.98
711 +	1.0761	4	91.42	1.0884	4	90.10
640 +	1.0658	2	92.56	1.0780	2	91.22
146	1.0557	<1	93.72	1.0676	<1	92.36
246 +	1.0269	3	97.20	1.0387	4	95.74
137 +	1.0006	5	100.68	1.0120	6	99.14
650	0.9840	<1	103.04	0.9951	--	101.44
156	.9761	<1	104.22	.9872	--	102.58
800	.9606	<1	106.62	.9716	<1	104.90
652 +	.9532	<1	107.82	.9640	--	106.08
733	.9389	1	110.26	.9496	1	108.42
644 +	.9320	3	111.48	.9426	3	109.62
247 +	.9252	<1	112.72	.9357	--	110.82
822 +	.9057	2	116.54	.9160	2	114.48
831 +	.8934	<1	119.14	.9035	<1	116.98
751 +	.8874	3	120.46	.8975	3	118.24
662	.8816	1	121.80	.8915	1	119.54
832 +	.8758	<1	123.18	.8857	--	120.84
048	.8592	1	127.40	.8690	1	124.86
753 +	.8436	4	131.88	.8532	4	129.08
842 +	.8385	2	133.46	.8481	2	130.54
664	.8193	1	140.18	.8285	1	136.78
931 +	.8056	2	145.94	.8148	3	141.96
844	.7844	1	158.26	.7933	1	152.34
Lattice constant	7.6852Å			7.7726Å		
Density (calc.)	3.208 g/cm^3			3.905 g/cm^3		

Calcium strontium nitrate, $Ca(NO_3)_2$-$Sr(NO_3)_2$, calculated solid solution series

Structure

Cubic, $P2_13$ (198), Z = 4. The structures of both $Ca(NO_3)_2$ and $Sr(NO_3)_2$ were determined by Vegard and Bilberg [1931], and the space group was given as Pa3. However, later work by Birnstock [1967] on the isomorph $Ba(NO_3)_2$ indicated that the space group is $P2_13$. The atomic positions given by Vegard and Bilberg have been modified here for the change in space group. The system $Ca(NO_3)_2$-$Sr(NO_3)_2$ forms a complete solid solution series [Protsenko and Belova, 1957].

Lattice constants

The constants were derived by interpolation on a molar ratio using the following: for $Sr(NO_3)_2$, a = 7.7813Å [McMurdie et al, 1974] and for $Ca(NO_3)_2$, a = 7.6005Å [Swanson et al., 1957, modified to conform to new wavelength measurements].

Thermal parameters

Isotropic: calcium B = 1.0, strontium B = 1.0, nitrogen B = 1.2, oxygen B = 1.2.

Scattering factors

Ca^{2+}, N^0, O^{-1} [International Tables, 1962].
Sr^{2+} [Cromer and Waber, 1965].
The factors used were proportional to the molar ratio, assuming random distribution of the cations.

References

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	$Ca_{.67}Sr_{.33}(NO_3)_2$			$Ca_{.33}Sr_{.67}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598	
111	4.423	100	20.06	4.458	100	19.90
200	3.831	2	23.20	3.860	7	23.02
210	3.424	49	26.00	3.453	35	25.78
211	3.127	38	28.52	3.153	22	28.28
220	2.709	14	33.04	2.730	20	32.78
221	2.553	10	35.12	2.574	5	34.82
311	2.310	68	38.96	2.328	66	38.64
222	2.211	74	40.78	2.229	58	40.44
321 +	2.047	2	44.20	2.063	2	43.84
400	1.915	22	47.44	1.930	18	47.04
410	1.858	--	49.00	1.873	<1	48.58
411	1.806	6	50.50	1.820	4	50.08
331	1.757	11	52.00	1.771	12	51.56
024 +	1.713	11	53.46	1.726	12	53.00
124	1.672	<1	54.88	1.685	<1	54.40
332	1.633	1	56.28	1.646	<1	55.80
422	1.564	5	59.02	1.576	6	58.52
430	1.532	1	60.38	1.544	1	59.84
134 +	1.502	1	61.70	1.514	1	61.16
511 +	1.4743	11	63.00	1.4861	11	62.44

Calcium strontium nitrate, $Ca(NO_3)_2$-$Sr(NO_3)_2$, calculated solid solution series - continued

	$Ca_{.67}Sr_{.33}(NO_3)_2$			$Ca_{.33}Sr_{.67}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598	
432	1.4224	2	65.58	1.4340	1	64.98
125	1.3986	<1	66.84	1.4098	<1	66.24
440	1.3541	8	69.34	1.3648	7	68.72
522 +	1.3334	<1	70.58	1.3443	<1	69.92
433	1.3137	1	71.80	1.3242	1	71.14
531 +	1.2947	10	73.02	1.3052	11	72.34
442 +	1.2767	3	74.22	1.2868	4	73.54
610	1.2593	<1	75.42	1.2694	<1	74.72
235 +	1.2426	1	76.62	1.2526	1	75.90
620 +	1.2113	2	78.98	1.2209	2	78.24
126 +	1.1964	1	80.16	1.2059	<1	79.40
541 +	1.1820	<1	81.34	1.1914	<1	80.56
533	1.1683	2	82.50	1.1774	3	81.72
622	1.1548	5	83.68	1.1641	5	82.86
542 +	1.1419	<1	84.84	1.1510	<1	84.02
136 +	1.1295	1	86.00	1.1385	<1	85.16
444	1.1057	1	88.32	1.1145	1	87.44
543	1.0833	<1	90.64	1.0920	<1	89.72
711 +	1.0727	3	91.80	1.0813	3	90.86
640 +	1.0623	1	92.96	1.0708	1	92.00
146 +	1.0522	<1	94.12	1.0607	<1	93.14
633	1.0425	<1	95.28	1.0509	<1	94.28
246 +	1.0236	3	97.62	1.0319	3	96.58
544	1.0147	<1	98.78	1.0228	<1	97.72
137 +	0.9973	5	101.14	1.0053	5	100.04
650	.9807	<1	103.52	0.9887	<1	102.36
156 +	.9729	<1	104.70	.9806	<1	103.54
800	.9575	<1	107.12	.9652	<1	105.90
652 +	.9501	1	108.34	.9578	1	107.08
147	.9429	<1	109.56	.9505	<1	108.28
733	.9358	1	110.80	.9434	1	109.48
028 +	.9289	3	112.04	.9364	3	110.70
247 +	.9222	1	113.30	.9296	<1	111.92
822 +	.9028	2	117.14	.9100	2	115.66
830	.8966	<1	118.44	.9037	--	116.94
831 +	.8905	1	119.78	.8976	<1	118.22
751 +	.8845	3	121.12	.8916	3	119.52
662	.8787	1	122.48	.8857	1	120.84
832 +	.8730	1	123.86	.8800	<1	122.18
048 +	.8565	1	128.16	.8633	1	126.32
744 +	.8511	<1	129.66	.8580	<1	127.74
753 +	.8408	4	132.74	.8475	4	130.70
842 +	.8358	2	134.34	.8425	2	132.22
761 +	.8260	<1	137.66	.8326	<1	135.38
664	.8166	1	141.24	.8231	1	138.72
922 +	.8120	<1	143.12	.8185	<1	140.48
158	.8075	<1	145.10	.8139	<1	142.32
931 +	.8030	2	147.18	.8094	2	144.22
844				.7881	1	155.62
Lattice constant	7.6602Å			7.7216Å		
Density (calc.)	2.657 g/cm³			2.827 g/cm³		

Gallium magnesium, Ga_2Mg

Structure
Orthorhombic, Pbam (55), Z=8. The structure was determined by Smith, Mucker, Johnson and Wood [1969].

Lattice constants: [ibid.]

a = 6.802(13)Å
b = 16.347(33)
(published value: b = 16.346)
c = 4.111(8)

Density
(calculated) 4.76 g/cm^3 [ibid.]

Thermal parameters
Isotropic [Smith et. al., 1969]

Scattering factors
Ga^0, Mg^0[International Tables, 1962], corrected for dispersion [Cromer, 1965].

Scale factor
(integrated intensities) 8.184×10^4

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Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.17	1	0 2 0	10.82
6.28	6	1 1 0	14.10
5.23	7	1 2 0	16.94
4.25	1	1 3 0	20.88
4.11	31	0 0 1	21.60
3.67	25	0 2 1	24.22
3.50	52	1 4 0	25.40
3.44	39	1 1 1	25.88
3.40	10	2 0 0	26.18
3.33	5	2 1 0	26.76
3.23	3	1 2 1	27.58
3.14	4	2 2 0	28.40
2.96	17	1 3 1	30.22
2.95	16	1 5 0	30.30
2.90	5	0 4 1	30.82
2.73	1	0 6 0	32.84
2.67	42	1 4 1	33.58
2.62	17	2 0 1	34.20
2.61	16	2 4 0	34.28
2.53	6	1 6 0	35.46
2.50	26	2 2 1	35.96
2.36	100	2 3 1	38.08
2.27	30	0 6 1	39.66
2.25	13	3 1 0	40.12
2.21	9	1 7 0 +	40.82
2.15	1	1 6 1	41.90
2.13	9	2 6 0	42.48
2.09	3	3 3 0	43.18
2.06	49	0 0 2	44.02
2.04	44	2 5 1 +	44.28
1.983	32	3 4 0	45.72
1.971	13	3 1 1	46.02
1.946	36	1 7 1	46.64
1.929	17	3 2 1	47.06
1.889	10	2 6 1	48.14
1.865	1	3 3 1	48.78
1.836	1	0 4 2	49.60
1.830	2	0 8 1	49.80
1.786	2	3 4 1	51.10
1.773	11	1 4 2	51.50
1.759	2	2 0 2	51.94
1.755	3	1 9 0	52.08
1.750	2	2 1 2	52.24
1.720	1	2 2 2	53.22
1.700	2	4 0 0	53.88
1.692	1	4 1 0	54.18
1.686	2	1 5 2	54.38
1.665	2	4 2 0	55.12
1.635	1	0 10 0	56.22
1.616	2	2 4 2	56.94
1.614	2	1 9 1	57.00
1.602	4	2 9 0	57.48
1.595	2	1 6 2	57.74
1.516	5	3 1 2	61.06
1.509	3	4 5 0	61.40
1.505	5	1 7 2	61.58
1.478	4	2 6 2	62.82
1.467	3	3 3 2 +	63.36
1.449	11	0 8 2	64.22
1.443	3	4 6 0	64.54
1.427	16	3 4 2	65.34
1.417	2	3 9 0	65.84
1.370	1	0 0 3	68.40
1.351	1	0 2 3	69.50
1.340	6	3 9 1 +	70.18
1.336	5	1 12 0 +	70.42
1.320	2	5 3 0	71.40
1.310	2	4 0 2	72.02
1.307	4	4 8 0 +	72.22
1.304	3	1 3 3	72.42

