Standard X-ray Diffraction Powder Patterns

Section 10—Data for 84 Substances

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Errata

Monograph 25

Section 5, pg. 12. The journal reference for Glasser and Dent Glasser (1963) should be J. Am. Ceram. Soc. 46, 377.

Section 8, pgs. iii, 135, 164, 166. On each page, change the subscript for silicon in the formula for meliphanite (sodium calcium beryllium aluminum fluorosilicate). The silicon subscript should be 1.87.

Section 9, pg. 36. In the 1st column of the table, line 15, 1.4287 should read 1.4096.

Section 9, pg. 6. In the 3rd column of the table, line 9, the entry 320 should read 230.

Section 9, pg. 1, column 2; 11th row of text from botton, Avogadro's number should read (6.02252×10^{23})

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

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Circular 539, Vol. 3	178 904
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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 10 - Data for 84 substances

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Eloise H. Evans,[2] and Boris Paretzkin[2]
Assisted by Johan H. deGroot[2] and Simon J. Carmel

Standard x-ray diffraction patterns are presented for 84 substances. Forty-seven of these patterns represent experimental data and 37 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,[3] the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, 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 84 compounds (47 experimental and 37 calculated patterns), and is the twentieth of the series of "Standard X-ray Diffraction Powder Patterns."[4]

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, recrystallizing, or heating in hydrothermal bombs improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

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, 1960].

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

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

Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944].

A computer program [Evans et al., 1963] assigned $hk\ell$'s and refined the lattice constants. Cell refinement was based only upon 2θ values which could be indexed without ambiguity. In indexing cubic patterns, multiple $hk\ell$'s were not reported; instead, we chose the single appropriate index having the largest $\underline{h}$. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample. Unit cell constants and their standard errors were based on least-squares refinement of the variance-covariance matrix derived from the unweighted $\Delta\theta$ residuals. These standard errors derived by the computer program should be increased in most cases. An increase should also be applied to all lattice constant errors in earlier publications of this series.

Densities. These were calculated from the NBS lattice constants, the Avogadro number (6.02252×10^{23}), and atomic weights based on carbon 12 [International Union, 1961].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard (approximately 5 wt. percent tungsten powder). If tungsten lines were found to interfere with lines from the sample, silver or occasionally cadmium oxide was

---

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

[3] 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.

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

used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid aberrations at the very top of the peak, the reading of 2θ was taken at a position about 20 percent of the way down from the top, and in the center of the peak width. The internal standard correction 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.

The internal standards used were of high purity (four 9's). 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 $CuK\alpha_1$ 1.54056Å

hkℓ	W a = 3.16516Å ±.00004	Ag a = 4.08641Å ±.00002	CdO a = 4.69576Å ±.00002
110	40.262		
111		38.112	33.013
200	58.251	44.295	38.304
211	73.184		
220	86.996	64.437	55.287
310	100.632		
311		77.390	65.920
222	114.923	81.533	69.255
321	131.171		
400	153.535	97.875	82.014
331		110.499	91.290
420		114.914	94.378
422		134.871	106.954
511		156.737	116.939
440			136.230
531			152.077
600			159.618

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a curved lithium fluoride crystal monochromator located between the sample and the Geiger counter. Copper radiation was used and the wavelength $K\alpha_1$ was assumed to be 1.54056 Å [Bearden, 1964].

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Fig. 1), and the powdered sample was 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 Fig. 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the intensity of the strongest line. At least three patterns for intensity measurements were prepared for each sample to check reproducibility.

Reference intensity, $I/I_{corundum}$. 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 Figs. 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 113 reflection). 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 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 somewhat at NBS.

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

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

Thermal parameters. The computer program used thermal parameter data of only two forms: the isotropic B's and anisotropic β_{ij}'s; other thermal parameters were converted to one of those 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, in place of using given anisotropic parameters, we used approximately equivalent isotropic parameters, calculated from the equation:

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

Integrated intensities. Intensity calculations were based on the copper $K\alpha_1$ wavelength, 1.54056 Å, determined by Bearden [1964]. 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

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

The intensities were scaled to the strongest line which was assigned a value of 100. Reflections were not reported which had scaled intensities of 0.7 or less.

Scale factor. For each compound, this factor multiplied by the reported integrated intensities will reproduce the unscaled intensities which had been derived using formula (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 value of the half-width was chosen as as 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 0.7 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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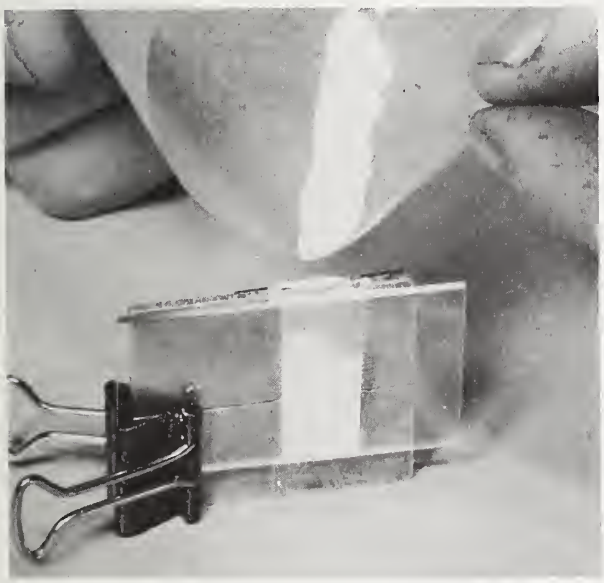

Figure 1

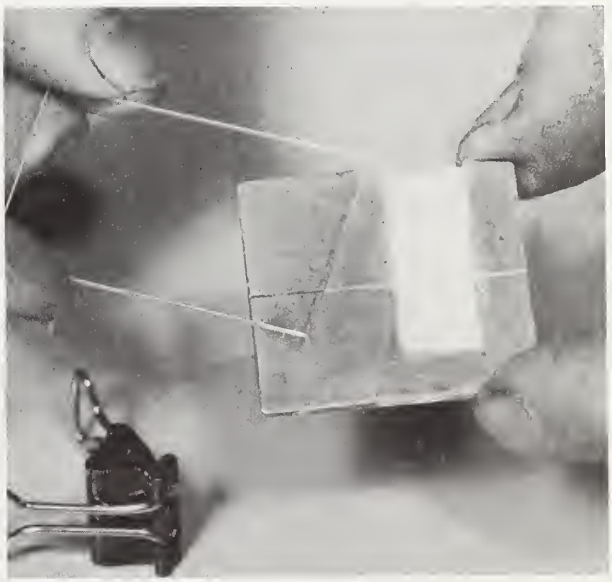

Figure 2

Ammonium aluminum sulfate, $NH_4Al(SO_4)_2$

Sample

Ammonium alum, $NH_4Al(SO_4)_2 \cdot 12H_2O$, was heated at 400 °C for five hours, then sealed in glass and heated at 500 °C for five hours. The sample was hygroscopic and patterns were prepared with the sample in a dry mount.

Color

Colorless

Structure

Hexagonal, P321 (150), Z=1, isostructural with many other dehydrated alums. The structure of $KAl(SO_4)_2$ was determined by Vegard and Maurstad [1929].

NBS lattice constants:

a= 4.7373(2)Å

c= 8.2814(4)

Density

(calculated) 2.446 g/cm^3

Reference intensity

$I/I_{corundum}$ = 3.2

Additional patterns

1. PDF card 3-320 [Dow Chemical Co., Midland, Michigan]

References

Vegard, L. and A. Maurstad (1929). Z. Krist. 69, 519.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
8.28	60	001	10.68
4.14	1	002	21.42
3.678	100	101	24.18
2.915	30	102	30.64
2.759	9	003	32.42
2.368	15	110	37.96
2.291	2	103	39.30
2.277	3	111	39.54
2.071	2	004	43.68
2.056	3	112	44.01
2.051	2	200	44.11
1.991	3	201	45.51
1.849	7	104	49.25
1.839	8	202	49.53
1.798	1	113	50.73
1.6563	1	005	55.43
1.6467	3	203	55.78
1.5587	2	114	59.23
1.5504	1	210	59.58
1.5362	2	105	60.19
1.5245	7	211	60.70
1.4574	4	204	63.81
1.4526	5	212	64.05
1.3805	1	006	67.83
1.3672	6	300	68.58
1.3572	5	115	69.16
1.3493	2	301	69.62
1.3084	1	106	72.13
1.2410	3	214	76.73
1.2254	1	303	77.89
1.1924	1	116	80.48
1.1842	2	220	81.15
1.1450	2	206	84.56
1.1367	1	107	85.32
1.1272	3	311	86.21
1.0971	2	312	89.19
1.0582	1	117	93.42
1.0545	1	305	93.85
1.0519	1	313	94.15
1.0310	1	216	96.68

Ammonium copper bromide hydrate, $(NH_4)_2CuBr_4 \cdot 2H_2O$

Sample

The sample was prepared by slow evaporation at room temperature of a 2:1 aqueous solution of NH_4Br and $CuBr_2$.

Color

Unground: medium olive green
Ground: brilliant yellow green

Optical data

Uniaxial (-), N_o=1.770, N_e=1.725

Structure

Tetragonal, $P4_2/mnm$ (136), Z=2, isostructural with $(NH_4)_2CuCl_4 \cdot 2H_2O$ [Rassenfosse et al.,1933, and Silbertstein, 1936]. The structure of $(NH_4)_2CuCl_4 \cdot 2H_2O$ was determined by Hendricks and Dickinson [1927].

NBS lattice constants:
a = 7.952(1)Å
c = 8.272(1)

Density

(calculated) 3.321 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.6

References

Chrobak, L. (1934). Z. Krist. 88, 35.
Hendricks, S.B. and R.G. Dickinson (1927). J. Am. Chem. Soc. 49, 2149.
Rassenfosse, A., J. Melon, and H. Brasseur (1933). Bull. Soc. Roy. Sci. Liège 2, 32.
Silberstein, A. (1936). Compt. Rend. 202A, 1196.

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

d (Å)	*I*	*hkl*	2θ(°)
5.73	40	101	15.46
5.62	20	110	15.76
4.133	90	002	21.48
3.978	35	200	22.33
3.557	30	210	25.01
3.334	11	112	26.72
3.269	11	211	27.26
2.864	100	202	31.20
2.812	75	220	31.80
2.696	25	212	33.20
2.606	4	103	34.39
2.527	2	301	35.50
2.515	2	310	35.67
2.325	35	222	38.69
2.206	5	320	40.88
2.178	3	213	41.42
2.131	5	321	42.39
2.068	18	004	43.74
1.988	12	400	45.60
1.946	7	322	46.63
1.942	8	114	46.74
1.929	10	410	47.07
1.875	4	330	48.51
1.834	6	204	49.66
1.788	11	214	51.03
1.7481	12	412	52.29
1.7221	2	323	53.14
1.7072	3	332	53.64
1.6659	17	224	55.08
1.6338	7	422	56.26
1.6200	2	105	56.78
1.5911	3	430	57.91
1.5597	3	510	59.19
1.5085	2	324	61.41
1.4997	2	215	61.81
1.4842	4	432	62.53
1.4591	2	512	63.73
1.4330	5	404	65.03
1.4107	6	414	66.19
1.3886	2	334	67.38
1.3786	2	006	67.94
1.3070	3	610	72.22
1.3025	4	206	72.51

Sample

The sample was prepared by evaporating a mixture of the solutions of NH_4OH and HIO_3.

Color

Colorless

Optical data

Biaxial (+) $N \simeq 1.785$, 2V is large. The sample was highly twinned.

Structure

Orthorhombic, $Pc2_1n$ (33), Z = 4 [Crane et al., 1969].

NBS lattice constants:

a = 6.4095(5)Å
b = 9.1706(5)
c = 6.3811(4)

Density

(calculated) 3.417 g/cm^3

Reference intensity

$I/I_{corundum} = 4.8$

Additional patterns

1. Crane et al. [1969]

Polymorphism

At 85 °C a first order transition to a non-polar phase occurs [Crane et al., 1969].

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

d (Å)	I	hkl	2θ(°)
5.26	1	110	16.84
4.586	65	020	19.34
4.523	90	101	19.61
4.057	3	111	21.89
3.220	100	121	27.68
3.190	35	002	27.95
3.013	3	012	29.62
2.865	1	201	31.19
2.760	1	130	32.41
2.732	2	211	32.75
2.626	14	220	34.11
2.618	11	022	34.22
2.533	1	131	35.41
2.427	1	221,122	37.01
2.292	14	040	39.27
2.260	20	202	39.85
2.206	2	032	40.87
2.088	1	132	43.30
2.046	18	141	44.24
2.027	25	222,301	44.67
2.019	18	103	44.86
1.971	<1	113	46.00
1.862	14	042	48.87
1.854	18	321	49.11
1.848	20	123	49.27
1.7428	1	312	52.46
1.7394	<1	213	52.57
1.6857	<1	133	54.38
1.6097	10	242	57.18
1.6022	4	400	57.47
1.5949	3	004	57.76
1.5283	3	060	60.53
1.5181	7	341	60.98
1.5150	10	143	61.12
1.5072	7	303,024	61.47
1.4872	1	313	62.39
1.4479	6	161	64.28
1.4318	8	323,402	65.09
1.4281	6	204	65.28
1.4115	<1	214	66.15
1.3914	<1	350	67.23
1.3794	3	260	67.89
1.3665	3	422	68.62
1.3638	4	224	68.78
1.3521	<1	333	69.46
1.3135	2	440	71.81
1.3094	1	044	72.07
1.2660	3	262,314	74.95
1.2596	3	343	75.40
1.2570	2	501	75.58
1.2187	4	163	78.40
1.2145	6	442	78.73
1.2121	6	244,521	78.91
1.2078	4	125	79.25
1.1463	<1	080	84.44
1.1303	<1	404	85.92
1.1112	1	181	87.77

Reference

Crane, G. R., J. G. Bergman Jr. and A. M. Glass (1969). J. Am. Ceram. Soc. 52, 655.

Sample

The sample was made by heating $NH_4Fe(SO_4)_2 \cdot 12H_2O$ at about 250 °C overnight.