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
1.293	11	2	11	1	+	73.16
1.287	6	5	1	1		73.50
1.279	1	0	10	2		74.04
1.276	6	5	2	1	+	74.28
1.272	3	2	0	3		74.52
1.264	3	2	9	2		75.12
1.262	4	3	10	1		75.24
1.256	4	5	3	1	+	75.64
1.241	1	4	9	0		76.72
1.238	7	2	3	3	+	76.98
1.224	2	0	6	3		77.98
1.216	2	4	5	2		78.60
1.188	1	4	9	1		80.82
1.185	3	2	5	3	+	81.12
1.181	3	4	6	2		81.42
1.176	1	5	7	0		81.88
1.170	2	3	1	3		82.38
1.167	3	3	12	0	+	82.60
1.164	5	1	7	3		82.84
1.161	3	3	2	3		83.12
1.152	1	2	6	3		83.94
1.134	2	2	13	1	+	85.60
1.130	3	5	7	1		85.92
1.124	2	5	2	2		86.56
1.120	2	1	12	2		86.90
1.111	1	5	3	2		87.82
1.103	3	4	8	2		88.60
1.083	1	6	2	1		90.66
1.072	1	5	5	2		91.90
1.063	1	4	9	2		92.92
1.060	2	1	13	2		93.26
1.053	1	5	9	1		94.08
1.041	3	1	15	1		95.46
1.037	2	6	5	1		96.00
1.029	1	4	12	1		96.90
1.028	2	0	0	4		97.10
1.020	1	5	7	2		98.04
1.015	2	3	12	2	+	98.70
1.013	1	5	10	1		99.02
.986	1	1	4	4		102.74
.985	2	3	9	3		102.86
.966	3	2	11	3		105.78
.964	3	5	1	3		106.14
.959	1	5	2	3		106.92
.957	1	7	3	0		107.28
.953	1	3	10	3		107.86
.952	1	2	16	1		108.04
.951	1	5	3	3		108.26
.937	1	5	12	1		110.54
.935	1	3	1	4		111.02

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
8.17	1	0	2	0	10.82
6.28	5	1	1	0	14.09
5.23	5	1	2	0	16.94
4.25	1	1	3	0	20.87
4.11	25	0	0	1	21.60
4.09	5	0	4	0	21.73
3.67	22	0	2	1	24.21
3.50	47	1	4	0	25.41
3.44	34	1	1	1	25.88
3.40	8	2	0	0	26.18
3.33	5	2	1	0	26.75
3.23	3	1	2	1	27.58
3.14	4	2	2	0	28.40
2.96	15	1	3	1	30.21
2.95	7	1	5	0	30.31
2.90	5	0	4	1	30.83
2.72	1	0	6	0	32.85
2.67	40	1	4	1	33.58
2.62	16	2	0	1	34.19
2.61	6	2	4	0	34.27
2.53	5	1	6	0	35.46
2.50	25	2	2	1	35.96
2.36	100	2	3	1	38.07
2.27	30	0	6	1	39.65
2.25	13	3	1	0	40.12
2.21	8	1	7	0	40.82
2.21	2	2	4	1	40.88
2.15	1	1	6	1	41.90
2.13	10	2	6	0	42.48
2.09	3	3	3	0	43.18
2.06	49	0	0	2	44.02
2.04	26	2	5	1	44.26
2.04	24	0	8	0	44.29
1.983	34	3	4	0	45.73
1.971	12	3	1	1	46.01
1.946	39	1	7	1	46.64
1.929	17	3	2	1	47.06
1.889	10	2	6	1	48.14
1.865	1	3	3	1	48.78
1.836	1	0	4	2	49.60
1.830	2	0	8	1	49.79
1.786	2	3	4	1	51.11
1.773	12	1	4	2	51.51
1.759	2	2	0	2	51.94
1.755	2	1	9	0	52.07
1.749	1	2	1	2	52.26
1.720	1	2	2	2	53.22
1.700	3	4	0	0	53.87
1.691	1	4	1	0	54.18
1.686	2	1	5	2	54.38

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.665	3	4 2 0	55.12
1.635	1	0 10 0	56.23
1.616	2	2 4 2	56.94
1.614	1	1 9 1	57.02
1.605	2	3 6 1	57.38
1.602	4	2 9 0	57.47
1.595	2	1 6 2	57.75
1.516	6	3 1 2	61.06
1.509	3	4 5 0	61.41
1.505	4	1 7 2	61.58
1.478	5	2 6 2	62.83
1.467	2	4 4 1	63.36
1.467	2	3 3 2	63.36
1.449	14	0 8 2	64.22
1.443	3	4 6 0	64.55
1.427	20	3 4 2	65.34
1.418	2	3 9 0	65.83
1.370	1	0 0 3	68.41
1.351	1	0 2 3	69.50
1.342	2	5 2 0	70.06
1.340	7	3 9 1	70.17
1.339	2	1 1 3	70.25
1.336	3	1 12 0	70.44
1.335	1	1 9 2	70.50
1.320	2	5 3 0	71.41
1.310	2	4 0 2	72.02
1.307	4	4 8 0	72.22
1.306	1	4 1 2	72.28
1.304	1	1 3 3	72.40
1.294	2	4 2 2	73.08
1.293	14	2 11 1	73.15
1.288	6	5 1 1	73.49
1.279	1	0 10 2	74.04
1.276	3	1 4 3	74.26
1.276	5	5 2 1	74.29
1.271	1	2 0 3	74.61
1.264	3	2 9 2	75.12
1.262	4	3 10 1	75.24
1.257	2	5 3 1	75.61
1.256	1	5 5 0	75.66
1.256	2	2 2 3	75.66
1.241	1	4 9 0	76.71
1.238	9	2 3 3	76.97
1.237	2	1 13 0	77.07
1.224	3	0 6 3	77.99
1.216	2	4 5 2	78.60
1.188	1	4 9 1	80.81
1.185	3	2 5 3	81.12
1.184	2	1 13 1	81.16
1.181	3	4 6 2	81.44

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.175	1	5 7 0	81.88
1.170	2	3 1 3	82.37
1.168	2	3 12 0	82.55
1.168	1	0 14 0	82.55
1.167	2	3 9 2	82.61
1.164	5	1 7 3	82.83
1.161	2	3 2 3	83.14
1.152	2	2 6 3	83.94
1.134	2	2 13 1	85.60
1.133	1	4 10 1	85.68
1.130	3	5 7 1	85.93
1.124	2	5 2 2	86.55
1.120	3	1 12 2	86.91
1.111	2	5 3 2	87.83
1.103	5	4 8 2	88.60
1.083	2	6 2 1	90.65
1.072	2	5 5 2	91.90
1.063	1	4 9 2	92.92
1.060	3	1 13 2	93.27
1.053	2	5 9 1	94.08
1.041	4	1 15 1	95.46
1.036	3	6 5 1	96.01
1.029	1	4 12 1	96.90
1.028	4	0 0 4	97.09
1.020	1	5 7 2	98.03
1.015	2	3 12 2	98.70
1.015	1	0 14 2	98.70
1.013	1	5 10 1	98.95
.991	1	6 1 2	102.05
.986	1	1 4 4	102.72
.985	3	3 9 3	102.86
.970	1	3 13 2	105.20
.966	5	2 11 3	105.78
.964	2	5 1 3	106.12
.959	2	5 2 3	106.92
.957	1	7 3 0	107.26
.953	2	3 10 3	107.87
.952	1	2 16 1	108.04
.951	1	5 3 3	108.25
.937	1	5 12 1	110.55
.935	1	3 1 4	111.03
.932	1	1 7 4	111.52

Gallium magnesium, Ga_5Mg_2

Structure
Tetragonal, I4/mmm (139), Z = 4. The structure was determined by Smith, Johnson and Wood [1969].

Lattice constants: [ibid.]

a = 8.627(26)Å
c = 7.111(21)

Density
(calculated) 4.98 g/cm^3 [ibid.]

Thermal parameters
Isotropic [Smith et. al., 1969].

Scattering factors
Ga^0, Mg^0[International Tables, 1962], corrected for dispersion [Cromer, 1965].

Scale factor
(integrated intensities) 11.81 x 10^4

References

Cromer, D. T. (1965). Acta Cryst. 18, 17.
International Tables for X-ray Crystallography III (1962), 202.
Smith, G. S., Johnson, Q. and Wood, D.H. (1969). Acta Cryst. B25, 554.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
6.10	1	1	1	0	14.52
5.49	2	1	0	1	16.14
4.31	18	2	0	0	20.58
3.56	66	0	0	2	25.02
3.39	62	2	1	1	26.26
3.05	37	2	2	0	29.26
2.74	47	2	0	2	32.62
2.73	55	3	1	0	32.80
2.67	47	3	0	1	33.60
2.31	26	2	2	2	38.88
2.29	7	1	0	3	39.40
2.27	9	3	2	1	39.72
2.16	44	3	1	2	41.70
2.16	63	4	0	0	41.84
2.03	61	3	3	0	44.52
2.02	100	2	1	3	44.84
1.84	22	4	0	2	49.38
1.83	18	3	0	3	49.82
1.77	19	3	3	2	51.74
1.71	2	1	1	4	53.66
1.69	6	5	1	0	54.16
1.68	6	4	3	1 +	54.70
1.57	1	4	1	3	58.82
1.56	6	5	2	1	59.06
1.54	4	2	2	4	60.20
1.53	4	5	1	2	60.56
1.52	6	4	4	0	60.68
1.44	8	6	0	0	64.78
1.402	3	4	4	2	66.68
1.395	4	4	3	3	67.04
1.366	3	5	3	2	68.66
1.334	14	2	1	5 +	70.52
1.327	37	5	2	3	70.96
1.324	22	5	4	1	71.16
1.275	4	3	0	5	74.34
1.266	1	6	3	1	74.98
1.226	2	5	1	4	77.88
1.222	3	3	2	5	78.12
1.220	4	7	1	0 +	78.30
1.217	3	6	1	3	78.54
1.214	2	7	0	1	78.74
1.196	3	6	4	0	80.16
1.185	2	0	0	6	81.08
1.176	1	4	1	5	81.82
1.171	3	5	4	3	82.24
1.154	5	7	1	2 +	83.76
1.133	9	7	3	0 +	85.68
1.130	5	6	3	3	85.94
1.105	2	2	2	6	88.42
1.097	2	4	3	5 +	89.16
1.093	2	7	0	3	89.58
1.091	1	6	5	1	89.84
1.079	4	7	3	2	91.08
1.064	7	5	2	5	92.82
1.058	1	8	1	1 +	93.44
1.046	1	8	2	0	94.84
1.039	1	4	0	6	95.74
1.032	1	8	0	2	96.56
1.024	2	3	3	6	97.58
1.006	1	5	5	4	99.94
1.004	2	8	2	2 +	100.26
1.001	2	6	5	3	100.60
.982	1	2	1	7	103.28
.978	2	5	4	5 +	103.92
.975	5	8	1	3 +	104.34
.971	2	5	1	6	105.04
.931	1	7	0	5	111.60
.928	1	9	2	1	112.26
.915	1	6	0	6	114.76
.881	1	9	3	2	121.94

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
6.10	1	1 1 0	14.51
5.49	1	1 0 1	16.14
4.31	14	2 0 0	20.57
3.56	56	0 0 2	25.02
3.39	53	2 1 1	26.26
3.05	33	2 2 0	29.26
2.74	42	2 0 2	32.61
2.73	47	3 1 0	32.80
2.67	45	3 0 1	33.59
2.31	26	2 2 2	38.87
2.29	7	1 0 3	39.39
2.27	9	3 2 1	39.71
2.16	40	3 1 2	41.70
2.16	54	4 0 0	41.85
2.03	61	3 3 0	44.52
2.02	100	2 1 3	44.84
2.01	1	4 1 1	45.13
1.84	24	4 0 2	49.38
1.83	20	3 0 3	49.81
1.77	21	3 3 2	51.75
1.71	2	1 1 4	53.66
1.70	1	4 2 2	54.04
1.69	6	5 1 0	54.17
1.68	2	5 0 1	54.70
1.68	5	4 3 1	54.70
1.57	1	4 1 3	58.82
1.56	6	5 2 1	59.06
1.54	5	2 2 4	60.20
1.53	4	5 1 2	60.56
1.53	6	4 4 0	60.68
1.44	10	6 0 0	64.79
1.402	4	4 4 2	66.68
1.395	5	4 3 3	67.04
1.366	3	5 3 2	68.65
1.334	15	2 1 5	70.52
1.333	6	6 0 2	70.60
1.327	49	5 2 3	70.95
1.324	2	5 4 1	71.17
1.275	6	3 0 5	74.35
1.266	1	6 3 1	74.99
1.226	2	5 1 4	77.88
1.223	3	3 2 5	78.11
1.220	3	7 1 0	78.30
1.220	2	5 5 0	78.30
1.217	1	6 1 3	78.53
1.214	3	7 0 1	78.74
1.196	4	6 4 0	80.16
1.185	3	0 0 6	81.08
1.176	1	4 1 5	81.82
1.171	4	5 4 3	82.24
1.163	1	1 1 6	82.92
1.154	4	7 1 2	83.75
1.154	3	5 5 2	83.75
1.134	3	6 4 2	85.59
1.133	13	7 3 0	85.69
1.130	2	6 3 3	85.91
1.105	3	2 2 6	88.42
1.097	1	5 0 5	89.16
1.097	1	4 3 5	89.16
1.093	3	7 0 3	89.57
1.091	1	6 5 1	89.78
1.079	6	7 3 2	91.07
1.064	11	5 2 5	92.82
1.058	1	8 1 1	93.43
1.058	1	7 4 1	93.43
1.046	1	8 2 0	94.83
1.039	2	4 0 6	95.74
1.032	1	8 0 2	96.57
1.024	4	3 3 6	97.58
1.017	1	6 6 0	98.51
1.010	1	4 2 6	99.43
1.006	1	5 5 4	99.95
1.004	1	6 1 5	100.18
1.004	2	8 2 2	100.26
1.001	3	6 5 3	100.60
.982	1	2 1 7	103.28
.978	3	5 4 5	103.91
.978	1	6 6 2	104.00
.975	2	7 4 3	104.34
.975	6	8 1 3	104.34
.971	3	5 1 6	105.04
.965	1	7 5 2	105.89
.931	2	7 0 5	111.59
.928	1	9 2 1	112.26
.915	2	6 0 6	114.76
.910	1	7 2 5	115.58
.909	1	9 3 0	115.79
.907	1	8 5 1	116.27
.902	1	8 2 4	117.37
.895	1	6 2 6	118.86
.889	1	0 0 8	120.13
.881	1	9 3 2	121.93
.872	3	6 5 5	124.01
.871	4	7 7 0	124.24
.870	6	9 2 3	124.51
.870	1	7 6 3	124.51
.863	5	10 0 0	126.48
.858	2	5 2 7	127.76
.855	1	7 4 5	128.55
.855	4	8 1 5	128.55

Lead strontium nitrate, $Pb(NO_3)_2$-$Sr(NO_3)_2$, calculated solid solution series

Structure

Cubic, $P2_13$ (198), Z=4. The structures of $Pb(NO_3)_2$ and $Sr(NO_3)_2$ were determined by Vegard [1922]. He found them to be isostructural with each other and with $Ba(NO_3)_2$ and $Ca(NO_3)_2$. Hamilton [1957] refined the structure of $Pb(NO_3)_2$. These earlier studies all assumed the space group to be Pa3 (205). However, Birnstock [1967] used neutron diffraction methods to refine the structure of $Ba(NO_3)_2$ and found weak reflections not permitted by Pa3. He assigned the space group $P2_13$ which we used here. The atom positions for $Sr(NO_3)_2$ used in these calculations were those given by Vegard and Bilberg [1931]; the $Pb(NO_3)_2$ positions were from Hamilton [1957]. The system $Pb(NO_3)_2$-$Sr(NO_3)_2$ forms a complete solid solution series [Laybourn et al., 1934].

Lattice constants

The constants were derived by interpolation on a molar ratio using the following: for $Pb(NO_3)_2$, a = 7.8573 [Swanson et al., 1955], modified to conform to new wavelength measurements; for $Sr(NO_3)_2$, a = 7.7813 [McMurdie et al., 1974].

Thermal parameters

Isotropic: barium B = .93; strontium B = 1.0; nitrogen B = 1.2; oxygen B = 1.16.

Scattering factors

N^0, O^- [International Tables, 1962].
Pb^{2+}, Sr^{2+} [Cromer and Waber, 1965].
The factors used were proportional to the molar ratio, assuming random distribution of the cations.

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	$Pb_{.67}Sr_{.33}(NO_3)_2$			$Pb_{.33}Sr_{.67}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598	
111	4.521	100	19.62	4.507	100	19.68
200	3.914	31	22.70	3.904	24	22.76
210	3.501	7	25.42	3.490	12	25.50
211	3.198	5	27.88	3.186	8	27.98
220	2.769	29	32.30	2.759	27	32.42
221	2.611	--	34.32	2.602	1	34.44
311	2.361	62	38.08	2.354	62	38.20
222	2.261	32	39.84	2.253	38	39.98
123 +	2.093	<1	43.18	2.086	<1	43.34
400	1.958	11	46.34	1.951	12	46.50
410	1.900	<1	47.84	1.893	<1	48.02
411	1.846	1	49.32	1.840	1	49.50
331	1.796	15	50.78	1.791	14	50.96
024 +	1.752	14	52.18	1.745	14	52.38
124	1.709	<1	53.58	1.704	<1	53.76
332	1.670	<1	54.94	1.664	<1	55.14
422	1.599	10	57.60	1.593	9	57.82
430	1.567	--	58.90	1.561	<1	59.12
134 +	1.536	<1	60.20	1.531	<1	60.42
511 +	1.508	11	61.46	1.502	11	61.70

Lead strontium nitrate, $Pb(NO_3)_2$-$Sr(NO_3)_2$, calculated solid solution series - continued

	$Pb_{.67}Sr_{.33}(NO_3)_2$			$Pb_{.33}Sr_{.67}(NO_3)_2$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
		λ=1.540598			λ=1.540598	
432	1.4544	<1	63.96	1.4496	<1	64.20
440	1.3847	5	67.60	1.3800	6	67.86
433	1.3433	<1	69.98	1.3386	<1	70.26
531 +	1.3239	12	71.16	1.3194	11	71.44
442 +	1.3055	5	72.32	1.3012	5	72.60
610	1.2877	--	73.48	1.2832	<1	73.78
611 +	1.2706	<1	74.64	1.2662	<1	74.94
620 +	1.2385	3	76.92	1.2344	3	77.22
533	1.1944	4	80.32	1.1905	4	80.64
622	1.1808	4	81.44	1.1770	4	81.76
542	1.1676	--	82.56	1.1637	<1	82.90
136	1.1548	--	83.68	1.1510	<1	84.02
444	1.1305	1	85.90	1.1267	1	86.26
711 +	1.0967	4	89.24	1.0932	4	89.60
640 +	1.0861	2	90.34	1.0826	2	90.72
146	1.0757	<1	91.46	1.0723	<1	91.84
246 +	1.0466	4	94.78	1.0431	4	95.20
553 +	1.0197	5	98.12	1.0164	5	98.56
800	0.9790	<1	103.78	0.9758	<1	104.26
733	.9569	1	107.22	.9537	1	107.74
644 +	.9497	3	108.40	.9467	3	108.92
128	.9429	--	109.56	.9398	<1	110.10
822 +	.9230	2	113.14	.9200	2	113.70
831	.9105	--	115.56	.9074	<1	116.18
751 +	.9044	3	116.80	.9014	3	117.42
662	.8984	1	118.06	.8955	1	118.68
832	.8925	--	119.32	.8896	<1	119.96
048 +	.8757	1	123.20	.8727	1	123.92
753 +	.8597	4	127.28	.8569	4	128.04
842 +	.8546	2	128.68	.8517	2	129.48
664	.8349	1	134.62	.8322	1	135.54
931 +	.8210	2	139.50	.8183	2	140.54
844	.7994	1	149.00	.7967	1	150.40
933 +	.7872	4	156.24	.7846	4	158.10
068 +	.7832	2	159.16			
Lattice constant	7.8322Å			7.8064Å		
Density (calc.)	4.033 g/cm^3			3.506 g/cm^3		

Lithium silver bromide, LiBr-AgBr, calculated solid solution series

Structure

Cubic, Fm3m (225), Z = 4, isostructural with NaCl. The system LiBr-AgBr forms a complete solid solution series [Sandonnini and Scarpa, 1913].

Lattice constants

The constants were derived by interpolation on a molar ratio, using the cell dimensions of LiBr (a = 5.5016Å) and AgBr (a = 5.7749Å). Those dimensions were determined by Swanson et al. [1955] and are modified to conform to new wavelength measurements.

Thermal parameters

Isotropic. Overall B = 1.6

Scattering factors

Li^+, Ag^+, Br^- [International Tables, 1962].