Color

Yellowish - white

Structure

Hexagonal, P321 (150), Z=1, isostructural with many other dehydrated alums. The structure of $KAl(SO_4)_2$ was determined by Vegard and Maurstad [1929].

NBS lattice constants

a = 4.8392(1)Å
c = 8.3138(3)

Density

(calculated) 2.620 g/cm^3

Reference intensity

$I/I_{corundum} = 0.6$

Additional patterns

1. PDF card 3-35 [Vegard and Maurstad, 1929]
2. PDF card 9-9 [Taylor and Bassett, 1952]

References

Taylor, D. and J. Bassett (1952). J. Chem. Soc. 1952, 4431.
Vegard, L.and A. Maurstad (1929). Z.Krist 69,519.

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

d (Å)	*I*	*hkl*	2θ(°)
8.30	65	001	10.65
4.191	6	100	21.18
3.742	100	101	23.76
2.951	45	102	30.26
2.772	6	003	32.27
2.420	30	110	37.12
2.324	8	111	38.72
2.313	9	103	38.91
2.091	8	112	43.23
2.033	7	201	44.54
1.871	14	202	48.63
1.861	12	104	48.89
1.822	4	113	50.02
1.672	5	203	54.88
1.663	2	005	55.19
1.583	3	210	58.22
1.577	8	114	58.49
1.556	12	211	59.35
1.546	2	105	59.77
1.480	8	212	62.71
1.476	6	204	62.91
1.397	11	300	66.92
1.386	2	006	67.55
1.377	5	301	68.02
1.3750	5	213	68.14
1.3702	8	115	68.41
1.3155	3	106	71.68
1.2597	4	214	75.39
1.2472	1	303	76.28
1.2098	3	220	79.09
1.2025	2	116	79.67
1.1975	1	221	80.07
1.1618	1	222	83.06
1.1592	2	304	83.29
1.1557	3	206	83.60
1.1512	5	311	84.00
1.1428	2	107	84.76
1.1194	3	312	86.96
1.0717	2	313	91.90
1.0694	3	305	92.16
1.0456	1	224	94.90
1.0428	2	216	95.23
1.0395	3	401,008	95.63
1.0334	1	207	96.39
1.0159	2	402	98.62
1.0146	2	314	98.79
1.0087	2	108	99.57
0.9838	1	306	103.07
.9800	2	403	103.62
.9782	3	225	103.90
.9551	1	321,118	107.51
.9526	1	315	107.92
.9503	2	217	108.30
.9367	4	322	110.63
.9356	4	404	110.83
.9310	1	208	111.66
.9145	5	410	114.77
.9113	3	226	115.39
.9084	2	323	115.98
.9020	<1	109	117.29
.8905	1	316	119.76
.8727	1	324	123.03
.8690	2	218	124.85
.8630	1	119	126.39

Ammonium magnesium aluminum fluoride, NH_4MgAlF_6

Sample

The sample was precipitated by adding HF solution to an aqueous solution of $MgCl_2$, $AlCl_3$, and NH_4Cl.

Color

Colorless

Optical data

Uniaxial, N <1.40

Structure

Cubic, face centered, structure similar to K_3FeF_6 and other hexafluorides, Z=4.

NBS lattice constant:
a = 9.9892(4)Å

Density

(calculated) 1.221 g/cm^3

Reference intensity

$I/I_{corundum} = 1.0$

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

d (Å)	*I*	*hkl*	2θ(°)
5.77	100	111	15.35
3.012	55	311	29.63
2.886	25	222	30.96
2.498	8	400	35.92
2.292	6	331	39.27
2.040	12	422	44.38
1.923	20	511	47.22
1.7660	20	440	51.72
1.6886	7	531	54.28
1.5796	4	620	58.37
1.5231	6	533	60.76
1.5059	6	622	61.53
1.4417	1	444	64.59
1.3987	8	711	66.83
1.3005	5	731	72.64
1.2486	1	800	76.18
1.1460	1	662	84.47
1.1169	1	840	87.21
1.0896	1	842	89.97
1.0647	<1	664	92.68

Additional patterns

1. PDF card 3-99 [Hanawalt et al., 1938]

References

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

Sample

The sample was prepared by melting a mixture of BaBr and BaF_2, grinding, and annealing at 400°C overnight.

Color

Colorless

Optical data

Uniaxial (-), N_o= 1.738, N_e= 1.724

Structure

Tetragonal, P4/nmm (129), Z=2, matlockite type, by analogy. The structure of PbClF (matlockite) was determined by Nieuwenkamp and Bijvoet[1932].

NBS lattice constants:

a= 4.5109(4)Å
c= 7.443(1)

Density

(calculated) 5.180 g/cm^3

Reference intensity

$I/I_{corundum}$ = 3.3

References

Nieuwenkamp, W. and J.M. Bijvoet (1932). Z.Krist. 81, 469.

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

d (Å)	*I*	*hkl*	2θ(°)
7.45	6	001	11.87
3.86	30	101	23.01
3.723	25	002	23.88
3.192	85	110	27.93
2.871	100	102	31.13
2.483	2	003	36.15
2.422	45	112	37.09
2.256	40	200	39.93
2.174	12	103	41.51
1.959	6	113	46.31
1.949	10	211	46.57
1.929	10	202	47.07
1.860	1	004	48.92
1.773	35	212	51.49
1.720	19	104	53.21
1.607	5	114	57.28
1.595	10	220	57.75
1.565	6	213	58.96
1.488	2	005	62.34
1.4736	3	301	63.03
1.4659	3	222	63.40
1.4264	9	310	65.37
1.4137	2	105	66.03
1.3941	6	302	67.08
1.3676	12	214	68.56
1.3488	3	115	69.65
1.3318	7	312	70.67
1.2854	1	303	73.63
1.2408	5	006	76.75
1.1960	2	106	80.19
1.1860	7	322	81.00
1.1695	3	304	82.39
1.1562	1	116	83.55

?BaF2 **Barium chloride fluoride, BaClF**

Sample
The sample was prepared by melting a stoichiometric mixture of BrF_2 and $BaCl_2$. The sample was then ground and heated to 400 °C overnight.

Color
Colorless

Optical data
Uniaxial (-), N_o= 1.660, N_e= 1.648

Structure
Tetragonal, P4/nmm (129), Z=2, matlockite type, by analogy. The structure of PbClF (matlockite) was determined by Nieuwenkamp and Bijvoet[1932]. Patel and Singh [1969] reported a somewhat larger cell and a different space group.

NBS lattice constants:
a= 4.3936(4)Å
c= 7.226(1)

Density
(calculated) 4.566 g/cm^3

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

Additional patterns
1. PDF card 3-0304 [Dow Chemical Co., Midland, Michigan].

References

Nieuwenkamp, W. and J.M. Bijvoet (1932). Z.Krist. **81**, 469.

Patel, A. R. and R. P. Singh (1969). J. Cryst. Growth **5**, 70.

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

d (Å)	*I*	*hkl*	2θ(°)
7.22	14	001	12.25
3.756	100	101	23.67
3.616	30	002	24.60
3.106	60	110	28.72
2.788	55	102	32.08
2.409	4	003	37.29
2.356	45	112	38.17
2.195	30	200	41.08
2.112	18	103	42.79
1.903	25	113	47.75
1.897	25	211	47.92
1.877	14	202	48.46
1.806	1	004	50.49
1.726	16	212	53.02
1.670	13	104	54.93
1.6229	2	203	56.67
1.5530	6	220	59.47
1.5226	8	213	60.78
1.4451	4	005	64.42
1.4350	5	301	64.93
1.4266	5	222	65.36
1.3894	6	310	67.34
1.3730	2	105	68.25
1.3575	4	302	69.14
1.3302	9	214	70.77
1.3108	4	115	71.98
1.2971	7	312	72.86
1.2518	2	303	75.95
1.2075	5	205	79.27
1.2042	6	006	79.53
1.1614	3	106	83.09
1.1545	2	322	83.70
1.1376	3	304	85.24

Sample

$BaCO_3$ was treated with H_2SO_4. Excess H_2SO_4 was then fumed off and the sample was annealed overnight at 690 °C.

Color

Colorless

Structure

Orthorhombic, Pbnm (62), Z = 4, isostructural with $PbSO_4$ and other bivalent sulfates. The structure was determined by Rinne et al.[1924].

NBS lattice constants:

a = 7.1565(3)Å
b = 8.8811(4)
c = 5.4541(3)

Density

(calculated) 4.472 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.6

Additional patterns

1. PDF card 5-448 [Swanson et al., 1954]

References

Rinne, F., H. Hentschel, and E. Schiebold (1924). Z. Krist. 61, 164.

Swanson, H. E., R. K. Fuyat, and G. M. Ugrinic (1954). Nat'l. Bur. Std. U.S., Circular 539, 3, 65.

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

d (Å)	*I*	*hkl*	2*θ*(°)
5.58	2	110	15.88
4.440	16	020	19.98
4.339	30	101	20.45
3.899	50	111	22.79
3.773	12	120	23.56
3.577	30	200	24.87
3.445	100	021	25.84
3.319	70	210	26.84
3.103	95	121	28.75
2.836	50	211	31.52
2.735	15	130	32.72
2.729	45	002	32.79
2.482	13	221	36.16
2.447	2	112,131	36.69
2.325	14	022	38.70
2.305	6	310	39.05
2.282	8	230	39.46
2.211	25	122	40.78
2.169	3	202	41.60
2.121	80	311,140	42.58
2.106	75	212,231	42.90
2.057	19	041	43.98
1.9486	1	222	46.57
1.9317	7	132	47.00
1.8575	18	330	49.00
1.7889	4	400	51.01
1.7616	8	103	51.86
1.7584	10	312,331	51.96
1.7540	8	410	52.10
1.7284	4	113	52.93
1.7239	5	150	53.08
1.6823	8	023	54.50
1.6741	14	142	54.79
1.6699	11	411	54.94
1.6596	2	420	55.31
1.6440	3	151	55.88
1.6378	8	123	56.11
1.6258	1	340	56.56
1.5944	8	213	57.78
1.5906	6	250	57.93

d (Å)	I	hkl	2θ(°)
1.5876	4	421	58.05
1.5350	15	332	60.24
1.5274	8	251	60.57
1.4958	3	402	61.99
1.4801	2	060	62.72
1.4751	10	412	62.96
1.4570	4	152	63.83
1.4495	1	160	64.20
1.4273	11	313	65.32
1.4246	12	350	65.46
1.4216	11	233	65.62
1.4179	6	422	65.81
1.4067	6	043	66.40
1.4008	8	161	66.72
1.3843	4	501	67.62
1.3786	5	351	67.94
1.3629	18	004,520	68.83
1.3497	4	441	69.60
1.3351	1	432	70.47
1.3265	2	261	71.00
1.3216	4	521	71.30
1.3086	1	243	72.12
1.3030	2	024	72.48
1.3008	4	062	72.62
1.2993	4	333	72.72
1.2886	1	530	73.42
1.2826	1	124	73.82
1.2799	1	162	74.00
1.2742	1	204	74.39
1.2626	10	352,413	75.19
1.2538	2	531,512	75.81
1.2510	1	153	76.01
1.2282	2	451	77.68
1.2249	2	224	77.93
1.2224	4	262	78.12
1.2185	4	522	78.42
1.2030	4	540	79.63
1.1960	4	270	80.19
1.1930	4	600	80.43

Cadmium ammine chloride, $Cd(NH_3)_2Cl_2$

Sample
The sample was made by adding a concentrated NH_4OH solution to a concentrated solution of $CdCl_2$.

Color
Colorless

Optical data
Biaxial, N_α= 1.656, N_γ= 1.705

Structure
Orthorhombic, Cmm2 (35), Z = 2, isostructural with $Cd(NH_3)_2Br_2$. The structure was determined by MacGillavry and Bijvoet [1936].

NBS lattice constants:
a = 8.199(1)Å
b = 8.307(1)
c = 3.960(1)

Density
(calculated) 2.677 g/cm^3

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

Additional patterns
1. MacGillavry and Bijvoet [1936]

References
MacGillavry, C. H. and J. M. Bijvoet (1936). Z. Krist. 94, 231.

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

d (Å)	I	hkl	2θ(°)
5.82	100	110	15.20
4.153	40	020	21.38
4.098	11	200	21.67
3.960	7	001	22.43
3.278	25	111	27.18
2.916	1	220	30.63
2.848	45	201	31.38
2.624	16	130	34.14
2.595	6	310	34.53
2.349	25	221	38.29
2.187	11	131	41.25
2.171	15	311	41.57
2.077	7	040	43.54
2.049	6	400	44.16
1.980	5	002	45.80
1.945	3	330	46.65
1.876	5	112	48.49
1.853	2	240	49.14
1.838	5	420	49.55
1.821	<1	401	50.05
1.787	4	022	51.06
1.746	6	331	52.35
1.678	9	241	54.65
1.668	1	421	55.01
1.628	1	150	56.48
1.609	2	510	57.20
1.580	3	132	58.34
1.576	3	312	58.52
1.5061	1	151	61.52
1.4900	1	511	62.26
1.4587	2	440	63.75
1.4330	2	042	65.03
1.4242	2	402	65.48
1.4200	2	350	65.70
1.4111	1	530	66.17
1.3879	1	332	67.42
1.3845	1	060	67.61
1.3686	<1	441	68.50
1.3471	2	422	69.75
1.3370	1	351	70.36

Cadmium fluoride, CdF_2

Sample
The sample was obtained from the K and K Laboratories Inc., Plainview, N.Y.

Color
Colorless

Optical data
Isotropic, N = 1.562

Structure
Cubic, Fm3m (225), Z=4, isostructural with CaF_2. The structure was determined by Haendler and Bernard [1951].

NBS lattice constant:
a = 5.3895(1)Å

Density
(calculated) 6.349 g/cm^3

Reference intensity
$I/I_{corundum}$ = 7.6

Additional patterns
1. PDF card 5-0567 [Haendler and Bernard, 1951].

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

d (Å)	*I*	*hkl*	2θ(°)
3.112	100	111	28.66
2.695	25	200	33.21
1.9058	60	220	47.68
1.6250	40	311	56.59
1.5559	5	222	59.35
1.3475	7	400	69.73
1.2367	12	331	77.05
1.2054	7	420	79.44
1.1002	10	422	88.87
1.0372	8	511	95.92
.9528	3	440	107.89
.9110	6	531	115.45
.8983	2	600	118.08
.8521	5	620	129.37
.8219	2	533	139.18
.8125	2	622	142.91

References
Haendler, H. M. and W. J. Bernard (1951). J. Am. Chem. Soc. 73, 5218.