Random distribution of the cations was assumed, and the factors used were proportional to the molar ratio.

References

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	$Li_{.8}Ag_{.2}Br$			$Li_{.6}Ag_{.4}Br$			$Li_{.4}Ag_{.6}Br$			$Li_{.2}Ag_{.8}Br$		
hkℓ	d(Å)	I	2θ(°) λ=1.540598	d(Å)	I	2θ(°) λ=1.540598	d(Å)	I	2θ(°) λ=1.540598	d(Å)	I	2θ(°) λ=1.540598
111	3.209	53	27.78	3.238	16	27.52	3.271	2	27.24	3.302	--	26.98
200	2.778	100	32.20	2.805	100	31.88	2.833	100	31.56	2.861	100	31.24
220	1.9642	55	46.18	1.9837	58	45.70	2.003	55	45.24	2.022	60	44.78
311	1.6755	15	54.74	1.6915	4	54.18	1.7084	--	53.60	1.7246	--	53.06
222	1.6040	16	57.40	1.6196	16	56.80	1.6354	16	56.20	1.6511	17	55.62
400	1.3890	6	67.36	1.4027	6	66.62	1.4162	6	65.90	1.4301	6	65.18
331	1.2747	4	74.36	1.2871	1	73.52	1.2999	--	72.68	1.3124	--	71.88
420	1.2423	13	76.64	1.2545	14	75.76	1.2668	14	74.90	1.2791	15	74.06
422	1.1342	9	85.56	1.1454	9	84.52	1.1566	9	83.52	1.1676	9	82.56
511 +	1.0692	2	92.18	1.0798	1	91.02	1.0903	--	89.90	1.1010	--	88.80
440	0.9822	2	103.30	0.9919	2	101.90	1.0016	2	100.54	1.0112	2	99.24
531	.9392	2	110.20	.9484	1	108.62	0.9576	--	107.10	0.9669	--	105.62
600 +	.9260	5	112.58	.9351	5	110.92	.9443	5	109.32	.9534	5	107.80
620	.8785	3	122.52	.8871	3	120.52	.8959	3	118.60	.9045	3	116.78
533	.8473	1	130.76	.8557	--	128.38	.8640	--	126.14	.8723	--	124.02
622	.8376	3	133.74	.8459	3	131.18	.8541	3	128.80	.8624	3	126.56
444	.8020	1	147.68	.8099	1	144.02	.8178	1	140.76	.8257	1	137.80
711 +				.7857	--	157.28	.7933	--	152.32	.8010	--	148.18
640							.7857	3	157.30	.7933	3	152.36
Lattice constant	5.5563Å			5.6110Å			5.6656Å			5.7203Å		
Density (calc.)	4.144 g/cm³			4.783 g/cm³			5.384 g/cm³			5.947 g/cm³		

Phosphoric acid hydrate, $H_3PO_4 \cdot \frac{1}{2}H_2O$

Structure
Monoclinic, $P2_1/a$ (14), Z=8. The structure was determined by Mighell, Smith and Brown [1969].

Lattice constants: [ibid.]

a = 7.922(10)Å
b = 12.987(20)
c = 7.470(10)
β = 109.9(1)°

Density
(calculated) 1.967 g/cm^3

Thermal parameters
Isotropic [ibid.]

Scattering factors
P^0, O^- [International Tables, 1962]

Scale factor
(integrated intensities) 2.663 x 10^4

Additional patterns
1. Lehr et al. [1967].
2. Norbert [1972].

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Calculated Pattern (Peak heights)

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
7.02	40	0	0	1		12.60
6.47	6	1	1	0	+	13.68
5.66	9	-1	1	1		15.64
4.89	46	1	2	0		18.12
4.52	74	-1	2	1		19.64
4.18	4	1	1	1		21.24
3.88	46	-2	0	1		22.88
3.72	52	2	0	0	+	23.88
3.68	15	0	3	1		24.14
3.65	100	1	2	1		24.36
3.56	44	-1	1	2	+	25.02
3.51	12	0	0	2		25.34
3.39	11	0	1	2		26.26
3.33	2	-2	2	1		26.74
3.25	68	0	4	0		27.46
3.21	44	-1	2	2		27.74
3.14	2	-2	0	2		28.36
3.09	6	0	2	2	+	28.88
3.06	9	-2	1	2		29.20
2.98	3	1	4	0		30.00
2.95	11	0	4	1		30.30
2.91	26	2	0	1		30.74
2.84	14	2	1	1		31.52
2.83	15	-2	2	2	+	31.58
2.81	4	-1	3	2		31.78
2.62	2	1	4	1		34.26
2.592	6	1	2	2	+	34.58
2.545	5	-2	3	2		35.24
2.490	4	-2	4	1		36.04
2.445	14	-3	2	1	+	36.72
2.438	12	0	5	1	+	36.84
2.418	4	-3	1	2		37.16
2.384	2	0	4	2		37.70
2.367	2	1	3	2		37.98
2.341	2	0	0	3	+	38.42
2.301	4	-3	2	2		39.12
2.254	8	-3	3	1	+	39.96
2.235	1	-2	2	3		40.32
2.207	2	2	0	2		40.86
2.203	4	0	2	3		40.94
2.176	1	2	1	2		41.46
2.158	7	-2	5	1	+	41.82
2.139	2	-3	3	2		42.22
2.130	2	2	5	0		42.40
2.125	4	-1	5	2		42.50
2.088	2	0	5	2	+	43.30
2.070	3	-3	1	3	+	43.70
2.060	3	0	3	3		43.92
2.047	2	-1	6	1		44.22
2.019	7	1	1	3		44.86
2.003	1	-2	5	2		45.24
1.975	8	-4	0	1	+	45.92
1.961	1	-3	4	2		46.26
1.951	3	-4	1	1		46.50
1.949	3	1	2	3		46.56
1.943	6	1	6	1	+	46.70
1.938	3	2	5	1		46.84
1.899	2	0	4	3		47.86
1.887	2	-3	3	3		48.18
1.868	6	-1	6	2		48.70
1.860	2	-4	2	2		48.92
1.848	3	1	3	3		49.28
1.843	5	0	6	2		49.42
1.831	1	-2	1	4		49.76
1.797	3	-1	5	3		50.76

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
1.792	2	4	2	0	+	50.92
1.783	1	-2	6	2		51.20
1.779	3	-2	2	4	+	51.32
1.766	3	-4	1	3		51.72
1.762	3	-3	4	3		51.86
1.729	2	1	4	3		52.90
1.719	2	2	1	3		53.26
1.702	4	3	2	2	+	53.82
1.687	1	-4	4	1		54.34
1.675	1	2	2	3		54.76
1.665	4	4	0	1		55.12
1.659	1	-1	7	2		55.34
1.633	2	3	3	2		56.28
1.631	2	-3	5	3		56.36
1.623	4	0	8	0	+	56.66
1.606	1	1	5	3		57.32
1.602	1	-2	6	3		57.48
1.581	2	1	1	4	+	58.32
1.572	1	-4	5	1		58.70
1.567	1	-5	1	2		58.90
1.561	2	-4	1	4		59.14
1.546	1	2	6	2		59.78
1.528	1	-4	2	4		60.54
1.518	1	-3	7	1		60.98
1.501	2	-5	1	3		61.74
1.498	3	-2	8	1		61.90
1.481	3	-3	7	2		62.66
1.478	3	-4	3	4		62.82
1.470	1	-4	5	3		63.22
1.452	4	5	2	0		64.08

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
7.02	33	0	0	1	12.59
6.49	4	0	2	0	13.63
6.46	4	1	1	0	13.69
5.66	9	-1	1	1	15.64
4.89	44	1	2	0	18.11
4.52	70	-1	2	1	19.63
4.18	4	1	1	1	21.24
3.88	47	-2	0	1	22.89
3.74	5	1	3	0	23.75
3.72	41	2	0	0	23.87
3.72	15	-2	1	1	23.90
3.69	11	0	3	1	24.13
3.65	100	1	2	1	24.36
3.58	1	2	1	0	24.85
3.57	7	-1	3	1	24.95
3.56	43	-1	1	2	25.01
3.51	11	0	0	2	25.34
3.39	12	0	1	2	26.27
3.33	1	-2	2	1	26.73
3.25	74	0	4	0	27.45
3.21	45	-1	2	2	27.73
3.14	2	-2	0	2	28.36
3.09	1	1	3	1	28.86
3.09	5	0	2	2	28.88
3.06	9	-2	1	2	29.20
2.98	3	1	4	0	30.00
2.95	12	0	4	1	30.30
2.91	28	2	0	1	30.74
2.89	3	-2	3	1	30.91
2.84	13	2	1	1	31.52
2.83	9	-2	2	2	31.59
2.82	2	2	3	0	31.67
2.81	3	-1	3	2	31.79
2.62	2	1	4	1	34.25
2.592	6	1	2	2	34.58
2.587	2	-3	1	1	34.64
2.544	6	-2	3	2	35.25
2.491	4	-2	4	1	36.03
2.453	2	1	5	0	36.61
2.446	11	-3	2	1	36.71
2.445	3	-1	1	3	36.73
2.439	2	3	1	0	36.82
2.436	7	0	5	1	36.87
2.417	4	-3	1	2	37.16
2.384	2	0	4	2	37.70
2.367	3	1	3	2	37.98
2.342	1	-2	1	3	38.41
2.341	2	0	0	3	38.42
2.301	4	-3	2	2	39.12
2.259	3	-2	4	2	39.88