Cadmium manganese oxide, $CdMn_2O_4$

Sample

The sample was prepared by heating a 1:1 mixture of CdO and Mn_2O_3 at 900 °C for 17 hours, grinding, and reheating at 900 °C for 3 hours.

Color

Brownish black

Structure

Tetragonal, $I4_1/amd$ (141), Z=4, distorted spinel type. Also, it was found to have the cations in the "normal" spinel positions, at room temperature [Sinha et al., 1957].

NBS lattice constants:
a = 5.832(1)Å
c = 9.754(1)

Density

(calculated) 5.731 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.0

Additional patterns

1. PDF card 20-185 [Toussaint, 1964]
2. Sinha et al. [1957b]

References

Sinha, A. P. B., N. R. Sanjana, and A. B. Biswas (1957a). Acta Cryst. 10, 439.

Sinha, A. P. B., N. R. Sanjana, and A. B. Biswas (1957b). Z. Krist. 109, 410.

Toussaint, J. (1964). Rev. Chim. Minerale 1, 141.

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

d (Å)	*I*	*hkl*	2θ(°)
5.01	4	101	17.69
3.150	80	112	28.31
2.915	35	200	30.64
2.839	70	103	31.49
2.520	100	211	35.60
2.440	3	004	36.81
2.062	3	220	43.88
2.034	5	213	44.51
1.906	3	301	47.68
1.8704	15	204	48.64
1.8504	20	105	49.20
1.7248	20	312	53.05
1.6685	11	303	54.99
1.5954	25	321	57.74
1.5745	35	224	58.58
1.5130	4	116	61.21
1.4581	14	400	63.78
1.4198	2	206	65.71
1.3773	5	305	68.01
1.3231	2	332	71.21
1.2973	8	413	72.85
1.2597	2	422	75.39
1.2289	5	217	77.63
1.2197	7	316,008	78.33
1.1501	4	424	84.10
1.1453	6	415	84.53
1.1247	2	208	86.45
1.1136	2	512	87.53
1.0977	5	433	89.13
1.0761	2	521	91.42
1.0555	3	327	93.73

Sample

The sample was prepared by melting together equimolar amounts of CaF_2 and $CaCl_2$, quenching to 750 °C and heating for 18 hours. The material was unstable in air, and all patterns were made with the material in a dry mount. Because of the instability and because of the incongruent melting (as reported by Wenz et al.[1969]), CaF_2 was often present; its estimated intensity has been deducted where there was overlap at one reflection.

Color

Colorless

Structure

Tetragonal, P4/nmm (129), Z=2, isostructural with matlockite. The structure of PbClF (matlockite) has been determined by Nieuwenkamp and Bijvoet [1932].

NBS lattice constants:

a = 3.8911(1)Å
c = 6.8228(2)

Density

(calculated) 3.039 g/cm^3

Additional patterns

1. PDF card 1-1100 [Hanawalt et al., 1938]

References

Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Nieuwenkamp, W. and J.M. Bijvoet (1932). Z.Krist. 81, 469.
Wenz, D.A., I. Johnson, and R.D. Wolson (1969). J. Chem. Eng. Data 14, 250.

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

d (Å)	*I*	*hkl*	2θ(°)
6.81	10	001	12.99
3.409	9	002	26.12
3.377	6	101	26.37
2.751	50	110	32.52
2.564	100	102	34.97
2.275	2	003	39.58
2.142	50	112	42.16
1.963	17	103	46.20
1.945	35	200	46.66
1.754	4	113	52.11
1.691	5	202	54.21
1.5621	16	104	59.09
1.5502	25	212	59.59
1.4497	5	114	64.19
1.3821	8	213	67.74
1.3757	11	220	68.10
1.3643	9	005	68.75
1.2875	2	105	73.49
1.2302	5	310	77.53
1.2227	5	115	78.10
1.2184	11	214	78.43
1.2124	8	302	78.89
1.1576	6	312	83.43
1.1370	1	006	85.29
1.1266	2	303	86.27
1.1172	12	205	87.18
1.0915	<1	106	89.77
1.0821	1	313	90.77
1.0738	2	215	91.67
1.0510	4	116	94.26
1.0325	3	304	96.50
1.0290	5	322	96.93
.9980	2	314	101.04
.9817	2	206	103.37
.9746	2	007	104.43
.9689	3	225	105.31
.9454	1	107	109.13
.9187	3	117	113.95
.9119	6	324	115.27
.9096	5	412	115.74
.8856	2	332	120.86
.8765	1	226	123.01
.8715	2	207	124.23
.8700	4	420	124.59
.8504	1	217	129.86
.8465	<1	325	131.00

Sample

The sample was prepared by Clyde McDaniel by heating a 1:4 mixture of platinum black and $CaCO_3$ at 1000 °C for several days.

Color

Medium gray

Structure

Hexagonal, $R\bar{3}c$ (167), Z=6, isostructural with Sr_4PtO_6 [McDaniel, 1972]. The structure of Sr_4PtO_6 was determined by Randall and Katz [1959].

NBS lattice constants:

a = 9.3308(1)Å
c = 11.246(1)

Density

(calculated) 5.304 g/cm^3

Reference intensity

$I/I_{corundum}$ = 5.4

Additional patterns

1. McDaniel [1972]

References

McDaniel , C. (1972), to be published in J. Am. Cer. Soc.
Randall, J.J. and L. Katz (1959). Acta Cryst. 12, 519.

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

d (Å)	*I*	*hkl*	2θ(°)
4.665	100	110	19.01
4.616	80	012	19.21
3.282	20	202	27.15
2.922	12	113	30.57
2.694	70	300	33.23
2.654	18	104	33.74
2.333	9	220	38.56
2.308	30	024	38.99
2.198	6	131	41.03
2.081	25	312	43.44
2.068	45	214	43.73
1.980	13	223	45.79
1.901	5	042	47.80
1.830	1	321	49.78
1.8108	1	125	50.35
1.7635	15	410	51.80
1.7524	14	134	52.15
1.7391	13	116	52.58
1.6402	5	404	56.02
1.5959	2	413	57.72
1.5873	<1	315	58.06
1.5549	10	330	59.39
1.5476	15	324	59.70
1.5387	1	306	60.08
1.5134	<1	241	61.19
1.4738	4	422	63.02
1.4613	8	226	63.62
1.4395	1	511	64.70
1.4049	4	152	66.50
1.4011	4	054	66.70
1.3847	4	018	67.60
1.3468	6	600	69.77
1.3418	3	244	70.07
1.3277	3	208	70.92
1.3056	1	137	72.31
1.2931	7	342	73.12
1.2897	4	514	73.35
1.2842	7	416	73.71
1.2770	5	128	74.20
1.2252	<1	161	77.91
1.2194	<1	155	78.35
1.2139	<1	327	78.77
1.2070	1	119	79.31
1.2037	3	612	79.57
1.2010	2	434	79.79
1.1967	1	336	80.13
1.1909	2	318	80.60
1.1664	1	440	82.66
1.1539	1	048	83.76
1.1309	1	072	85.86

d (Å)	*I*	*hkl*	2θ(°)
1.1286	2	164	86.08
1.1202	4	238	86.89
1.1139	1	1·0·10,443	87.50
1.1069	<1	247	88.20
1.1014	1	229	88.75
1.0990	1	262	89.00
1.0936	<1	606	89.55
1.0833	<1	0·2·10	90.64
1.0809	<1	615	90.90
1.0705	2	710	92.04
1.0679	7	354	92.32
1.0647	6	526	92.68
1.0607	3	508	93.14
1.0555	1	2·1·10	93.74
1.0410	3	624	95.45
1.0344	2	428	96.26
1.0180	4	630	98.34
1.0098	2	158	99.42
1.0053	1	1·3·10	100.03
0.9941	<1	802	101.58
.9903	1	446	102.12
.9827	1	4·0·10,633	103.23
.9724	1	722	104.78
.9709	1	544	105.00
.9656	1	348	105.82
.9615	<1	3·2·10	106.47
.9506	2	084	108.25
.9399	<1	455	110.08
.9371	1	0·0·12	110.56
.9330	1	550	111.29
.9314	1	274	111.58
.9294	3	716	111.95
.9268	2	618	112.43
.9189	1	1·1·12	113.92
.9145	1	642	114.76
.9056	1	2·4·10,553	116.55
.9039	1	725	116.90
.8989	1	529	117.94
.8976	1	372	118.23
.8964	1	814	118.47
.8922	5	538	119.38
.8890	2	5·1·10	120.09
.8851	4	3·0·12	120.98
.8817	1	820	121.77
.8802	1	464	122.11
.8762	2	268	123.07
.8696	1	2·2·12	124.70
.8650	1	734	125.88
.8583	1	4·3·10,823	127.64
.8447	1	191	131.54
.8377	3	912	133.71

Sample

The sample was prepared by fusing together CsBr and $CdBr_2$.

Color

Colorless

Structure

Hexagonal, $P6_3/mmc$ (194), Z=2, isostructural with $CsNiCl_3$ and other similar ABX_3 compounds. Tischenko [1955] determined the structure of $CsNiCl_3$, and Soling [1968] reported a refined structure for $CsCoCl_3$.

NBS lattice constants:

a = 7.6767(3)Å
c = 6.7231(4)

Density

(calculated) 4.694 g/cm^3

Reference intensity

$I/I_{corundum} = 5.3$

Polymorphism

A cubic form of $CsCdBr_3$ has been reported by Natta and Passerini [1928], and is represented on PDF card 2-1314.

References

Natta, G. and J. Passerini (1928). Gazz. Chim. Ital. 58, 472

Soling, H. (1968). Acta Chem. Scan. 22, 2793.

Tischenko, G.N. (1955). Tr. Inst. Kristallogr. Akad. Nauk SSSR 1955, 93.

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

d (Å)	*I*	*hkl*	2θ(°)
6.64	30	100	13.32
4.731	6	101	18.74
3.839	35	110	23.15
3.362	17	002	26.49
3.325	5	200	26.79
3.000	10	102	29.76
2.979	100	201	29.97
2.530	4	112	35.45
2.513	6	210	35.70
2.364	35	202	38.04
2.216	6	300	40.69
2.124	1	103	42.52
2.012	8	212	45.01
1.919	25	220	47.34
1.8585	13	203	48.97
1.8441	5	310	49.38
1.7788	<1	311	51.32
1.6809	5	004	54.55
1.6671	6	222	55.04
1.6298	2	104	56.41
1.6128	12	401	57.06
1.5394	2	114	60.05
1.5256	1	320	60.65
1.4900	5	402	62.26
1.4874	4	321	62.38
1.4507	2	410	64.14
1.3973	1	214	66.91
1.3894	2	322	67.34
1.3391	2	304	70.23
1.3351	3	403	70.47
1.2796	1	330	74.02
1.2642	4	224	75.08
1.2566	2	420	75.61
1.2467	2	205	76.32
1.2349	6	421	77.18
1.1941	1	510	80.34
1.1767	3	422	81.78
1.1293	<1	324	86.01
1.1253	1	512	86.39
1.1079	2	600	88.10
1.0983	2	414	89.07
1.0960	2	423	89.31
1.0646	1	520	92.70
1.0616	1	206	93.03
1.0521	1	602	94.13

Cesium manganese fluoride, $CsMnF_3$

Sample

The sample was prepared by V. Minkiewicz at the University of California.

Major impurities

0.01 –0.1 % each: Ca, Li and Na

0.1 –1.0 % each: K and Rb

Color

Light pink

Optical data

Very low double refraction, $N_O \cong 1.527$.

Structure

Hexagonal, $P6_3/mmc$ (194), Z=6, isostructural with hexagonal $BaTiO_3$ and with $RbMnCl_3$ [Simanov et al., 1957] and [Zalkin et al., 1962].

NBS lattice constants:
a = 6.2249(1)Å
c =15.113(1)

Density

(calculated) 4.810 g/cm^3

Reference intensity

$I/I_{corundum} = 3.3$

References

Simanov, Yu. P., L. P. Batsanova, and L. M. Kovba (1957). Zh. Neorgan. Khim. 2, 2410. Russ. J. Inorg. Chem. (English transl.) 2 [10], 207.

Zalkin, A., K. Lee, and D.H. Templeton (1962). J. Chem. Phys. 37, 697.

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

d (Å)	I	hkl	2θ(°)
5.07	2	101	17.47
4.38	9	102	20.25
3.781	5	004	23.51
3.682	35	103	24.15
3.110	100	110	28.68
3.093	70	104	28.84
2.654	7	201	33.75
2.638	5	105	33.96
2.538	16	202	35.33
2.518	12	006	35.62
2.402	7	114	37.41
2.377	30	203	37.82
2.195	40	204	41.09
2.019	8	211	44.86
2.012	11	205	45.02
2.004	12	107	45.20
1.967	5	212	46.11
1.958	5	116	46.33
1.889	7	0·0·8,213	48.14
1.797	20	300	50.77
1.793	30	214	50.88
1.690	6	215	54.23
1.6849	9	207	54.41
1.6229	2	304	56.67
1.6146	7	118	56.99
1.6035	5	109	57.42
1.5561	15	220	59.34
1.5473	5	208	59.71
1.4816	7	217	62.65
1.4669	2	312	63.35
1.4630	2	306	63.54
1.4550	1	1·0·10	63.93
1.4389	2	224	64.73
1.4336	4	313	65.00
1.4254	5	209	65.42
1.3903	8	314	67.29
1.3851	2	218	67.58
1.3601	1	1·1·10	68.99
1.3426	1	401	70.02
1.3401	1	315	70.17
1.3310	2	1·0·11	70.72
1.3269	2	402	70.97
1.3237	1	226	71.17
1.3185	1	2·0·10	71.49
1.3019	6	3·0·8,403	72.55
1.2954	2	219	72.97
1.2694	4	404	74.72
1.2592	2	0·0·12	75.43
1.2305	2	405	77.51
1.2293	4	317	77.60

d (Å)	I	hkl	2θ(°)
1.2204	1	322	78.27
1.2133	1	2·1·10	78.82
1.2011	4	2·2·8,323	79.78
1.1761	7	410	81.83
1.1674	2	1·1·12	82.57
1.1568	1	3·0·10	83.50
1.1433	1	407	84.71
1.1387	2	2·1·11	85.13
1.1234	<1	414	86.58
1.1165	1	319	87.25
1.0973	1	408	89.17
1.0732	1	327	91.74
1.0675	2	2·0·13,502	92.37
1.0658	2	416	92.56
1.0631	2	3·1·10	92.87
1.0543	1	503	93.88
1.0513	2	409	94.23
1.0374	2	330	95.89
1.0316	1	3·0·12	96.61
1.0197	1	1·1·14	98.12
1.0166	1	421	98.53
1.0117	2	3·1·11	99.17
1.0095	2	2·1·13,422	99.46
0.9987	2	4 1 8,423	100.94
.9959	2	329	101.33
.9838	2	424	103.07
.9790	2	2·2·12	103.77
.9647	1	507	105.97
.9604	2	512	106.65
.9573	1	3·2·10	107.15
.9508	1	513	108.22
.9380	1	514	110.41
.9305	1	1·0·16	111.75
.9252	2	3·0·14	112.73
.9213	1	427	113.45
.9192	2	3·2·11	113.86
.9177	1	3·1·13	114.15
.9093	1	338	115.79
.9071	1	509	116.24
.8985	4	600	118.03
.8967	2	428	118.42
.8914	2	2·0·16	119.56
.8870	1	2·2·14	120.56
.8835	2	517	121.36
.8802	2	4·0·13,432	122.12

Holmium fluoride, HoF_3

Sample
The sample was obtained from Pfaltz and Bauer, Inc., Flushing, N.Y.