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.254	8	-3	3	1	39.96
2.235	1	-2	2	3	40.32
2.207	2	2	0	2	40.85
2.203	4	0	2	3	40.94
2.176	1	2	1	2	41.46
2.159	8	-2	5	1	41.81
2.158	1	-1	3	3	41.83
2.139	2	-3	3	2	42.22
2.130	1	2	5	0	42.39
2.126	4	-1	5	2	42.49
2.088	2	0	5	2	43.29
2.086	1	-2	3	3	43.34
2.079	1	1	6	0	43.51
2.070	2	-3	1	3	43.70
2.069	1	0	6	1	43.73
2.059	4	0	3	3	43.93
2.047	2	-1	6	1	44.22
2.019	9	1	1	3	44.87
2.003	1	-2	5	2	45.24
1.975	3	-1	4	3	45.90
1.974	8	-4	0	1	45.93
1.961	1	-3	4	2	46.26
1.952	2	-4	1	1	46.49
1.949	2	1	2	3	46.55
1.943	5	1	6	1	46.70
1.941	1	-4	0	2	46.76
1.937	1	2	5	1	46.87
1.899	3	0	4	3	47.86
1.887	2	-3	3	3	48.19
1.868	8	-1	6	2	48.70
1.860	2	-4	2	2	48.93
1.848	3	1	3	3	49.27
1.843	4	0	6	2	49.42
1.831	1	-2	1	4	49.75
1.797	4	-1	5	3	50.76
1.794	1	0	7	1	50.86
1.790	1	4	2	0	50.98
1.783	1	-2	6	2	51.19
1.779	1	-1	7	1	51.30
1.779	3	-2	2	4	51.32
1.766	4	-4	1	3	51.72
1.761	2	-3	4	3	51.87
1.748	1	3	1	2	52.29
1.729	2	1	4	3	52.90
1.719	2	2	1	3	53.25
1.702	5	3	2	2	53.81
1.701	2	-2	3	4	53.86
1.687	1	-4	4	1	54.34
1.675	1	2	2	3	54.75
1.665	5	4	0	1	55.11
1.658	1	-1	7	2	55.35
1.634	3	3	3	2	56.27
1.631	2	-3	5	3	56.35
1.625	1	-3	6	2	56.59
1.623	5	0	8	0	56.65
1.606	1	1	5	3	57.32
1.602	1	-2	6	3	57.50
1.582	2	0	8	1	58.29
1.581	2	1	1	4	58.34
1.572	1	-4	5	1	58.69
1.567	1	-5	1	2	58.90
1.561	3	-4	1	4	59.14
1.546	1	2	6	2	59.79
1.528	1	-4	2	4	60.54
1.518	2	-3	7	1	60.99
1.501	3	-5	1	3	61.74
1.498	2	-2	8	1	61.90
1.481	3	-3	7	2	62.67
1.478	3	-4	3	4	62.83
1.470	1	-4	5	3	63.21
1.454	1	0	7	3	63.98
1.452	5	5	2	0	64.08

Potassium cerium fluoride, β-$KCeF_4$

Structure

Orthorhombic, Pnam (62), Z=4. The structure was determined by Brunton [1969].

Lattice constants: (published values: 6.2895, 15.596, 3.8040 [ibid.])

a = 6.2899(3)Å
b = 15.597(2)
c = 3.8042(3)

Density

(calculated) 4.542 g/cm^3

Thermal parameters

Isotropic: potassium B = 1.02; cerium B = 0.55; fluorine (1) B = 1.17; fluorine (2) B = 0.96; fluorine (3) B = 1.03; fluorine (4) B = 1.28.

Polymorphism

Two other forms have been described. At the stoichiometric composition, β-$KCeF_4$ becomes the cubic, fluorite-type α-$KCeF_4$ above 755 °C. A hexagonal phase, β_1-$KCeF_4$ does not occur as an equilibrium compound [Brunton, 1969].

Scattering factors

K^+, Ce^{3+}, F^- [Cromer and Waber,1965]; the cerium factors were corrected for dispersion [Dauben and Templeton, 1955].

Scale factor

(integrated intensities) 6.570 x 10^4

References

Brunton, G. (1969). Acta Cryst. B25, 600.

Cromer, D. T. and Waber, J. T. (1965) Acta Cryst. 18, 104.

Dauben, C. H. and Templeton, D. H. (1955). Acta Cryst. 8, 241.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
7.797	100	0 2 0	11.34
4.897	74	1 2 0	18.10
3.314	81	1 4 0	26.88
3.186	93	1 1 1	27.98
3.144	33	2 0 0	28.36
3.0703	45	0 3 1	29.06
2.9173	9	2 2 0	30.62
2.7946	1	1 5 0	32.00
2.5991	5	0 6 0	34.48
2.4994	7	1 4 1	35.90
2.4238	9	2 0 1	37.06
2.4125	27	0 5 1	37.24
2.4051	17	1 6 0	37.36
2.3952	3	2 1 1	37.52
2.2140	2	2 5 0	40.72
2.1965	63	2 3 1	41.06
2.0999	2	1 7 0	43.04
2.0779	1	3 1 0	43.52
2.0309	2	1 6 1	44.58
2.0248	3	3 2 0	44.72
2.0036	5	2 6 0	45.22
1.9498	12	0 8 0	46.54
1.9451	8	3 3 0	46.66
1.9225	3	0 7 1	47.24
1.9141	25	2 5 1	47.46
1.9021	20	0 0 2	47.78
1.8469	24	3 4 0 +	49.30
1.8385	35	1 7 1	49.54
1.8234	23	3 1 1	49.98
1.7731	7	1 2 2	51.50
1.7312	1	3 3 1	52.84
1.6571	8	2 8 0	55.40
1.6495	15	1 4 2	55.68
1.6402	2	2 7 1	56.02
1.6317	2	3 6 0	56.34
1.6274	8	2 0 2	56.50
1.5934	2	2 2 2	57.82
1.5824	1	3 5 1	58.26
1.5726	3	4 0 0	58.66
1.5600	1	0 10 0	59.18
1.5415	2	4 2 0	59.96
1.5350	2	0 6 2	60.24
1.5295	6	1 9 1	60.48
1.5137	3	1 10 0	61.18
1.4913	1	1 6 2	62.20
1.4170	6	3 7 1	65.86
1.4098	1	1 7 2	66.24
1.3997	6	4 3 1	66.78
1.3960	3	2 10 0	66.98
1.3861	1	3 2 2	67.52
1.3797	2	2 6 2	67.88
1.3614	5	0 8 2	68.92
1.3453	2	4 6 0	69.86
1.3284	3	0 11 1	70.88
1.3249	11	3 4 2	71.10
1.3172	2	4 5 1	71.58
1.2729	3	1 12 0	74.48
1.2602	3	3 9 1	75.36
1.2512	2	3 10 0	76.00
1.2495	5	2 8 2	76.12
1.2418	1	5 2 0	76.68
1.2390	4	1 1 3 +	76.88
1.2320	2	0 3 3	77.40
1.2240	8	2 11 1 +	78.00
1.2120	2	4 0 2	78.92

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
1.2062	1	0	10	2		79.38
1.1974	3	5	4	0	+	80.08
1.1910	4	5	1	1		80.60
1.1844	2	1	10	2		81.14
1.1746	2	0	5	3		81.96
1.1470	4	2	3	3		84.38
1.1443	3	0	13	1		84.62
1.1224	1	3	11	1		86.68
1.1047	2	3	12	0		88.42
1.1004	3	2	5	3		88.86
1.0984	2	4	6	2		89.06
1.0856	3	1	7	3		90.40
1.0826	4	3	1	3		90.72
1.0752	2	2	13	1		91.52
1.0579	3	1	12	2		93.46
1.0527	2	5	7	1		94.06
1.0500	2	2	14	0		94.38
1.0483	1	6	0	0		94.58
1.0455	1	3	10	2		94.92
1.0400	1	5	2	2		95.58
1.0293	3	4	8	2		96.90
1.0148	2	4	11	1		98.76
1.0132	3	5	4	2		98.98
1.0105	2	1	9	3		99.34
.9920	2	6	3	1		101.88
.9905	3	1	15	1		102.10
.9835	1	5	9	1		103.12
.9755	2	3	7	3	+	104.30
.9730	2	5	6	2		104.68
.9698	2	4	3	3		105.18
.9614	2	6	5	1	+	106.50
.9553	2	3	12	2	+	107.48
.9511	1	0	0	4	+	108.18
.9452	1	0	11	3		109.16
.9412	1	4	5	3		109.86
.9311	1	2	16	0		111.64
.9253	1	4	13	1		112.72
.9232	1	6	8	0		113.10
.9195	2	3	9	3	+	113.80
.9181	1	6	0	2		114.08
.9141	2	1	4	4		114.84
.9118	1	6	2	2		115.30
.9103	1	2	0	4		115.60
.9091	1	4	14	0		115.84
.9051	3	2	11	3	+	116.66
.8916	2	5	1	3		119.52

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
7.799	84	0	2	0	11.34
4.896	73	1	2	0	18.10
3.314	86	1	4	0	26.88
3.186	100	1	1	1	27.98
3.145	35	2	0	0	28.36
3.0701	49	0	3	1	29.06
2.9167	10	2	2	0	30.63
2.7946	1	1	5	0	32.00
2.5995	6	0	6	0	34.47
2.4988	9	1	4	1	35.91
2.4239	9	2	0	1	37.06
2.4121	32	0	5	1	37.25
2.4024	3	1	6	0	37.40
2.3952	1	2	1	1	37.52
2.2147	1	2	5	0	40.71
2.1969	79	2	3	1	41.05
2.1003	3	1	7	0	43.03
2.0779	1	3	1	0	43.52
2.0313	2	1	6	1	44.57
2.0247	3	3	2	0	44.72
2.0037	6	2	6	0	45.22
1.9496	16	0	8	0	46.54
1.9445	1	3	3	0	46.68
1.9226	3	0	7	1	47.24
1.9140	32	2	5	1	47.46
1.9021	25	0	0	2	47.78
1.8479	4	0	2	2	49.27
1.8466	29	3	4	0	49.31
1.8387	44	1	7	1	49.54
1.8236	31	3	1	1	49.97
1.7730	9	1	2	2	51.50
1.7314	1	3	3	1	52.83
1.6570	10	2	8	0	55.40
1.6497	21	1	4	2	55.67
1.6404	1	2	7	1	56.01
1.6320	3	3	6	0	56.33
1.6276	10	2	0	2	56.49
1.5932	4	2	2	2	57.83
1.5824	1	3	5	1	58.26
1.5725	4	4	0	0	58.66
1.5597	1	0	10	0	59.19
1.5414	2	4	2	0	59.96
1.5350	2	0	6	2	60.24
1.5297	9	1	9	1	60.47
1.5139	4	1	10	0	61.17
1.4913	2	1	6	2	62.20
1.4170	9	3	7	1	65.86
1.4099	1	1	7	2	66.24
1.3996	9	4	3	1	66.79
1.3973	1	2	10	0	66.91