Color
Pale pink

Structure
Orthorhombic, Pnma (62), Z=4, isostructural with other rare earth fluorides and with YF_3. The structure of YF_3 was determined by Zalkin and Templeton [1953].

NBS lattice constants:

a= 6.396(1)Å
b= 6.874(1)
c= 4.382(1)

Density
(calculated) 7.651 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.4

Polymorphism
A hexagonal form of HoF_3 is reported by Zalkin and Templeton [1953] and is represented by PDF card 5-0572.

Additional patterns
1. PDF card 5-0725 [Zalkin, 1951]

References
Zalkin, A. (1951). Thesis-Univ. of Calf. Berkeley
Zalkin, A. and D.H. Templeton (1953). J.Am. Chem. Soc. **75**, 2453.

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

d (Å)	*I*	*hkl*	2θ(°)
3.697	25	011	24.05
3.617	65	101	24.59
3.437	75	020	25.90
3.203	100	111,200	27.83
2.899	65	210	30.82
2.584	3	201	34.69
2.491	18	121	36.02
2.420	4	211	37.12
2.342	3	220	38.41
2.192	10	002	41.15
2.066	20	221	43.79
1.985	20	112	45.67
1.935	45	131	46.91
1.916	30	301	47.40
1.862	35	230	48.88
1.847	25	022,311	49.29
1.774	14	122	51.46
1.748	15	212	52.30
1.718	12	040	53.27
1.674	14	321	54.78
1.598	6	400	57.62
1.552	6	141	59.52
1.537	5	132	60.16
1.529	3	302	60.51
1.492	5	312	62.17
1.471	8	331	63.16
1.467	8	411	63.34
1.449	4	420	64.22
1.429	7	013	65.23
1.4193	8	232	65.74
1.3965	4	322	66.95
1.3941	3	113	67.08
1.3519	3	042	69.47
1.3287	4	203	70.86
1.3229	4	142	71.22
1.3117	4	051,430	71.92
1.2920	4	402	73.19
1.2850	4	151	73.66
1.2801	7	341	73.99
1.2633	4	250	75.14
1.2394	6	223	76.85
1.2096	5	133,422	79.11

Iron oxalate hydrate (humboldtine), $FeC_2O_4 \cdot 2H_2O$

Sample
The sample was prepared by precipitation from a mixture of $Fe(OH)_2$ and $C_2H_6O_6$.

Color
Brilliant yellow

Structure
Monoclinic, I2/c (15), Z=4. The structure was determined by Deyrieux and Peneloux [1969] who gave 2 possible cells in the C2/c arrangement.

NBS lattice constants:

a= 9.707(1)Å
b= 5.556(1)
c= 9.921(1)
β= 104.50(1)°

Density
(calculated) 2.307 g/cm^3

Reference intensity
$I/I_{corundum} = 1.5$

Polymorphism
Deyrieux and Peneloux described an orthorhombic polymorph which they designated the beta form, referring to their monoclinic form as alpha.

Additional patterns
1. PDF card 14-703 [Hanawalt et al., 1938].
2. Deyrieux and Peneloux [1969]

References

Deyrieux, R. and A. Peneloux (1969). Bull. Soc. Chim. France, 2675.

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

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

d (Å)	*I*	*hkl*	2θ(°)
4.80	100	011,002	18.45
4.70	65	200	18.85
3.880	25	$\bar{2}02$	22.90
3.629	20	$\bar{1}12$	24.51
3.597	25	$\bar{2}11$	24.73
3.172	4	211	28.11
3.004	50	202	29.72
2.778	4	020	32.20
2.654	30	$\bar{2}13$	33.74
2.634	16	$\bar{3}12$	34.01
2.616	25	$\bar{1}21$	34.25
2.396	3	$\bar{2}04$	37.50
2.355	3	$\bar{4}02$	38.19
2.258	13	$\bar{2}22$	39.89
2.224	3	$\bar{4}11$	40.52
2.190	4	213	41.18
2.122	9	$\bar{1}23$	42.56
2.106	8	$\bar{3}21$	42.91
2.037	7	$\bar{3}14$	44.43
2.021	14	$\bar{4}13$	44.80
1.980	3	123	45.80
1.949	11	204	46.56
1.929	9	402	47.07
1.893	15	$\bar{3}23$	48.03
1.847	2	$\bar{2}15$	49.30
1.816	21	$\bar{5}12$,015	50.21
1.795	4	420	50.83
1.779	2	510	51.30
1.727	3	$\bar{1}32$	52.98
1.673	2	132	54.83
1.635	4	$\bar{4}15$,314	56.21
1.625	3	323	56.59
1.6125	2	$\bar{1}25$,$\bar{6}02$	57.07
1.5901	5	$\bar{4}24$,$\bar{5}21$	57.95
1.5473	3	$\bar{6}11$	59.71
1.5302	1	$\bar{5}23$	60.45
1.5081	5	125	61.43
1.4889	3	521	62.31
1.4583	3	332	63.77
1.4370	1	611	64.83
1.4143	2	$\bar{3}34$	66.00
1.3718	3	$\bar{2}17$	68.32
1.3669	5	$\bar{1}41$	68.60
1.3534	2	141	69.38
1.3315	2	017,240	70.69
1.2930	1	$\bar{6}06$	73.13

Lead bromide fluoride, PbBrF

Sample

The sample was prepared by melting a stoichiometric mixture of $PbBr_2$ and PbF_2 at about 550°C. The pattern was sharpened by heating the sample at 300 °C for 72 hours, after grinding.

Optical data

The indices are very high (greater than 2.15).

Color

Yellowish white

Structure

Tetragonal, P4/nmm (129), Z= 2, isostructural with PbClF (matlockite). The structure was determined by Nieuwenkamp and Bijvoet [1932]. Their calculated intensities vary widely from those measured at NBS.

NBS lattice constants:

a= 4.1905(2)Å
c= 7.5913(4)

Density

(calculated) 7.625 g/cm^3

Reference intensity

$I/I_{corundum}$ = 4.8

Additional patterns

1. PDF card 3-1166 [Nieuwenkamp and Bijvoet, 1932].

References

Niewenkamp, W. and J.M. Bijvoet (1932). Z.Krist. 82, 157.

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

d (Å)	I	hkl	2θ(°)
7.62	11	001	11.61
3.797	30	002	23.41
3.670	70	101	24.23
2.964	80	110	30.13
2.814	100	102	31.77
2.531	2	003	35.43
2.336	50	112	38.51
2.167	13	103	41.65
2.095	30	200	43.14
2.020	2	201	44.83
1.924	8	113	47.19
1.834	11	202	49.66
1.820	13	211	50.09
1.729	18	104	52.90
1.681	25	212	54.55
1.614	2	203	57.02
1.599	1	114	57.61
1.5186	4	005	60.96
1.5061	6	213	61.52
1.4814	7	220	62.66
1.4542	1	221	63.97
1.3800	4	222	67.86
1.3739	4	301	68.20
1.3510	4	115	69.52
1.3334	12	214	70.57
1.3252	8	310	71.08
1.3108	5	302	71.98
1.2787	1	221	74.08
1.2647	2	006	75.04
1.2507	5	312	76.03
1.2296	4	205	77.58
1.2229	2	303	78.08
1.2112	2	106	78.98
1.1736	2	313	82.04
1.1636	2	116	82.90
1.1489	2	321	84.20
1.1249	3	304	86.43
1.1114	4	322	87.75
1.0844	2	007	90.52
1.0829	2	206	90.68
1.0603	2	225	93.18

Sample
The sample was prepared by heating a stoichiometric mixture of PbI_2 and PbF_2 in a sealed tube at 450 °C for two hours.

Color
Vivid yellow

Optical data
Extremely high indices (greater than 2.1)

Structure
Tetragonal, P4/nmm (129), Z=2, matlockite type by analogy. The structure of matlockite, PbClF was determined by Nieuwenkamp and Bijvoet[1932].

NBS lattice constants:

a= 4.2382(2)Å
c= 8.800(1)

Density
(calculated) 7.418 g/cm^3

Reference intensity
$I/I_{corundum}$ = 7.1

References
Nieuwenkamp, W. and J.M. Bijvoet (1932). Z. Krist. 81, 469.

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

d (Å)	*I*	*hkl*	2θ(°)
8.81	7	001	10.03
4.399	14	002	20.17
3.818	8	101	23.28
3.052	100	102	29.24
2.996	55	110	29.80
2.932	<1	003	30.46
2.477	20	112	36.24
2.201	3	004	40.98
2.118	25	200	42.66
2.096	3	113	43.12
2.018	1	201	43.87
1.953	18	104	46.46
1.909	5	202	47.59
1.853	1	211	49.14
1.773	7	114	51.49
1.741	30	212	52.53
1.719	1	203	53.26
1.6256	<1	105	56.57
1.5263	2	204	60.62
1.4982	5	220	61.88
1.4667	2	006	63.36
1.4362	10	214	64.87
1.4187	1	222	65.77
1.3451	6	302	69.87
1.3406	7	310	70.14
1.3171	4	116	71.58
1.2819	2	312	73.87
1.2383	1	224	76.93
1.2058	3	206	79.40
1.1887	2	304	80.78
1.1445	2	314	84.60
1.1358	4	322	85.40

Lead oxide sulfate, $Pb_5O_4SO_4$

Sample

The sample was prepared by heating a 4 : 1 mixture of PbO and $PbSO_4$ at 750 °C for one hour, grinding, and reheating at 750 °C for 15 minutes.

Color

Yellowish white

Structure

Monoclinic, $P2_1/a$ (14), Z = 4 [Billhardt, 1970]

NBS lattice constants:

a = 11.532(2)Å
b = 11.717(1)
c = 7.307(1)
β = 91.00(1)°

Density

(calculated) 8.047 g/cm^3

Reference intensity

$I/I_{corundum}$ = 4.9

Additional patterns

1. PDF card 2-1276 [Clark et al.,1936]
2. PDF card 6-0283 [Lander, 1949]
3. PDF card 6-0308, Shell Petroleum Co.
4. Billhardt [1970]
5. Lamb and Miebylski [1951]
6. Zimkina and Shchemelev [1960]

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

d (Å)	*I*	*hkl*	2θ(°)
8.23	10	110	10.74
7.32	4	001	12.08
6.21	4	011	14.26
5.86	1	020	15.10
5.77	3	200	15.34
5.48	2	$\bar{1}11$	16.15
5.43	4	111	16.30
5.175	2	210	17.12
4.491	1	201	19.75
4.269	4	$\bar{1}21$	20.79
3.700	<1	130	24.03
3.489	1	012	25.51
3.444	1	031	25.85
3.326	2	112	26.78
3.294	6	131,$\bar{3}11$	27.05
3.232	100	230	27.58
3.111	45	$\bar{2}02$	28.67
3.060	45	202	29.16
3.006	2	$\bar{2}12$,$\bar{1}22$	29.69
2.967	1	$\bar{2}31$	30.09
2.947	1	231	30.30
2.929	1	040,321	30.49
2.883	.30	400	30.99
2.841	1	140	31.46
2.746	<1	$\bar{2}22$	32.58
2.719	1	041	32.91
2.668	45	032,401	33.56
2.606	3	$\bar{1}32$,$\bar{3}12$	34.39
2.576	2	$\bar{3}31$	34.80
2.563	2	312	34.98
2.465	1	$\bar{2}41$	36.42
2.453	2	241,$\bar{4}21$	36.61
2.433	1	$\bar{2}32$,$\bar{3}22$	36.92
2.397	<1	322	37.49
2.343	1	$\bar{1}13$	38.39
2.329	1	340,113	38.63
2.320	1	430	38.79
2.297	1	150	39.19
2.285	1	042	39.40
2.262	1	510	39.81
2.258	1	$\bar{2}03$	39.90
2.245	2	$\bar{1}42$,402	40.14
2.238	1	142,051	40.26
2.218	2	$\bar{4}31$,$\bar{2}13$	40.65
2.212	2	$\bar{1}23$,341	40.75

References

Billhardt, H.W. (1970). J. Electrochem. Soc. 117, 690.

Clark, G. L., J. N. Mrgudich, and N. C. Schedtz (1936). Z. Anorg. Allgem. Chem. 229, 401.

Lamb, F.W. and L.N. Miebylski (1951). Anal. Chem. 23, 1388.

Lander, J. J. (1949). J. Electrochem. Soc. 95, 174.