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.3863	2	3 2 2	67.51
1.3795	3	2 6 2	67.89
1.3615	8	0 8 2	68.91
1.3455	3	4 6 0	69.85
1.3286	4	0 11 1	70.87
1.3249	16	3 4 2	71.10
1.3173	3	4 5 1	71.57
1.2729	5	1 12 0	74.48
1.2603	5	3 9 1	75.35
1.2514	2	3 10 0	75.98
1.2494	7	2 8 2	76.13
1.2419	1	5 2 0	76.67
1.2391	5	1 1 3	76.87
1.2386	2	3 6 2	76.91
1.2319	3	0 3 3	77.40
1.2240	5	4 8 0	78.00
1.2239	10	2 11 1	78.01
1.2120	3	4 0 2	78.93
1.2061	1	0 10 2	79.39
1.1976	2	4 2 2	80.06
1.1972	4	5 4 0	80.09
1.1909	7	5 1 1	80.61
1.1845	3	1 10 2	81.13
1.1747	3	0 5 3	81.95
1.1471	7	2 3 3	84.37
1.1442	1	0 13 1	84.63
1.1324	1	5 6 0	85.73
1.1261	1	2 10 2	86.32
1.1223	1	3 11 1	86.69
1.1141	1	0 14 0	87.49
1.1047	3	3 12 0	88.42
1.1004	5	2 5 3	88.85
1.0984	3	4 6 2	89.06
1.0970	1	1 14 0	89.21
1.0855	6	1 7 3	90.40
1.0824	5	3 1 3	90.74
1.0753	3	2 13 1	91.51
1.0579	5	1 12 2	93.47
1.0527	5	5 7 1	94.07
1.0501	1	2 14 0	94.37
1.0483	1	6 0 0	94.58
1.0454	2	3 10 2	94.92
1.0399	2	5 2 2	95.59
1.0293	6	4 8 2	96.90
1.0149	5	4 11 1	98.75
1.0132	5	5 4 2	98.97
1.0101	2	1 9 3	99.39
.9921	3	6 3 1	101.87
.9905	5	1 15 1	102.10
.9834	3	5 9 1	103.12

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.9792	1	5 10 0	103.75
.9755	3	3 7 3	104.30
.9748	1	0 16 0	104.41
.9730	2	5 6 2	104.69
.9698	3	4 3 3	105.18
.9614	4	6 5 1	106.49
.9613	1	0 14 2	106.51
.9570	1	4 10 2	107.20
.9556	1	2 15 1	107.43
.9553	4	3 12 2	107.48
.9510	2	0 0 4	108.18
.9503	1	1 14 2	108.31
.9452	2	0 11 3	109.16
.9411	2	4 5 3	109.87
.9336	1	1 2 4	111.19
.9311	1	2 16 0	111.64
.9252	2	4 13 1	112.73
.9233	2	6 8 0	113.08
.9197	3	3 9 3	113.77
.9193	2	2 14 2	113.84
.9181	2	6 0 2	114.07
.9141	4	1 4 4	114.84
.9118	1	6 2 2	115.30
.9103	2	2 0 4	115.60
.9091	1	4 14 0	115.85
.9052	5	2 11 3	116.63
.9048	4	3 15 1	116.72
.9042	1	2 2 4	116.84
.9039	2	5 12 0	116.90
.8927	1	7 2 0	119.30
.8916	4	5 1 3	119.52

Potassium sodium bromide, KBr-NaBr, calculated solid solution series

Structure

Cubic, Fm3m (225), Z = 4, isostructural with NaCl. The system KBr-NaBr forms a complete solid solution series [Bellanca, 1939].

Lattice constants

The constants were derived by interpolation on a molar ratio, using the cell dimensions of KBr [Swanson and Tatge, 1953] and NaBr [Swanson et al.,1954]. For KBr, a=6.6004Å and for NaBr, a=5.9776Å; the original values have been modified to conform to new wavelength measurements.

Thermal parameters

Isotropic: overall B = 1.6.

Scattering factors

K^+, Na^+, Br^- [International Tables, 1962].

Random distribution of the cations was assumed, and the factors used were proportional to the molar ratio.

References

Bellanca, A. (1939). Periodico Mineral. 10, 18.

International Tables for X-ray Crystallography III (1962), 202, 204, 206.

Swanson, H. E., Fuyat, R. K., and Ugrinic, G. M. (1954). Natl. Bur. Std. U.S. Circ. 539, 3, 47.

Swanson, H. E. and Tatge, E. (1953). Natl. Bur. Std. U.S. Circ. 539, 1, 66.

	$K_{.8}Na_{.2}Br$			$K_{.6}Na_{.4}Br$			$K_{.4}Na_{.6}Br$			$K_{.2}Na_{.8}Br$		
hkℓ	d(Å)	I	2θ(°) λ=1.540598	d(Å)	I	2θ(°) λ=1.540598	d(Å)	I	2θ(°) λ=1.540598	d(Å)	I	2θ(°) λ=1.540598
111	3.74	29	23.78	3.67	34	24.26	3.60	43	24.74	3.52	54	25.26
200	3.238	100	27.52	3.175	100	28.08	3.112	100	28.66	3.052	100	29.24
220	2.290	63	39.32	2.246	60	40.12	2.202	63	40.96	2.157	62	41.84
311	1.952	10	46.48	1.915	12	47.44	1.878	14	48.44	1.840	17	49.50
222	1.870	18	48.66	1.834	17	49.68	1.797	17	50.76	1.762	18	51.86
400	1.619	7	56.82	1.588	7	58.04	1.557	7	59.32	1.525	7	60.66
331	1.486	3	62.46	1.457	4	63.82	1.429	4	65.26	1.400	5	66.76
420	1.448	17	64.28	1.420	16	65.70	1.392	16	67.18	1.364	16	68.74
422	1.322	10	71.28	1.296	10	72.90	1.271	10	74.60	1.246	10	76.40
511 +	1.246	2	76.36	1.222	2	78.14	1.198	3	80.00	1.174	3	81.98
440	1.1448	3	84.58	1.1228	2	86.64	1.1008	2	88.82	1.0787	2	91.14
531	1.0945	2	89.46	1.0736	2	91.70	1.0526	2	94.08	1.0315	2	96.62
442 +	1.0792	5	91.08	1.0586	5	93.38	1.0378	5	95.84	1.0170	5	98.48
620	1.0239	3	97.58	1.0042	3	100.18	0.9845	3	102.96	0.9649	3	105.94
533	0.9876	--	102.52	0.9686	--	105.36	.9496	1	108.42	.9306	1	111.74
622	.9763	2	104.18	.9575	2	107.12	.9388	3	110.28	.9199	3	113.72
444	.9347	1	111.00	.9167	1	114.34	.8988	1	117.98	.8808	1	121.98
711 +	.9068	1	116.30	.8894	1	120.02	.8719	1	124.12	.8545	1	128.70
640	.8980	2	118.14	.8807	2	122.00	.8635	2	126.28	.8462	2	131.08
642	.8654	4	125.78	.8488	4	130.34	.8321	4	135.56	.8154	4	141.70
731 +	.8431	1	132.04	.8269	1	137.36	.8106	2	143.70	.7944	2	151.68
820 +	.7853	3	157.56									
Lattice constant	6.4758Å			6.3513Å			6.2267Å			6.1022Å		
Density (calc.)	2.832 g/cm³			2.918 g/cm³			3.008 g/cm³			3.102 g/cm³		

Potassium sodium chloride, KCl-NaCl, calculated solid solution series

Structure

Cubic, Fm3m (225), Z = 4. The system KCl-NaCl forms a solid solution series, complete only between 480° and 650 °C [Scheil and Stadelmaier, 1952].

Lattice constants

The constants were derived by interpolation on a molar ratio, using the cell dimensions of KCl [Swanson and Tatge, 1953] and NaCl [Swanson and Fuyat, 1953]. The original values were modified to a = 6.2935Å (KCl) and a = 5.6406Å (NaCl), to conform to new wavelength measurements.

Thermal parameters

Isotropic: potassium B = 1.6; sodium B = 1.9; chlorine B = 1.6.

Scattering factors

K^+, Na^+, Cl^- [International Tables, 1962]. The factors used were proportional to the molar ratio, assuming random distribution of the cations.

References

International Tables for X-ray Crystallography III (1962), 202, 204.

Scheil, E. and Stadelmaier, Z. (1952). Z. Metallk. 43, 227.

Swanson, H. E. and Fuyat, R. K. (1953). Natl. Bur. Std. U. S. Circ. 539, II, 41.

Swanson, H. E. and Tatge, E. (1953). Natl. Bur. Std. U. S. Circ. 539, I, 65.

	$K_{.8}Na_{.2}Cl$			$K_{.6}Na_{.4}Cl$			$K_{.4}Na_{.6}Cl$			$K_{.2}Na_{.8}Cl$		
hkℓ	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)	d(Å)	I	2θ(°)
	λ=1.540598			λ=1.540598			λ=1.540598			λ=1.540598		
111	3.56	--	25.00	3.48	--	25.56	3.41	2	26.14	3.33	6	26.74
200	3.081	100	28.96	3.016	100	29.60	2.951	100	30.26	2.886	100	30.96
220	2.179	53	41.40	2.133	53	42.34	2.087	50	43.32	2.040	52	44.36
222	1.779	14	51.32	1.742	14	52.50	1.704	14	53.76	1.666	14	55.08
400	1.541	5	60.00	1.508	5	61.44	1.476	5	62.94	1.443	5	64.54
420	1.378	12	67.96	1.349	11	69.66	1.320	11	71.42	1.290	11	73.30
422	1.258	7	75.52	1.232	7	77.44	1.205	7	79.50	1.178	6	81.68
440	1.0894	2	90.00	1.0664	2	92.50	1.0433	2	95.18	1.0202	2	98.06
442 +	1.0271	4	97.18	1.0054	3	100.02	0.9836	3	103.10	0.9619	3	106.42
620	0.9745	2	104.46	0.9538	2	107.72	.9331	2	111.28	.9125	2	115.16
622	.9290	2	112.02	.9094	2	115.78	.8897	2	119.94	.8700	2	124.60
640	.8546	2	128.66	.8365	2	134.10	.8184	2	140.50	.8003	2	148.52
642	.8236	3	138.56	.8061	3	145.72	.7887	4	155.22			
Lattice constant	6.1629Å			6.0323Å			5.9018Å			5.7712Å		
Density (calc.)	2.024 g/cm³			2.061 g/cm³			2.097 g/cm³			2.131 g/cm³		

Thorium cobalt, Th_2Co_{17}

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3 isostructural with Th_2Zn_{17}. The structure was determined by Johnson. Smith and Wood [1969].

Lattice constants: [ibid.]

a = 8.438(5)Å
c = 12.254(8)

Density
(calculated) 9.664 g/cm^3

Thermal parameters
Isotropic [Johnson et. al., 1969].

Scattering factors
Th^0, Co^0[International Tables, 1962], corrected for anomalous dispersion [Dauben and Templeton, 1955].

Scale factor
(integrated intensities) 56.46 x 10^4

References

Dauben, C. H. and Templeton, D. H. (1955). Acta Cryst. 8, 241.

International Tables for X-ray Crystallography III (1962), 202, 212.

Johnson, Q., Smith, G. S., and Wood, D.H. (1969). Acta Cryst. B25, 464.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
6.28	9	1	0	1	14.10
4.697	6	0	1	2	18.88
4.219	30	1	1	0	21.04
4.085	11	0	0	3	21.74
3.501	18	0	2	1	25.42
3.138	8	2	0	2	28.42
2.934	80	1	1	3	30.44
2.826	18	1	0	4	31.64
2.695	18	2	1	1	33.22
2.518	10	1	2	2	35.62
2.435	50	3	0	0	36.88
2.347	36	0	2	4	38.32
2.324	1	0	1	5	38.72
2.109	68	2	2	0	42.84
2.093	100	3	0	3 +	43.20
2.051	25	2	1	4	44.12
2.042	32	0	0	6	44.32
2.036	24	2	0	5	44.46
1.874	4	2	2	3	48.54
1.833	5	1	2	5	49.70
1.751	1	0	4	2	52.20
1.703	6	1	0	7	53.80
1.690	5	1	3	4	54.22
1.661	5	3	2	1	55.26
1.617	6	2	3	2	56.90
1.594	6	4	1	0	57.78
1.579	4	0	2	7	58.40
1.569	2	4	0	4	58.80
1.565	9	0	3	6 +	58.98
1.485	22	1	4	3 +	62.48
1.478	12	2	1	7	62.80
1.470	12	3	2	4	63.18
1.467	21	2	2	6	63.34
1.451	2	0	5	1	64.12
1.422	1	5	0	2	65.62
1.406	4	3	3	0	66.42
1.384	2	2	3	5	67.66
1.372	1	2	4	1	68.30
1.362	1	0	0	9	68.90
1.330	12	3	3	3	70.80
1.325	5	1	3	7	71.10
1.319	3	0	5	4	71.46
1.305	2	5	1	1	72.36
1.296	4	1	1	9	72.96
1.283	2	1	5	2	73.78
1.259	6	2	4	4	75.44
1.256	4	5	0	5 +	75.68
1.218	10	6	0	0	78.46
1.211	6	3	2	7	79.02
1.208	4	1	0	10	79.26
1.206	5	5	1	4	79.36
1.203	5	4	2	5	79.62
1.189	10	3	0	9 +	80.80
1.174	2	0	4	8	82.04
1.170	2	5	2	0	82.34
1.162	2	0	2	10	83.06
1.158	2	3	3	6	83.36
1.157	2	1	5	5	83.48
1.131	1	2	3	8	85.88
1.125	6	5	2	3 +	86.44
1.122	5	0	5	7	86.72
1.120	2	2	1	10	86.90
1.084	1	2	4	7	90.54
1.055	6	4	4	0	93.82
1.050	4	5	1	7	94.36
1.047	4	1	6	4	94.70
1.046	7	6	0	6 +	94.84
1.040	1	3	5	1	95.56
1.035	6	1	4	9 +	96.14
1.033	3	1	2	11	96.44

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
1.021	2	0	0	12		97.94
1.010	1	6	2	1		99.42
.990	1	4	3	7		102.12
.989	2	3	2	10		102.28
.988	2	3	5	4		102.44
.978	4	3	3	9		103.90
.976	3	3	1	11		104.24
.968	2	7	1	0		105.46
.962	3	6	2	4		106.38
.960	2	5	3	5		106.76
.942	8	1	7	3	+	109.74
.939	5	1	6	7	+	110.16
.937	6	4	4	6	+	110.56
.935	4	1	0	13		110.98
.933	1	5	4	1		111.32
.925	1	4	5	2		112.78
.921	1	6	3	0		113.58
.919	3	2	2	12		113.88
.917	3	2	4	10		114.36
.898	4	3	6	3	+	118.12
.897	3	3	5	7		118.44
.896	4	5	1	10		118.62
.895	3	5	4	4		118.82
.892	3	2	1	13		119.42
.890	2	2	7	1		119.90
.887	4	5	2	9	+	120.46
.877	2	6	2	7		122.88
.875	2	7	1	6	+	123.44
.860	1	4	1	12	+	127.20
.855	2	1	3	13		128.64
.857	1	2	7	4		127.98
.853	1	8	1	1		129.06
.851	1	2	0	14		129.64
.839	1	7	2	5		133.34
.826	3	5	5	3	+	137.56
.825	3	5	4	7		137.98
.824	3	1	6	10		138.30
.824	3	8	1	4		138.48
.822	4	3	2	13		139.26
.817	2	3	4	11		141.12
.808	1	4	6	4		144.64
.808	1	1	8	5		145.06

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
6.28	9	1	0	1	14.10
4.695	7	0	1	2	18.89
4.219	33	1	1	0	21.04
4.085	12	0	0	3	21.74
3.501	21	0	2	1	25.42
3.138	9	2	0	2	28.42
2.935	100	1	1	3	30.44
2.825	23	1	0	4	31.64
2.694	23	2	1	1	33.22
2.518	14	1	2	2	35.63
2.436	69	3	0	0	36.87
2.348	50	0	2	4	38.31
2.324	1	0	1	5	38.72
2.109	95	2	2	0	42.83
2.092	74	3	0	3	43.21
2.092	72	0	3	3	43.21
2.051	34	2	1	4	44.11
2.042	40	0	0	6	44.32
2.035	19	2	0	5	44.48
1.874	6	2	2	3	48.53
1.833	7	1	2	5	49.69
1.807	1	4	0	1	50.47
1.751	2	0	4	2	52.21
1.702	9	1	0	7	53.81
1.690	7	1	3	4	54.22
1.661	7	3	2	1	55.26
1.617	9	2	3	2	56.90
1.595	11	4	1	0	57.77
1.579	6	0	2	7	58.41
1.569	2	4	0	4	58.80
1.565	7	3	0	6	58.97
1.565	8	0	3	6	58.97
1.485	19	4	1	3	62.47
1.485	19	1	4	3	62.47
1.479	19	2	1	7	62.79
1.471	17	3	2	4	63.17
1.467	27	2	2	6	63.33
1.451	3	0	5	1	64.12
1.422	1	5	0	2	65.62
1.406	7	3	3	0	66.42
1.384	3	2	3	5	67.66
1.372	2	2	4	1	68.29
1.362	1	0	0	9	68.91
1.347	1	4	2	2	69.75
1.330	21	3	3	3	70.80
1.325	6	1	3	7	71.10
1.319	4	0	5	4	71.46
1.305	5	5	1	1	72.35
1.296	8	1	1	9	72.95
1.283	3	1	5	2	73.77

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.259	11	2 4 4	75.45
1.257	1	4 1 6	75.59
1.257	1	1 4 6	75.59
1.255	1	5 0 5	75.71
1.218	20	6 0 0	78.47
1.211	11	3 2 7	79.02
1.209	1	1 0 10	79.19
1.206	9	5 1 4	79.36
1.203	5	4 2 5	79.62
1.188	11	3 0 9	80.80
1.188	10	0 3 9	80.80
1.174	3	0 4 8	82.03
1.170	3	5 2 0	82.34
1.162	4	0 2 10	83.06
1.158	3	3 3 6	83.37
1.157	3	1 5 5	83.48
1.131	1	2 3 8	85.87
1.125	7	5 2 3	86.44
1.125	7	2 5 3	86.44
1.122	4	0 5 7	86.72
1.120	3	2 1 10	86.90
1.101	1	0 1 11	88.77
1.084	3	2 4 7	90.54
1.055	15	4 4 0	93.83
1.050	9	5 1 7	94.37
1.049	1	1 3 10	94.54
1.047	3	1 6 4	94.71
1.046	7	6 0 6	94.85
1.046	7	0 6 6	94.85
1.040	1	3 5 1	95.56
1.035	6	4 1 9	96.13
1.035	7	1 4 9	96.13
1.033	1	1 2 11	96.42
1.029	1	5 3 2	96.92
1.021	4	0 0 12	97.93
1.010	2	6 2 1	99.41
1.000	1	2 6 2	100.79
.997	1	1 5 8	101.23
.991	1	4 3 7	102.09
.989	3	3 2 10	102.27
.988	4	3 5 4	102.44
.978	10	3 3 9	103.90
.976	3	3 1 11	104.19
.968	5	7 1 0	105.47
.962	8	6 2 4	106.38
.960	1	5 3 5	106.65
.942	8	7 1 3	109.75
.942	9	1 7 3	109.75
.942	3	0 3 12	109.76
.942	3	3 0 12	109.76

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.940	3	1 6 7	110.05
.939	1	0 5 10	110.24
.937	15	4 4 6	110.56
.936	4	2 6 5	110.68
.935	2	1 0 13	110.97
.933	1	5 4 1	111.32
.925	2	4 5 2	112.78
.921	3	6 3 0	113.58
.919	7	2 2 12	113.87
.917	6	2 4 10	114.37
.913	2	0 2 13	115.12
.898	6	6 3 3	118.11
.898	6	3 6 3	118.11
.897	6	3 5 7	118.44
.896	4	5 1 10	118.63
.895	6	5 4 4	118.82
.892	6	2 1 13	119.42
.890	2	2 7 1	119.79
.887	5	2 5 9	120.45
.887	6	5 2 9	120.45
.883	1	7 2 2	121.37
.877	5	6 2 7	122.88
.875	2	0 8 4	123.28
.875	2	1 7 6	123.45
.875	2	7 1 6	123.45
.874	1	4 5 5	123.59
.860	2	4 1 12	127.21
.860	2	1 4 12	127.21
.857	4	2 7 4	127.98
.856	1	8 0 5	128.31
.855	4	1 3 13	128.65
.853	3	8 1 1	129.07
.851	2	2 0 14	129.63
.847	2	1 8 2	130.84
.844	1	5 5 0	131.82
.839	1	6 3 6	133.20
.839	2	7 2 5	133.36
.834	1	4 4 9	134.98
.826	6	5 5 3	137.55
.826	5	3 3 12	137.57
.825	9	5 4 7	137.98
.824	2	1 6 10	138.24
.824	7	8 1 4	138.48
.822	11	3 2 13	139.28
.817	6	3 4 11	141.13
.812	2	9 0 0	143.14
.810	1	0 8 7	144.05
.809	5	4 6 4	144.63
.808	3	1 8 5	145.07
.802	1	1 1 15	147.66

Thorium iron, Th_2Fe_{17}

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with Th_2Zn_{17}. The structure was determined by Johnson, Smith and Wood [1969].

Lattice constants: [ibid.]

a = 8.565(2)Å
c = 12.469(3)

Density
(calculated) 8.888 g/cm^3

Thermal parameters
Isotropic [Johnson et. al., 1969]

Scattering factors
Th^0, Fe^0 [International Tables, 1962], corrected for anomalous dispersion [Dauben and Templeton, 1955].

Scale factor
(integrated intensities) 58.61 x 10^4

References

Dauben, C. H. and Templeton, D. H. (1955). Acta Cryst. 8, 241.

International Tables for X-ray Crystallography III (1962), 202, 212.