Zimkina, T.M. and V.N. Shchemelev (1960). Soviet Physics-solid State, (English transl.) 2, 1489.

d (Å)	I	hkl	2θ(°)
2.204	2	412,431	40.92
2.188	1	151	41.23
2.151	1	511	41.96
2.147	1	520	42.05
2.132	1	$\bar{2}42$	42.36
2.127	1	$\bar{4}22$	42.46
2.116	1	242	42.69
2.068	1	$\bar{5}21$,033	43.74
2.054	1	440	44.05
2.049	1	521	44.16
2.040	<1	$\bar{1}33$	44.36
2.010	1	313	45.06
1.984	2	530,$\bar{4}41$	45.69
1.971	18	441,$\bar{4}32$	46.02
1.952	14	060	46.48
1.945	20	432	46.65
1.923	1	$\bar{5}31$,600	47.23
1.909	1	531,512	47.60
1.886	1	061	48.21
1.872	2	043,$\bar{2}52$	48.59
1.863	3	$\bar{5}22$,$\bar{1}61$	48.84
1.849	1	260	49.24
1.838	1	522	49.56
1.8267	10	611,004	49.88
1.8088	<1	333	50.41
1.7955	1	$\bar{2}61$	50.81
1.7892	2	$\bar{2}43$,$\bar{1}14$	51.00
1.7644	<1	621,541	51.77
1.7603	<1	451,423	51.90
1.7478	<1	352	52.30
1.7239	11	630	53.08
1.7137	5	214,$\bar{6}02$	53.42
1.6886	6	053,602	54.28
1.6710	1	$\bar{5}13$,612	54.90
1.6676	1	153,433	55.02
1.6537	8	$\bar{2}62$	55.52
1.6464	9	262	55.79
1.6316	1	$\bar{5}42$,071,+	56.34
1.6158	6	$\bar{1}71$,253,+	56.94
1.6068	1	270,640,+	57.29
1.5971	8	523,$\bar{2}34$,+	57.67
1.5836	8	234	58.21
1.5720	1	$\bar{2}71$	58.68
1.5552	2	$\bar{4}04$,$\bar{7}21$	59.38
1.5304	3	404	60.44

Lead tin oxide, Pb_2SnO_4

Sample
$PbCO_3$ and SnO_2 in the molar ratio of 2:1 were ground together, heated one week at 750 °C, and one hour at 1000 °C.

Color
Pale greenish yellow

Structure
Tetragonal, $P4_2/mbc$ (135), Z=4, The structure was determined by Byström and Westgren [1943].

NBS lattice constants:
a = 8.7371(4)Å
c = 6.307(1)

Density
(calculated) 8.237 g/cm^3

Reference intensity
$I/I_{corundum} = 1.7$

Additional patterns
1. PDF card 3-1120 Byström and Westgren [1943].
2. PDF card 11-233 Venevcev and Zhdanov [1956].

References

Byström, A. and A. Westgren (1943). Arkiv. Kemi. Mineral. Geol. 16, 7.

Venevcev, Ya.N. and G.S. Zhdanov (1956). Zh. Fiz. Khim. 30, 1324.

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

d (Å)	*I*	*hkl*	2θ(°)
6.180	1	110	14.32
4.365	<1	200	20.33
3.909	1	210	22.73
3.591	2	201	24.77
3.323	100	211	26.81
3.154	9	002	28.27
3.089	7	220	28.88
2.808	20	112	31.84
2.762	30	310	32.39
2.557	14	202	35.07
2.533	<1	311	35.41
2.454	<1	212	36.59
2.423	2	320	37.08
2.261	4	321	39.84
2.206	2	222	40.88
2.183	4	400	41.32
2.078	3	312	43.52
2.059	3	330	43.94
2.008	8	411	45.11
1.954	6	420	46.44
1.921	2	322	47.27
1.867	1	421	48.74
1.851	16	213	49.18
1.795	14	402	50.81
1.759	1	412	51.93
1.748	<1	430	52.29
1.724	17	332	53.07
1.713	1	510	53.45
1.684	1	431	54.44
1.661	<1	422	55.24
1.654	1	511	55.51
1.5878	1	323	58.04
1.5764	5	004	58.50
1.5713	11	521	58.71
1.5443	3	440	59.84
1.5286	<1	432,114	60.52
1.5052	2	521	61.56
1.4980	1	530	61.89
1.4925	3	413	62.14
1.4562	3	600	63.87
1.4183	1	601	65.79
1.4041	1	224	66.54
1.4010	2	611	66.71
1.3876	1	442	67.44
1.3695	5	314	68.45

d (Å)	*I*	*hkl*	2θ(°)
1.3536	<1	532	69.37
1.3338	3	541	70.55
1.3221	1	602,324	71.27
1.3077	<1	612	72.18
1.2845	5	523	73.69
1.2650	2	414,622	75.02
1.2517	1	334,542	75.96
1.2355	<1	550	77.14
1.2269	2	424	77.78
1.2118	<1	205,640	78.94
1.2002	3	720,215	79.85
1.1896	1	641	80.71
1.1862	1	613	80.99
1.1790	<1	721	81.59
1.1602	<1	514	83.20
1.1505	2	552	84.06
1.1473	3	730,315	84.35
1.1446	2	543	84.59
1.1311	3	642,524	85.84
1.1218	<1	722	86.73
1.1190	1	325,650	87.00
1.1033	2	444	88.56
1.1012	1	651	88.77

Lithium gallium oxide, $LiGaO_2$

Sample
The sample was prepared by H. Parker at NBS by heating Li_2CO_3 and Ga_2O_3 together at 900 °C for 8 hours. It was then ground and reheated at 900 °C for 8 hours.

Color
Colorless

Structure
Orthorhombic, $Pna2_1$ (33), Z=4. The structure was determined by Marezio [1965].

NBS lattice constants:

a= 5.4063(1)Å
b= 6.3786(2)
c= 5.0129(1)

Density
(calculated) 4.175 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.4

Polymorphism
Under high pressure $LiGaO_2$ forms a hexagonal polymorph, given on PDF card 18-729 [Marezio and Remeika, 1965]. Chang and Margrave reported an additional high pressure form (called beta $LiGaO_2$);however the data did not index on their reported cell and closely resemble the form studied here.

Additional patterns
1. PDF card 21-494 [Hoffman and Brown, 1968]
2. PDF card 21-495 [Chang and Margrave, 1968]

References

Chang, C.H. and J.L. Margrave (1968).J. Am. Chem. Soc. 90, 2020.
Hoffman, C.W.W. and J. J. Brown (1968). J. Inorg. Nucl. Chem. 30, 63.
Marezio, M. (1965). Acta Cryst. 18, 481.
Marezio, M. and J. P. Remeika (1965). J. Phys. Chem. Solids 26, 1277.

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

d (Å)	*I*	*hkl*	2θ(°)
4.126	80	110	21.52
3.940	100	011	22.55
3.187	25	020,111	27.97
2.749	45	120	32.55
2.703	25	200	33.12
2.508	45	002	35.77
2.491	18	210	36.02
2.411	45	121	37.27
2.381	20	201	37.57
2.230	8	211	40.41
2.142	18	112	42.15
1.979	7	130	45.81
1.959	8	031	46.32
1.852	15	122	49.16
1.839	12	202	49.53
1.766	9	212	51.72
1.672	4	230	54.86
1.639	10	311	56.05
1.617	6	013	56.91
1.595	10	040	57.77
1.586	4	231	58.13
1.569	20	320	58.81
1.553	7	132	59.46
1.549	5	113	59.63
1.4274	17	123	65.32
1.4217	12	203	65.61
1.3903	4	232	67.29
1.3870	3	213	67.47
1.3738	3	240	68.21
1.3514	2	400	69.50
1.3453	6	042	69.86
1.3297	15	322	70.80
1.3258	15	331	71.04
1.3143	3	033	71.76
1.3052	3	142,401	72.32
1.2783	2	411	74.11
1.2764	2	133	74.24
1.2530	1	004	75.87
1.2416	1	150	76.69
1.2364	2	051	77.07
1.2044	5	242	79.52
1.2034	5	313	79.60
1.1991	4	114	79.94
1.1893	1	402	80.73
1.1815	1	233	81.38
1.1695	2	412	82.39
1.1539	1	250	83.76
1.1406	2	430,124	84.96
1.1371	1	204	85.28
1.1244	1	251	86.48

d (Å)	I	hkl	2θ(°)
1.1193	2	214	86.97
1.1122	2	152,431	87.67
1.0660	2	510	92.54
1.0612	6	243	93.08
1.0587	5	134	93.37
1.0508	2	403	94.28
1.0480	3	252	94.62
1.0430	3	160,511	95.21
1.0382	2	432	95.79
1.0367	2	413	95.98
1.0310	1	440	96.68
1.0241	1	520	97.56
1.0213	3	161	97.92
1.0195	2	351	98.15
1.0139	1	053	98.88
1.0098	2	441	99.42
1.0033	2	521	100.31
0.9968	<1	153	101.21
.9904	<1	015	102.11
.9852	1	044	102.86
.9811	1	512	103.47
.9793	2	324	103.73
.9742	1	115	104.50
.9631	1	162	106.22
.9535	1	442	107.78
.9494	1	253	108.45
.9478	2	522	108.72
.9466	2	531	108.93
.9417	4	125	109.76
.9399	3	205	110.07
.9300	1	215	111.84
.9278	1	450	112.25
.9259	1	244	112.60
.9190	<1	404	113.90
.9157	2	360	114.54
.9121	1	451	115.23
.9095	1	414	115.75
.9069	1	035	116.28
.9011	1	600	117.49
.8986	1	513,170	118.00
.8943	<1	135	118.94
.8848	3	163	121.05
.8838	3	353	121.28
.8783	3	611	122.56
.8775	3	443	122.76
.8731	3	523	123.82
.8700	2	452	124.59
.8680	2	315	125.10
.8634	1	270	126.29
.8600	2	362	127.18

Lithium iodate, $LiIO_3$ (tetragonal)

Sample

The sample was made by heating the hexagonal form (City Chemical Co., N. Y.) for 1 hour at 275 °C.

Color

Colorless

Structure

Tetragonal, Z=8, (from measured density) [Unezawa et al., 1970]

NBS lattice constants:

a = 9.727(1)Å
c = 6.153(1)

Density

(calculated) 4.149 g/cm^3

Reference intensity

$I/I_{corundum}$ = 3.4

Polymorphism

On being heated to 255 °C, the hexagonal form changes irreversibly to the tetragonal form, [Unezawa et al., 1970]. The hexagonal form is represented on PDF card 8-465.

References

Unezawa, T., Y. Ninomiya, and S. Tatuoka (1970). J. Appl. Cryst. 3, 417.

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

d (Å)	*I*	*hkl*	2θ(°)
6.90	12	110	12.83
5.21	17	101	17.02
4.87	<1	200	18.22
3.815	70	201	23.30
3.555	40	211	25.03
3.437	100	220	25.90
3.075	8	002,310	29.01
3.002	2	221	29.73
2.935	25	102	30.43
2.869	16	301	31.15
2.751	10	311	32.52
2.513	6	212	35.70
2.432	17	400	36.93
2.293	8	222,330	39.25
2.261	1	401	39.84
2.204	3	411	40.92
2.176	3	312,420	41.47
2.051	25	003,421	44.11
2.029	30	322	44.62
1.908	6	402,510	47.61
1.889	4	203	48.13
1.871	6	412	48.62
1.855	17	431,213	49.07
1.823	4	511	49.99
1.733	16	521,303	52.79
1.720	4	440	53.21
1.707	2	313	53.65
1.644	11	432	55.89
1.610	9	531	57.17
1.567	3	601,403	58.87
1.547	2	611,413	59.71
1.538	6	620,004	60.11
1.491	4	621,423	62.20
1.411	4	631,433	66.17
1.404	4	224	66.54
1.375	6	710,622	68.14
1.361	8	542	68.91
1.3550	9	701,523	69.29
1.3423	5	551	70.04
1.3174	1	641,443	71.56
1.3116	2	632	71.93
1.3005	2	404	72.64
1.2936	<1	533	73.09
1.2769	5	730,334	74.20
1.2254	7	722	77.89
1.2207	4	543,651,+	78.25
1.1929	3	801,205	80.44
1.1838	3	741,633,+	81.19
1.1792	3	820,732	81.57

Sample

The sample was obtained from the City Chemical Corporation, New York, N.Y.

Color

Colorless

Optical data

Biaxial (+) N_α=1.465, N_β=1.53, N_γ=1.696 (as reported in National Research Council Bulletin 107)

Structure

Monoclinic, $P2_1/n$ (14), Z =2. The structure was determined by Beagley and Small [1964].

NBS lattice constants:

a = 3.4029(4)Å
b = 5.1502(4)
c = 9.058(1)
β = 95.60(1)°

Density

(calculated) 2.142 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.0

Additional patterns

1. PDF card 14-759 [Hanawalt et al., 1938].

Reference

Beagley, B. and R.W.H. Small (1964). Acta Cryst. 17, 783.

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

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

d (Å)	*I*	*hkl*	2θ(°)
4.503	20	002	19.70
4.469	65	011	19.85
3.393	1	012	26.24
3.278	18	$\bar{1}$01	27.18
3.073	25	101	29.03
2.829	16	110	31.60
2.765	40	$\bar{1}$11	32.35
2.639	100	111	33.94
2.595	10	013	34.53
2.573	40	020	34.84
2.477	<1	021	36.24
2.367	<1	$\bar{1}$03	37.99
2.255	10	004	39.94
2.237	3	022	40.28
2.149	16	$\bar{1}$13	42.00
2.064	7	014	43.82
2.050	8	120	44.13
2.026	4	$\bar{1}$21	44.69
1.982	2	113	45.74
1.974	3	121	45.94
1.910	<1	$\bar{1}$22	47.58
1.837	2	$\bar{1}$14	49.58
1.826	2	122	49.91
1.742	7	$\bar{1}$23	52.48
1.695	16	024	54.05
1.686	8	031	54.37
1.661	1	$\bar{1}$05	55.27
1.638	<1	$\bar{2}$02	56.10
1.609	6	$\bar{2}$11,210	57.22
1.580	1	$\bar{1}$15	58.36
1.564	1	$\bar{1}$24	59.02
1.5614	1	$\bar{2}$12	59.12
1.5368	2	202	60.16
1.5213	<1	$\bar{1}$31	60.84
1.4986	4	131	61.86
1.4769	3	025,$\bar{2}$13	62.87
1.4734	5	124	63.04
1.4678	4	115	63.31
1.4311	2	132	65.13
1.4154	2	$\bar{2}$21,220	65.94
1.3892	3	$\bar{1}$33	67.35
1.3807	2	221	67.82
1.3741	2	$\bar{1}$16	68.19
1.3708	2	$\bar{2}$14	68.38
1.3406	1	133	70.14
1.2941	1	204	73.06
1.2872	1	040	73.51
1.2493	2	017	76.13
1.2448	4	$\bar{2}$24,$\bar{1}$07	76.46
1.2379	2	042	76.96

Magnesium manganese oxide, $MgMn_2O_4$

Sample

The sample was prepared by heating MgO and Mn_3O_4 in the proportions of 3:2 at 800 °C for 16 hours, then at 1100 °C for one and one half hours and cooled very slowly.

Color

Black

Structure

Tetragonal, $I4_1/amd$ (141), Z=4, distorted spinel type [Sinha et al., 1957]. Also, it was found to have the cations in the "normal"spinel positions, at room temperature [Mănăilă and Păușescu, 1965].

NBS lattice constants:

a = 5.728(1) Å

c = 9.346(1)

Density

(calculated) 4.293 g/cm^3

Reference intensity

$I/I_{corundum} = 1.4$

Polymorphism

The cell size of the tetragonal form varies considerably with thermal history of the sample. Above about 950 °C $MgMn_2O_4$,transforms reversibly to a cubic spinel structure [Mănăilă and Păușescu, 1965].

References

Mănăilă, R. and P. Păușescu (1965). Phys. stat. sol. 9, 385.

Sinha, A. P. B., N. R. Sanjana, and A. B. Biswas (1957). Acta Cryst. 10, 439.

Internal standard W, a = 3.16516 Å

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

d (Å)	*I*	*hkl*	2θ (°)
4.884	100	101	18.15
3.061	20	112	29.15
2.863	10	200	31.21
2.736	70	103	32.70
2.470	95	211	36.34
2.442	20	202	36.78
2.336	30	004	38.50
2.025	40	220	44.71
1.979	6	213	45.81
1.872	4	301	48.60
1.8108	5	204	50.35
1.7769	17	105	51.38
1.6892	7	312	54.26
1.6277	8	303	56.49
1.5664	25	321	58.91
1.5306	50	224	60.43
1.5103	8	215	61.33
1.4538	5	116	63.99
1.4320	25	400,314	65.08
1.4151	6	323	65.96
1.3741	5	411	68.19
1.3683	6	402,206	68.52
1.3358	6	305	70.43
1.2972	4	332	72.85
1.2811	3	420	73.92
1.2689	13	413	74.75
1.2355	8	422	77.14
1.2210	11	404	78.23
1.2107	6	325	79.02
1.1839	11	217	81.18
1.1811	4	316	81.41
1.1682	6	008	82.50
1.1369	9	431	85.30
1.1232	4	424	86.60
1.1150	9	415	87.39
1.0920	6	512	89.72
1.0750	9	433	91.54
1.0569	5	521	93.57
1.0220	8	327,109	97.82
1.0123	10	514,228	99.09
0.9892	6	426	102.28
.9766	7	435	104.13
.9623	5	219	106.35
.9370	6	611	110.59
.9355	5	602	110.85
.9290	3	444	112.01
.9053	11	408	116.60

Magnesium nickel oxide, $MgNiO_2$

Sample
The sample was prepared by heating MgO and NiO together, then reheating the product at 1000 °C for 70 hours.

Color
Grayish-yellow green

Structure
Cubic, Fm3m (225),Z=2, isostructural with NaCl. $MgNiO_2$ is the midpoint in the complete solid solution series from NiO to MgO [Wartenburg and Prophet, 1932]

NBS lattice constant:
a = 4.1926(1)Å

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

d (Å)	*I*	*hkl*	2θ(°)
2.421	45	111	37.11
2.097	100	200	43.10
1.4827	50	220	62.60
1.2640	14	311	75.09
1.2103	15	222	79.05
1.0482	6	400	94.59
0.9620	5	331	106.40
.9375	15	420	110.50
.8557	11	422	128.35
.8068	3	511	145.37

Density
(calculated) 5.183 g/cm^3

Reference intensity
$I/I_{corundum}$ = 3.6

Additional patterns
1. PDF card 3-999 [Holgersson and Karlsson, 1929]

References

Holgersson, S. and A. Karlsson (1929). Z. anorg. u. allgem. Chem. 182, 255.

Wartenburg, V.H.,and E. Prophet (1932). Z. anorg. u. allgem. Chem. 208, 379.

Magnesium tin oxide, Mg_2SnO_4

Sample
The sample was prepared by heating a 2 : 1 mixture of MgO and SnO_2 for 17 hours at 1500 °C, followed by regrinding and reheating at 1500 °C for one hour.

Color
Light bluish white

Optical data
Isotropic, N = 1.79

Structure
Cubic, Fd3m (227), Z = 8, inverse spinel type [Natta and Passerini, 1929].

NBS lattice constants:
a = 8.6376(1)Å

Density
(calculated) 4.768 g/cm^3

Reference intensity
$I/I_{corundum}$ = 3.6

Additional patterns
1. Natta and Passerini [1929]
2. Colin [1963]

References

Colin, M-L. (1963). Bull. Soc. Roy. Sci. Liege 32, 110.

Natta, G. and L. Passerini (1929). Rend. Accad. Naz. Lincei 9, 557.

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

d (Å)	*I*	*hkl*	2θ(°)
4.98	85	111	17.79
3.055	8	220	29.21
2.604	100	311	34.41
2.493	20	222	35.99
2.160	55	400	41.79
1.981	11	331	45.76
1.764	2	422	51.79
1.6623	30	511	55.21
1.5270	45	440	60.59
1.4599	11	531	63.69
1.3657	1	620	68.67
1.3173	8	533	71.57
1.3022	9	622	72.53
1.2467	8	444	76.32
1.2094	4	711	79.12
1.1542	1	642	83.73
1.1244	12	731	86.48
1.0796	5	800	91.04
1.0553	1	733	93.76
1.0179	<1	822	98.35
0.9975	7	751	101.11
.9907	4	662	102.06
.9657	8	840	105.81
.9480	3	911	108.68
.9207	<1	664	113.57
.9055	5	931	116.56
.8816	12	844	121.80
.8681	3	933	125.07
.8470	1	10·2·0	130.84
.8350	7	951	134.58
.8312	5	10·2·2	135.87
.8055	3	953	146.00

Sample

The sample of MnO_2, obtained from T. Baker Chemical Co., Phillipsburg, N.J., was prepared by heating to 1000 °C for three days.

Color

Unground: purplish black
ground: dark brown

Structure

Tetragonal, $I4_1/amd$ (141), Z=4, distorted spinel type [Aminoff, 1926].

NBS lattice constants:
a = 5.7621(1)Å
c = 9.4696(4)

Density

(calculated) 4.834 g/cm^3

Reference intensity

$I/I_{corundum} = 1.5$

Polymorphism

Mn_3O_4 transforms reversibly at 1170 °C to a cubic spinel, represented by card 4-732 [McMurdie and Golovato, 1948].

Additional patterns

1. PDF card 16-154 (from a natural mineral) [Nuffield, 1962].

References

Aminoff, G. (1926). Z. Krist. 64, 475.
McMurdie, H.F. and E.Golovato (1948). J.Res. Nat. Bur. Std. 41, 589.
Nuffield, E.W. (1962). Geol. Soc. Amer. Mem. 85, 195.

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

d (Å)	*I*	*hkl*	2θ(°)
4.924	30	101	18.00
3.089	40	112	28.88
2.881	17	200	31.01
2.768	85	103	32.31
2.487	100	211	36.08
2.463	20	202	36.45
2.367	20	004	37.99
2.0369	20	220	44.44
1.8288	7	204	49.82
1.7988	25	105	50.71
1.7008	10	312	53.86
1.6405	8	303	56.01
1.5762	25	321	58.51
1.5443	50	224	59.84
1.5260	2	215	60.63
1.4721	3	116	63.10
1.4405	20	400	64.65
1.4260	3	323	65.39
1.3841	4	206	67.63
1.3823	2	411	67.74
1.3487	6	305	69.66
1.3055	1	332	72.32
1.2777	10	413	74.15
1.2431	6	422	76.58
1.2305	5	404	77.51
1.2212	1	325	78.21
1.1978	5	217	80.05
1.1935	4	316	80.39
1.1836	4	008	81.20
1.1439	2	431	84.66
1.1316	4	424	85.80
1.1245	8	415	86.47
1.0993	2	512	88.97
1.0826	8	503	90.72
1.0632	3	521	92.85
1.0325	5	327	96.50
1.0235	3	228	97.63
1.0185	6	440	98.27
0.9981	1	426	101.02
.9845	5	435	102.97
.9743	5	219	104.49
.9674	2	532	105.55
.9425	3	611	109.62
.9357	2	444	110.81
.9222	2	1·1·10	113.28
.9189	2	516	113.92
.9146	6	408	114.74

Manganese oxide (pyrolusite), β-MnO_2

Sample

The sample was obtained from Baker Chemical Co. Phillipsburg, N.J.

Color

Dark grey

Structure

Tetragonal, $P4_2/mnm$ (136), Z = 2, rutile type, determined by Goldschmidt [1926] and Ferrari [1926].

NBS lattice constants: Å
a = 4.3999(1)A
c = 2.8740(1)

Density

(calculated) 5.189 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.7

Polymorphism

MnO_2 occurs in several crystal modifications. The mineral ramsdellite, α-MnO_2, is represented by PDF card 7-222. A number of poorly crystallized synthetic polymorphs are represented by PDF cards 12-141, 12-714, 12-720, 14-644, and 18-802.

Additional patterns

1. PDF card 12-716 [Sorem and Cameron, 1960]
2. McMurdie and Golovato [1948]

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

d (Å)	I	hkl	2θ(°)
3.110	100	110	28.68
2.407	55	101	37.33
2.199	8	200	41.01
2.110	16	111	42.82
1.9681	5	210	46.08
1.6234	55	211	56.65
1.5554	14	220	59.37
1.4370	8	002	64.83
1.3912	8	310	67.24
1.3677	<1	221	68.55
1.3064	20	301	72.26
1.3045	20	112	72.38
1.2524	1	311	75.91
1.2029	3	202	79.64
1.1604	1	212	83.18
1.1232	5	321	86.60
1.1000	2	400	88.89
1.0556	6	222	93.72
1.0370	3	330	95.94
0.9998	11	312,411	100.78
.9838	3	420	103.06
.9360	3	103	110.77
.8734	3	402	123.75
.8629	3	510	126.41
.8614	8	213	126.81
.8567	<1	412	128.09
.8410	7	332,431	132.67

References

Ferrari, A. (1926). Rend. Accad. Naz. Lincei, 3, 224.

Goldschmidt, V.M. (1926). Skrifter Norske Videns-kaps-Akad. Oslo, I Mat.-Naturv. Kl. 1926, No. 1

McMurdie, H. F. and E. Golovato (1948). J. Res. Nat. Bur. Std. 41, 589.

Sorem, R.K. and E.N. Cameron (1960). Econ. Geol. 55, 278.

Mercury amide chloride, $HgNH_2Cl$

Sample
The sample was prepared by adding a concentrated NH_4OH solution to a concentrated $HgCl_2$ solution.

Color
Colorless

Structure
Orthorhombic, Pmm2 (25), Z=2. The structure of $HgNH_2Cl$ was determined by Lipscomb [1951].

NBS lattice constants:
a = 5.1558(3)Å
b = 6.7158(3)
c = 4.3529(2)

Density
(calculated) 5.554 g/cm^3

Reference intensity
$I/I_{corundum}$ = 5.3

Additional patterns
1. PDF card 6-265 [Lipscomb,1951]

References
Lipscomb, W.N. (1951). Acta Cryst. 4, 244.

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

d (Å)	*I*	*hkl*	2θ(°)
5.16	100	100	17.17
4.352	65	001	20.39
4.088	2	110	21.72
3.356	30	020	26.54
3.327	70	101	26.77
2.980	10	111	29.96
2.813	50	120	31.79
2.658	45	021	33.69
2.577	9	200	34.78
2.362	40	121	38.06
2.218	30	201	40.64
2.176	15	002	41.46
2.106	<1	211	42.91
2.044	25	220	44.27
2.005	11	102	45.18
1.922	1	112	47.26
1.857	4	131	49.01
1.850	17	221	49.21
1.826	5	022	49.89
1.721	14	122	53.18
1.6792	6	040	54.61
1.6634	4	202	55.17
1.5971	8	140	57.67
1.5667	4	041	58.90
1.5553	1	311	59.37
1.5302	3	320	60.45
1.4984	8	141	61.87
1.4940	7	132	62.07
1.4900	12	222	62.26
1.4507	1	003	64.14
1.4433	7	321	64.51
1.4066	2	240	66.41
1.3967	2	103	66.94
1.3671	<1	113	68.59
1.3627	1	330	68.84
1.3488	3	302	69.65
1.3388	6	241	70.25
1.3350	5	232	70.48
1.3320	5	023	70.66
1.3297	5	042	70.80

d (Å)	I	hkl	2θ(°)
1.2893	5	123,400	73.37
1.2872	6	142	73.51
1.2646	2	203	75.05
1.2518	2	322	75.95
1.2360	1	401	77.10
1.2030	2	420	79.63
1.2010	2	340	79.79
1.1830	2	223	81.25
1.1816	2	242	81.37
1.1596	2	421	83.25
1.1578	3	341	83.41
1.1193	1	060	86.97
1.1089	2	402,303	88.00
1.0977	<1	043	89.13
1.0937	1	313,160	89.54
1.0840	1	061	90.57
1.0735	1	143	91.70
1.0646	1	104	92.69
1.0609	2	161	93.11
1.0528	2	422,323	94.05
1.0517	2	114,342	94.18
1.0313	<1	500	96.64
1.0267	1	260	97.23
1.0223	1	440	97.78
1.0151	<1	124	98.72
1.0100	1	243	99.40
1.0028	1	204	100.37
0.9994	1	261	100.84
.9955	1	062,441	101.39
.9858	<1	520,053	102.77

Potassium magnesium fluoride, K_2MgF_4

Sample
The sample was prepared by heating a 2:1 mixture of KF and MgF_2 for 1½ hours at 750 °C. The material was somewhat hygroscopic.