Johnson, Q., Smith, G. S., and Wood, D.H. (1969). Acta Cryst. B25, 464.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
6.375	8	1	0	1		13.88
4.772	5	0	1	2		18.58
4.283	27	1	1	0		20.72
4.157	10	0	0	3		21.36
3.553	17	0	2	1		25.04
3.186	9	2	0	2		27.98
2.982	76	1	1	3		29.94
2.873	18	1	0	4		31.10
2.735	16	2	1	1		32.72
2.557	10	1	2	2		35.06
2.473	50	3	0	0		36.30
2.387	33	0	2	4		37.66
2.364	2	0	1	5		38.04
2.142	63	2	2	0		42.16
2.125	100	3	0	3	+	42.50
2.084	26	2	1	4		43.38
2.079	40	0	0	6		43.50
2.070	15	2	0	5		43.70
1.904	4	2	2	3		47.74
1.863	5	1	2	5		48.84
1.778	1	0	4	2		51.36
1.732	5	1	0	7		52.80
1.717	4	1	3	4		53.30
1.686	4	3	2	1		54.38
1.6419	5	2	3	2		55.96
1.6185	6	4	1	0		56.84
1.6056	4	0	2	7		57.34
1.5909	9	0	3	6	+	57.92
1.5083	22	1	4	3	+	61.42
1.5039	17	2	1	7		61.62
1.4935	13	3	2	4		62.10
1.4913	19	2	2	6		62.20
1.4730	1	0	5	1		63.06
1.4431	1	5	0	2		64.52
1.4274	4	3	3	0		65.32
1.4057	2	2	3	5		66.46
1.3931	1	2	4	1		67.14
1.3501	12	3	3	3		69.58
1.3467	9	1	3	7		69.78
1.3396	2	0	5	4		70.20
1.3246	2	5	1	1		71.12
1.3181	4	1	1	9		71.52
1.3027	2	1	5	2		72.50
1.2785	5	2	4	4		74.10
1.2752	3	5	0	5		74.32
1.2363	10	6	0	0		77.08
1.2304	6	3	2	7	+	77.52
1.2251	5	5	1	4		77.92
1.2219	4	4	2	5		78.16
1.2087	11	3	0	9	+	79.18
1.1932	1	0	4	8		80.42
1.1878	2	5	2	0		80.86
1.1820	2	0	2	10		81.34
1.1767	2	3	3	6		81.78
1.1751	2	1	5	5		81.92
1.1419	6	5	2	3	+	84.84
1.1393	5	0	5	7	+	85.08
1.1015	1	2	4	7		88.74
1.0707	6	4	4	0		92.02
1.0669	4	5	1	7		92.44
1.0625	7	6	0	6	+	92.94
1.0558	1	3	5	1		93.70
1.0526	5	1	4	9	+	94.08
1.0392	2	0	0	12		95.68
1.0252	1	6	2	1		97.42
1.0059	2	3	2	10	+	99.96
1.0034	2	3	5	4		100.30
.9943	4	3	3	9		101.56
.9929	1	3	1	11		101.76
.9825	2	7	1	0		103.26

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
.9769	3	6	2	4		104.10
.9745	1	5	3	5		104.46
.9580	2	0	3	12	+	107.04
.9562	6	1	7	3	+	107.34
.9549	3	1	6	7	+	107.54
.9518	6	4	4	6	+	108.06
.9470	1	5	4	1		108.86
.9389	1	4	5	2		110.26
.9348	3	2	2	12	+	110.98
.9318	2	2	4	10		111.52
.9293	1	0	2	13		111.98
.9117	4	3	6	3	+	115.32
.9106	3	3	5	7	+	115.54
.9084	3	5	4	4		115.98
.9076	3	2	1	13		116.14
.9038	1	2	7	1		116.92
.9018	3	5	2	9	+	******
.8908	1	6	2	7		119.70
.8885	2	0	8	4	+	120.22
.8744	1	4	1	12	+	123.50
.8702	1	2	7	4		124.56
.8694	1	1	3	13		124.76
.8661	1	8	1	1		125.60
.8402	1	3	3	12		132.94
.8388	2	5	5	3		133.36
.8381	3	5	4	7	+	133.60
.8363	3	8	1	4		134.18
.8356	3	3	2	13		134.38
.8303	1	3	4	11		136.18
.8208	1	4	6	4		139.58
.8199	1	1	8	5		139.94
.8093	6	8	2	0		144.28
.8084	3	9	0	3	+	144.66
.8074	4	2	7	7	+	145.14

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
6.375	9	1	0	1	13.88
4.773	6	0	1	2	18.58
4.283	32	1	1	0	20.72
4.157	11	0	0	3	21.36
3.555	22	0	2	1	25.03
3.187	12	2	0	2	27.97
2.983	100	1	1	3	29.93
2.874	24	1	0	4	31.09
2.735	22	2	1	1	32.71
2.557	14	1	2	2	35.07
2.473	70	3	0	0	36.30
2.386	46	0	2	4	37.66
2.364	2	0	1	5	38.03
2.141	94	2	2	0	42.17
2.125	75	3	0	3	42.51
2.125	74	0	3	3	42.51
2.085	35	2	1	4	43.37
2.078	43	0	0	6	43.51
2.070	16	2	0	5	43.70
1.904	7	2	2	3	47.74
1.863	8	1	2	5	48.84
1.834	1	4	0	1	49.66
1.777	1	0	4	2	51.36
1.732	8	1	0	7	52.81
1.717	7	1	3	4	53.31
1.686	8	3	2	1	54.37
1.6416	8	2	3	2	55.97
1.6186	10	4	1	0	56.84
1.6058	7	0	2	7	57.33
1.5937	2	4	0	4	57.81
1.5909	7	3	0	6	57.92
1.5909	7	0	3	6	57.92
1.5083	18	4	1	3	61.42
1.5083	19	1	4	3	61.42
1.5036	17	2	1	7	61.64
1.4937	17	3	2	4	62.09
1.4914	28	2	2	6	62.20
1.4731	2	0	5	1	63.05
1.4432	1	5	0	2	64.52
1.4275	7	3	3	0	65.31
1.4057	4	2	3	5	66.46
1.3930	2	2	4	1	67.14
1.3856	1	0	0	9	67.55
1.3676	1	4	2	2	68.56
1.3501	22	3	3	3	69.58
1.3467	5	1	3	7	69.78
1.3396	4	0	5	4	70.20
1.3247	4	5	1	1	71.11
1.3183	9	1	1	9	71.51
1.3028	3	1	5	2	72.49

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.2785	10	2 4 4	74.10
1.2750	2	5 0 5	74.34
1.2363	20	6 0 0	77.08
1.2305	11	3 2 7	77.51
1.2297	1	1 0 10	77.57
1.2251	8	5 1 4	77.92
1.2220	4	4 2 5	78.15
1.2087	11	3 0 9	79.18
1.2087	11	0 3 9	79.18
1.1932	2	0 4 8	80.42
1.1878	3	5 2 0	80.86
1.1820	4	0 2 10	81.34
1.1767	3	3 3 6	81.78
1.1751	3	1 5 5	81.92
1.1494	1	2 3 8	84.16
1.1420	7	5 2 3	84.83
1.1420	6	2 5 3	84.83
1.1400	4	0 5 7	85.02
1.1394	3	2 1 10	85.07
1.1206	1	0 1 11	86.85
1.1016	3	2 4 7	88.73
1.0706	14	4 4 0	92.02
1.0669	8	5 1 7	92.44
1.0633	2	1 6 4	92.84
1.0625	8	6 0 6	92.94
1.0625	8	0 6 6	92.94
1.0558	1	3 5 1	93.70
1.0526	6	1 4 9	94.08
1.0526	6	4 1 9	94.08
1.0447	1	5 3 2	95.01
1.0392	4	0 0 12	95.68
1.0251	2	6 2 1	97.42
1.0149	1	2 6 2	98.75
1.0127	1	1 5 8	99.04
1.0063	1	4 3 7	99.90
1.0058	3	3 2 10	99.96
1.0033	4	3 5 4	100.31
.9942	9	3 3 9	101.57
.9929	2	3 1 11	101.76
.9825	4	7 1 0	103.26
.9768	7	6 2 4	104.11
.9753	1	5 3 5	104.34
.9604	1	3 4 8	106.65
.9580	3	0 3 12	107.04
.9580	2	3 0 12	107.04
.9561	7	7 1 3	107.35
.9561	8	1 7 3	107.35
.9549	3	1 6 7	107.54
.9546	1	0 5 10	107.60
.9518	14	4 4 6	108.06

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.9513	2	1 0 13	108.14
.9509	3	2 6 5	108.20
.9470	1	5 4 1	108.87
.9389	2	4 5 2	110.26
.9349	8	2 2 12	110.96
.9345	3	6 3 0	111.03
.9317	5	2 4 10	111.54
.9287	1	0 2 13	112.09
.9118	5	6 3 3	115.31
.9118	5	3 6 3	115.31
.9107	5	3 5 7	115.52
.9104	3	5 1 10	115.58
.9085	5	5 4 4	115.97
.9076	6	2 1 13	116.15
.9038	2	2 7 1	116.92
.9018	5	5 2 9	117.35
.9018	5	2 5 9	117.35
.8968	1	7 2 2	118.40
.8908	4	6 2 7	119.71
.8887	2	0 8 4	120.17
.8882	1	1 7 6	120.28
.8882	1	7 1 6	120.28
.8875	1	4 5 5	120.43
.8745	1	4 1 12	123.50
.8745	1	1 4 12	123.50
.8702	4	2 7 4	124.56
.8694	3	1 3 13	124.76
.8661	2	8 1 1	125.60
.8599	2	1 8 2	127.23
.8565	1	5 5 0	128.15
.8517	2	7 2 5	129.49
.8472	1	4 4 9	130.80
.8401	4	3 3 12	132.95
.8389	5	5 5 3	133.34
.8381	7	5 4 7	133.60
.8378	1	1 6 10	133.68
.8363	6	8 1 4	134.16
.8356	9	3 2 13	134.39
.8303	4	3 4 11	136.18
.8242	1	9 0 0	138.34
.8225	1	0 8 7	138.97
.8208	3	4 6 4	139.58
.8199	3	1 8 5	139.94
.8161	1	1 1 15	141.43
.8110	1	4 5 8	143.53
.8093	25	8 2 0	144.27
.8084	4	9 0 3	144.66
.8084	4	0 9 3	144.66
.8077	9	2 7 7	144.99
.8075	4	3 5 10	145.09

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

m - Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

*Natural mineral.

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16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

Standard x-ray diffraction patterns are presented for 57 substances. Twenty-five of these patterns represent experimental data and 32 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)*

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

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