Color
Colorless

Optical data
Very low double refraction, N <1.4

Structure
Tetragonal, I4/mmm (139), Z=2. The structure was determined by Brehler and Winkler [1954].

NBS lattice constants:
a = 3.9731(2)Å
c = 13.172(1)

Density
(calculated) 2.851 g/cm^3

Additional patterns
1. PDF card 6-0589 [DeVries and Roy, 1953].
2. Remy and Hansen [1956].

References

Brehler, B. and H.G.F. Winkler (1954). Heidelberger Beitr. Mineral. Petrog. 4, 6.

DeVries, R.C. and R. Roy (1953). J. Am. Chem. Soc. 75, 2479.

Remy, H. and F. Hansen (1956). Z. Anorg. Allgem. Chem. 283, 277.

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

d (Å)	*I*	*hkl*	2θ(°)
6.57	30	002	13.46
3.292	11	004	27.06
2.945	85	103	30.32
2.810	100	110	31.82
2.585	35	112	34.67
2.194	70	105,006	41.10
2.137	85	114	42.25
1.987	85	200	45.61
1.902	12	202	47.79
1.7300	20	211,116	52.88
1.7008	4	204,107	53.86
1.6464	25	213,008	55.79
1.4734	35	215,206	63.04
1.4204	1	118	65.68
1.4049	16	220	66.50
1.3734	3	222,109	68.23
1.3171	<1	301,0·0·10	71.58
1.2915	1	224,217	73.23
1.2676	8	303,208	74.84
1.2563	6	310	75.63
1.2344	1	312	77.22
1.1928	6	1·1·10	80.45
1.1833	9	305,226	81.23
1.1737	7	314	82.03
1.1466	2	1·0·11	84.41
1.1296	2	219	85.99
1.0977	2	2·0·10,0·0·12	89.13
1.0905	5	316	89.88
1.0687	6	323,228	92.24
1.0223	<1	1·1·12	97.78
0.9932	4	400,2·1·11	101.71
.9816	<1	1·0·13,411	103.39
.9607	2	2·2·10,2·0·12	106.61
.9409	3	0·0·14	109.91
.9090	3	3·1·10	115.85
.9049	3	415,406	116.70
.8923	3	1·1·14	119.37
.8884	5	420,3·0·11	120.24

Potassium magnesium selenate hydrate, $K_2Mg(SeO_4)_2 \cdot 6H_2O$

Sample
The sample was prepared by slow evaporation of a 1:1 aqueous solution of K_2SeO_4 and $MgSeO_4$ at room temperature.

Color
Colorless

Optical data
Biaxial (+) N_α= 1.4969, N_β= 1.4991, N_γ= 1.5139, 2V= 39° 42' (Tutton, 1901).

Structure
Monoclinic, $P2_1/a$ (14), Z=2. $K_2Mg(SeO_4)_2 \cdot 6H_2O$ is a "Tutton Salt" [Tutton, 1901]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton [1962].

NBS lattice constants:

a= 9.273(1)Å
b=12.431(1)
c= 6.258(1)
β= 104.33(1)°

Density
(calculated) 2.359 g/cm^3

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

References

Margulis, T. N. and D. H. Templeton (1962). Z. Krist. 117, 334.

Tutton, A.E.H. (1901). Proc. Roy. Soc. London, series A, 97, 255.

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

d (Å)	*I*	*hkl*	2θ(°)
7.28	45	110	12.15
5.453	45	011	16.24
5.196	6	$\bar{1}11$	17.05
5.116	14	120	17.32
4.494	16	200	19.74
4.346	10	021	20.42
4.263	75	111	20.82
4.219	60	210,$\bar{1}21$	21.04
4.132	85	$\bar{2}01$	21.49
3.923	15	$\bar{2}11$	22.65
3.764	100	130	23.62
3.663	25	121	24.28
3.423	20	031	26.01
3.359	15	$\bar{1}31$	26.51
3.248	40	201	27.44
3.144	25	211	28.36
3.108	40	040	28.70
3.059	20	131	29.17
3.025	60	$\bar{1}12$	29.50
2.926	18	$\bar{2}31$	30.53
2.912	30	$\bar{3}11$,310	30.68
2.879	20	221	31.04
2.863	25	$\bar{2}02$	31.22
2.790	8	$\bar{2}12$	32.05
2.785	14	$\bar{1}22$	32.11
2.731	4	$\bar{1}41$	32.76
2.725	2	022	32.84
2.699	12	$\bar{3}21$,320	33.17
2.616	2	112	34.25
2.564	9	141	34.97
2.556	12	240,231	35.08
2.491	15	$\bar{1}32$	36.02
2.483	15	$\bar{2}41$	36.14
2.445	6	032	36.72
2.426	40	$\bar{3}31$,330	37.02
2.407	2	$\bar{3}12$,311	37.32
2.355	2	$\bar{2}32$	38.19
2.300	2	051,$\bar{4}01$	39.14
2.246	30	400,241	40.11
2.210	7	410	40.79
2.170	17	042	41.58
2.156	11	$\bar{3}41$,340,+	41.86
2.130	2	$\bar{2}51$,222	42.41
2.111	16	420,331,+	42.80
2.105	14	$\bar{2}42$	42.93
2.072	2	060	43.65
2.066	2	$\bar{4}02$	43.78
2.037	2	$\bar{4}12$	44.43
2.021	8	003	44.81
1.994	3	013	45.45

d (Å)	*I*	*hkl*	2θ(°)
1.978	2	$\bar{1}23$	45.83
1.974	6	430,251	45.94
1.948	5	$\bar{1}61$	46.58
1.943	3	$\bar{1}52$	46.70
1.926	4	$\bar{3}42$,341	47.16
1.922	4	052,023	47.26
1.914	6	$\bar{3}51$,350	47.47
1.885	13	312,161	48.24
1.862	2	$\bar{1}33$	48.87
1.852	8	$\bar{2}61$	49.16
1.847	7	$\bar{4}32$,$\bar{4}41$	49.29
1.831	8	$\bar{2}33$,242	49.77
1.824	11	$\bar{3}23$,322,+	49.97
1.820	13	440	50.09
1.795	4	123	50.83
1.779	9	510	51.32
1.774	6	$\bar{5}21$	51.46
1.747	4	351,261,+	52.34
1.742	4	170	52.49
1.733	9	$\bar{3}33$,332,+	52.79
1.729	9	$\bar{4}03$,$\bar{5}12$	52.90
1.721	5	$\bar{4}42$	53.17
1.708	10	133	53.62
1.703	9	$\bar{3}61$,360,+	53.77
1.693	4	043,203	54.11
1.681	2	$\bar{5}22$,$\bar{2}62$	54.56
1.674	3	252	54.78
1.666	5	$\bar{4}23$,450	55.09
1.653	6	441,171	55.55
1.648	6	530	55.72
1.639	2	162	56.06
1.609	5	$\bar{5}32$,412	57.20
1.596	1	$\bar{4}33$	57.70
1.591	1	$\bar{5}41$	57.90
1.589	3	$\bar{4}52$	58.00
1.583	2	$\bar{3}62$,361	58.22
1.567	4	233	58.88
1.565	5	521	58.98
1.557	3	271,$\bar{2}04$	59.31
1.542	5	$\bar{1}72$	59.93
1.533	5	072	60.34

Sample

The sample was prepared by treating a 2:1 mixture of KF and Ni with HF, drying at 120 °C and heating for one half hour at 900 °C.

Color

Pale yellowish green

Optical data

Very low double refraction, N ≅ 1.432.

Structure

Tetragonal, I4/mmm (139), Z=2, isostructural with K_2MgF_4 and similar tetrafluorides. The structure was determined Balz [1953].

NBS lattice constants:
a = 4.0099(1)Å
c = 13.087(1)

Density

(calculated) 3.360 g/cm^3

Reference intensity

$I/I_{corundum}$ = 5.1

Additional patterns

1. PDF card 10-107 [Insley et al., 1956].

References

Balz, D. (1953). Naturwiss. 40, 241.
Insley, H., T. N. McVay, R. E. Thoma, and G.D. White (1956). ORNL-2192, 34.

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

d (Å)	*I*	*hkl*	2θ(°)
6.53	100	002	13.54
3.837	10	101	23.16
2.953	60	103	30.24
2.836	40	110	31.52
2.603	2	112	34.42
2.192	18	105	41.14
2.181	45	006	41.36
2.143	15	114	42.13
2.005	35	200	45.19
1.918	5	202	47.37
1.777	2	211	51.37
1.7287	13	116	52.92
1.6585	13	213	55.35
1.6359	8	008	56.18
1.4791	9	215	62.77
1.4757	18	206	62.93
1.4173	9	220,118	65.84
1.3856	1	222	67.55
1.3669	2	109	68.60
1.2782	2	303	74.12
1.2679	8	310,208	74.82
1.1886	6	226,1·1·10	80.79
1.1826	2	314	81.29
1.1406	4	1·0·11	84.96
1.1297	2	219	85.98
1.0960	3	316,2·0·10	89.31
1.0907	2	0·0·12	89.86
1.0777	2	323	91.24
1.0715	1	228	91.92
1.0235	1	325	97.63
1.0179	1	1·1·12	98.35
1.0023	2	400,318	100.44
0.9913	2	2·1·11	101.98
.9840	<1	309	103.04
.9581	1	2·0·12	107.02
.9492	2	413	108.49
.9452	1	330	109.17
.9347	<1	0·0·14	110.98
.9108	3	406,3·1·10	115.50
.8967	3	420	118.42
.8886	2	3·0·11	120.18
.8877	2	1·1·14	120.38
.8834	1	329	121.37
.8671	1	336	125.32
.8644	<1	2·2·12	126.03
.8547	1	408	128.62
.8472	3	2·0·14	130.79

Potassium zinc fluoride, K_2ZnF_4

Sample

Hydrofluoric acid was added to a 1:2 mixture of zinc and potassium fluoride and the solution was evaporated. More hydrofluoric acid was added. The evaporation was repeated, the product dried at 200 °C, and heated for one hour at 480 °C.

Color

Colorless

Structure

Tetragonal, I4/mmm (139), Z=2 [Schmitz-DuMont and Bornefeld, 1956], isostructural with K_2MgF_4 and similar tetrafluorides.

NBS lattice constants:

a = 4.0564(1)Å
c = 13.110(1)

Density

(calculated) 3.380 g/cm^3

Reference intensity

$I/I_{corundum} = 2.1$

Additional patterns

1. PDF card 13-95 [Schmitz-DuMont and Bornefeld 1956]

References

Schmitz-DuMont O. and H. Bornefeld (1956). Z. Anorg. Allgem. Chem. 287, 120.

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

d (Å)	*I*	*hkl*	2θ(°)
6.56	80	002	13.49
3.88	30	101	22.91
2.973	100	103	30.03
2.868	95	110	31.16
2.203	25	105	40.93
2.185	40	006	41.28
2.159	15	114	41.80
2.029	60	200	44.63
1.938	11	202	46.84
1.797	5	211	50.75
1.738	19	116	52.61
1.700	1	107	53.87
1.676	25	213	54.73
1.639	5	008	56.07
1.492	13	215	62.17
1.4869	25	206	62.40
1.4342	11	220	64.97
1.4233	4	118	65.53
1.4010	2	222	66.71
1.3711	3	109	68.36
1.3448	1	301	69.89
1.3141	<1	224	71.77
1.3030	<1	217	72.48
1.2918	4	303	73.21
1.2829	6	310	73.80
1.2747	5	208	74.35
1.1991	8	226	79.94
1.1926	3	1·1·10	80.46
1.1435	3	1·0·11	84.69
1.1358	2	219	85.40
1.1211	<1	321	86.80
1.1061	4	316	88.28
1.0924	1	0·0·12	89.68
1.0894	4	323	89.99
1.0793	2	228	91.07
1.0340	1	325	96.31
1.0209	<1	1·1·12	97.96
1.0141	2	400	98.85
1.0101	2	318	99.38
1.0022	1	402	100.46
.9960	3	2·1·11	101.32
.9618	2	2·0·12	106.42
.9596	4	413	106.78
.9561	2	330	107.35
.9364	<1	0·0·14	110.70
.9208	3	415	113.55
.9198	2	406	113.74
.9071	3	420	116.25
.8984	<1	422	118.04
.8940	2	3·0·11	119.00
.8902	2	1·1·14,329	119.83

Sample

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

Color

Very light bluish green

Optical data

Uniaxial (-), $N_o = 1.648$, $N_e = 1.621$

Structure

Tetragonal, $P4_2/mnm$ (136), Z = 2, isostructural with $K_2CuCl_4 \cdot 2H_2O$ [Hendricks and Dickinson, 1927]. The structure of $K_2CuCl_4 \cdot 2H_2O$ was refined by Chrobak [1934].

NBS lattice constants:
a = 7.609(1)Å
c = 8.042(1)

Density

(calculated) 2.941 g/cm^3

Reference intensity

$I/I_{corundum} = 2.0$

References

Chrobak, L. (1934). Z. Krist 88, 35
Hendricks, S.B. and R.G. Dickinson (1927). J. Am. Chem. Soc. 49, 2149.

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

d (Å)	I	hkl	2θ(°)
5.524	45	101	16.03
5.378	15	110	16.47
3.805	25	200	23.36
3.404	10	210	26.16
3.221	95	112	27.67
3.137	13	211	28.43
2.763	100	202	32.37
2.689	80	220	33.29
2.598	9	212	34.50
2.529	6	103	35.47
2.417	5	301	37.16
2.407	6	310	37.33
2.106	5	213	42.91
2.065	25	312	43.80
2.043	6	321	44.31
2.012	20	004	45.03
1.902	12	400	47.78
1.884	3	114	48.27
1.846	2	410	49.32
1.842	3	303	49.44
1.799	2	411	50.71
1.793	1	330	50.88
1.778	5	204	51.33
1.730	2	214	52.87
1.7014	4	420	53.84
1.6772	3	412	54.68
1.6579	2	323	55.37
1.6378	8	332	56.11
1.6104	19	224	57.15
1.5737	5	105	58.61
1.5669	8	422	58.89
1.5429	2	314	59.90
1.5199	1	413	60.90
1.4544	2	215	63.96
1.3984	5	512	66.85
1.3820	6	404	67.75
1.3596	1	414	69.02
1.3451	1	440	69.87
1.3052	2	530	72.34
1.3002	6	116	72.66
1.2642	4	206	75.08

Sodium calcium silicate, Na_2CaSiO_4

Sample

The sample was prepared by heating $Na_2C_2O_4$, and $CaCO_3$, and silica gel at 1300 °C for one half hour. It was then ground and heated at 1100 °C for 17 hours.

Major impurities

0.01 –0.1 % each: Ag,Al,Cu,Mn,

0.1 –1.0 % each: Fe

Color

Bluish white

Optical data

Isotropic, N = 1.594

Structure

Cubic, $P2_13$ (198), Z = 4, closely related to the structure of high cristobalite. The structure of Na_2CaSiO_4 was determined by Barth and Posnjak [1932].

NBS lattice constant:
a = 7.497(1)Å

Density

(calculated) 2.807 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.4

Additional patterns

1. PDF card 2-951 [Barth, 1935], [Wyckoff and Morey, 1926]
2. PDF card 3-816 [McMurdie, 1941]
3. Barth and Posnjak [1932]
4. Hughes [1966]

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

d (Å)	I	hkl	2θ(°)
4.333	25	111	20.48
3.753	3	200	23.69
2.651	100	220	33.78
2.165	7	222	41.68
1.875	19	400	48.51
1.5302	15	422	60.45
1.4427	2	511	64.54
1.3253	4	440	71.07
1.2672	2	531	74.87
1.2499	<1	600	76.09
1.1854	2	620	81.05
1.1432	1	533	84.72
1.0820	1	444	90.78

References

Barth, T. F. W. (1935). J. Phys. Chem. 3, 324.
Barth, T. F. W. and E. Posnjak (1932). Z. Krist. 81, 370.
Hughes, H. (1966). Trans. Brit. Ceram. Soc. 65, 661.
McMurdie, H.F.(1941). J.Res. Nat. Bur. Std.27,502
Wyckoff, R. W. G., and G. W. Morey (1926). Am. J. Sci. 12, 420.

Sodium lanthanum molybdenum oxide, $NaLa(MoO_4)_2$

Sample

The sample was prepared by W. S. Brower at NBS by pulling a single crystal from a melt obtained from a stoichiometric mixture of $Na_2MoO_4 \cdot H_2O$, $La(OH)_3$, and MoO_3.

Color

Colorless

Structure

Tetragonal, $I4_1/a$ (88), Z = 2, isostructural with $CaWO_4$, [Sillén and Sundvall, 1943].

NBS lattice constants:

a = 5.3430(1)Å
c = 11.7437(3)

Density

(calculated) 4.772 g/cm^3

Reference intensity

$I/I_{corundum}$ = 3.7

References

Sillén, L.G. and H. Sundvall (1943). Arkiv Kemi, 17 A, No. 10.

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

d (Å)	*I*	*hkl*	2*θ*(°)
4.87	5	101	18.19
3.177	100	112	28.06
2.938	12	004	30.40
2.672	18	200	33.51
2.432	1	202	36.93
2.342	3	211	38.40
2.318	3	114	38.81
2.039	1	213	44.39
1.976	25	204	45.88
1.890	10	220	48.10
1.738	13	116	52.63
1.675	1	215	54.74
1.6240	17	312	56.63
1.5888	8	224	58.00
1.4682	1	008	63.29
1.4189	<1	305	65.76
1.3857	<1	323	67.54
1.3729	<1	217	68.26
1.3683	<1	118	68.51
1.3361	2	400	70.41
1.3026	<1	402	72.51
1.2868	4	208	73.54
1.2792	7	316	74.05
1.2676	<1	109	74.84
1.2314	4	332	77.44
1.2212	<1	307	78.21
1.2163	3	404	78.59
1.1944	3	420	80.32
1.1705	<1	422	82.30
1.1591	3	228	83.30
1.1454	<1	219	84.52
1.1214	2	1·1·10	86.77
1.1068	3	424	88.21
1.0643	<1	431	92.73
1.0589	1	336	93.34
1.0315	3	512	96.62
0.9880	1	408	102.46
.9786	<1	0·0·12	103.83
.9748	<1	2·1·11	104.41
.9725	<1	435	104.75
.9644	3	3·1·10	106.02
.9445	<1	440	109.28
.9266	2	428	112.46
.9238	3	516	112.98
.9190	2	2·0·12	113.89
.9054	3	532	116.58
.8991	3	444	117.91
.8905	<1	600	119.76
.8821	<1	4·0·10	121.67
.8689	1	2·2·12	124.88
.8589	1	3·3·10	127.48
.8521	1	604	129.36
.8448	<1	6·2·10	131.50
.8299	2	536	136.30
.8227	<1	615	138.87
.8189	<1	1·1·14	140.31
.8118	2	624	143.18
.7932	1	448	151.76
.7894	<1	4·0·12	154.72

Strontium aluminum hydroxide, $Sr_3Al_2(OH)_{12}$

Sample

The sample was prepared by adding $AlCl_3$ to a boiling solution of $Sr(OH)_2$.

Major impurities

0.01 –0.1 % each: Mg and Si

0.1 –1.0 % each: Ca,

Color

Colorless

Optical data

Isotropic, N = 1.605

Structure

Cubic, Ia3d (230), Z = 8, isostructural with $Ca_3Al_2(OH)_{12}$ and garnet [Flint et al., 1941].

NBS lattice constant:
a = 13.0395(2)Å

Density

(calculated) 3.121 g/cm^3

Reference intensity

$I/I_{corundum} = 2.9$

Additional patterns

1. PDF card 2-0148 [Imperical Chemical Industries, Northwich, England]
2. Carlson [1955]

References

Carlson, E.T. (1955). J. Res. Nat. Bur. Std. 54, 329.

Flint, E.P., H.F. McMurdie, and L.S. Wells (1941) J. Res. Nat. Bur. Std. 26, 13.

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

d (Å)	*I*	*hkl*	2θ(°)
5.33	95	211	16.61
4.612	1	220	19.23
3.486	75	321	25.53
3.261	25	400	27.33
2.916	100	420	30.63
2.782	2	332	32.15
2.662	18	422	33.64
2.559	9	431	35.04
2.380	65	521	37.76
2.305	7	440	39.04
2.116	65	611	42.70
2.063	<1	620	43.85
2.014	<1	541	44.98
1.923	6	631	47.22
1.883	18	444	48.30
1.8444	2	543	49.37
1.8084	30	640	50.42
1.7740	20	721	51.47
1.7428	30	642	52.46
1.6563	15	732	55.43
1.6300	12	800	56.40
1.5809	<1	820	58.32
1.5590	4	653	59.22
1.5163	1	831	61.06
1.4767	2	752	62.88
1.4581	9	840	63.78
1.4227	12	842	65.56
1.4060	8	921	66.44
1.3901	6	664	67.30
1.3743	<1	851	68.18
1.3450	8	932	69.88
1.3175	2	941	71.56
1.2913	4	10·1·1	73.24
1.2787	2	10·2·0	74.08
1.2433	8	10·3·1	76.56
1.2107	14	10·4·0	79.02
1.2003	5	10·3·3	79.84
1.1903	6	10·4·2	80.65
1.1805	1	954	81.46
1.1618	9	11·2·1	83.06

d (Å)	*I*	*hkl*	2θ(°)
1.1527	5	880	83.86
1.1265	6	11·3·2	86.28
1.1183	1	10·6·0	87.07
1.0943	2	965	89.48
1.0866	2	12·0·0	90.29
1.0793	1	12·1·1	91.07
1.0718	2	12·2·0	91.89
1.0646	3	11·5·2	92.69
1.0577	4	12·2·2	93.48
1.0507	<1	12·3·1	94.30
1.0375	1	11·6·1	95.88
1.0120	4	11·6·3	99.13
1.0060	3	10·8·2	99.93
0.9885	3	13·2·1	102.38
.9829	3	12·4·4	103.20
.9719	8	12·6·0	104.85
.9665	3	13·3·2	105.68
.9613	2	12·6·2	106.50
.9561	<1	13·4·1	107.34
.9458	1	10·9·3	109.06
.9410	2	888	109.88
.9267	3	14·1·1	112.45
.9084	4	14·3·1	115.97
.9041	1	12·8·0	116.85
.8956	4	14·4·0	118.65
.8913	1	14·3·3	119.59
.8871	6	14·4·2	120.52
.8751	3	14·5·1	123.33
.8597	5	15·2·1	127.28

Strontium aluminum oxide, $Sr_3Al_2O_6$

Sample

The sample was prepared by heating δ-Al_2O_3 and $SrCO_3$ together at 1000 °C overnight. It was then ground and reheated twice at 1600 °C for four hours. It was annealed at 800 °C for two hours after a final grinding.

Color

Colorless

Optical data

Isotropic N= 1.728

Structure

Cubic, Pa3 (205), Z = 24, isostructural with $Ca_3Al_2O_6$ [Lagerqvist et al., 1937]. The structure of $Ca_3Al_2O_6$ was determined by Ordway[1952]

NBS lattice constants:

a = 15.8440(4)Å

Density

(calculated) 4.136 g/cm^3

Reference intensity

$I/I_{corundum}$ = 5.2

Additional patterns

1. PDF card 3-0741 [McMurdie, 1941]
2. Lagerqvist et al. [1937]

References

Lagerqvist, K., S. Wallmark, and A. Westgren (1937). Z. anorg. allgem. Chem., 234, 1.

McMurdie, H.F. (1941). J. Research NBS, 27, 499.

Ordway, F. (1952). Proceedings of the 3rd international symposium on the chemistry of cement, page 91.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
7.10	4	210	12.46
6.49	2	211	13.64
5.60	10	220	15.82
5.29	2	221	16.75
4.782	2	311	18.54
4.397	5	230	20.18
4.235	12	321	20.96
3.964	8	400	22.41
3.845	1	410	23.11
3.635	2	331	24.47
3.458	5	421	25.74
3.235	2	422	27.55
3.171	2	430	28.12
3.050	1	511	29.26
2.943	3	432	30.35
2.892	5	521	30.89
2.799	100	440	31.95
2.675	<1	531	33.47
2.506	8	620	35.80
2.476	3	621	36.25
2.447	<1	541	36.70
2.362	1	630	38.07
2.336	1	631	38.50
2.286	15	444	39.39
2.263	1	632	39.80
2.219	1	711	40.63
2.176	1	641	41.47
2.156	1	721	41.87
2.118	10	642	42.66
2.100	1	722	43.03
2.063	3	731	43.84
2.029	2	650	44.62
2.012	2	732	45.02
1.981	30	800	45.77
1.965	2	810	46.16
1.936	2	733	46.89
1.908	2	821	47.63
1.895	2	653	47.98
1.867	4	822	48.72
1.855	<1	830	49.08
1.806	2	832	50.49
1.794	1	752	50.85
1.771	6	840	51.56
1.760	2	841	51.90
1.739	1	911	52.57
1.7087	1	921	53.59
1.6892	2	664	54.26
1.6797	1	922	54.59
1.6429	<1	852	55.92

d (Å)	I	hkl	2θ(°)
1.6338	1	932	56.26
1.6172	35	844	56.89
1.5923	<1	933	57.86
1.5764	<1	10·1·0	58.50
1.5537	3	10·2·0	59.44
1.5464	2	10·2·1	59.75
1.5315	1	951	60.39
1.5177	<1	10·3·0	61.00
1.5110	1	10·3·1	61.30
1.4906	1	10·3·2	62.23
1.4778	<1	953	62.83
1.4644	1	10·4·1	63.47
1.4463	1	10·4·2	64.36
1.4279	<1	11·1·1	65.29
1.4168	1	10·5·0	65.87
1.4118	1	11·2·1	66.13
1.4000	15	880	66.76
1.3841	1	11·3·1	67.63
1.3685	<1	11·3·2	68.51
1.3584	1	10·6·0	69.09
1.3441	<1	11·3·3	69.93
1.3345	<1	11·4·2	70.51
1.3198	2	12·0·0	71.41
1.3155	2	12·1·0	71.68
1.3069	<1	11·5·1	72.23
1.2979	<1	12·2·1	72.81
1.2850	2	12·2·2	73.66
1.2808	2	12·3·0	73.94
1.2646	<1	12·3·2	75.05
1.2605	<1	11·6·1	75.34
1.2524	12	12·4·0	75.91
1.2450	<1	12·3·3	76.44
1.2332	<1	10·8·1	77.31
1.2224	<1	10·8·2	78.12
1.2186	1	12·5·0	78.41
1.2116	1	13·1·1	78.95
1.2044	<1	12·5·2	79.52
1.2013	1	13·2·1	79.76
1.1941	2	12·4·4	80.34
1.1842	<1	13·3·1	81.15
1.1680	2	12·6·2	82.52
1.1649	1	12·5·4	82.79
1.1526	<1	13·4·2	83.87
1.1434	4	888	84.70

Sample

The sample was prepared by melting a stoichiometric mixture of $SrBr_2 \cdot 6H_2O$ and SrF_2. After being ground, the sample was annealed at 500 °C overnight, then reheated at 400 °C for about 65 hours.

Color

Colorless

Optical data

Uniaxial (-), N_o= 1.728, N_e= 1.711

Structure

Tetragonal, P4/nmm (129), Z=2, matlockite type, by analogy. The structure of PbClF (matlockite) was determined by Nieuwenkamp and Bijvoet[1932].

NBS lattice constants:

a= 4.2180(3)Å
c= 7.3425(4)

Density

(calculated) 4.742 g/cm^3

Reference intensity

$I/I_{corundum}$ = 5.1

References

Nieuwenkamp, W. and J.M. Bijvoet(1932). Z. Krist. 81, 469.

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

d (Å)	I	hkl	2θ(°)
7.32	2	001	12.08
3.670	20	002	24.23
2.981	55	110	29.95
2.769	100	102,111	32.30
2.447	1	003	36.69
2.314	30	112	38.88
2.117	18	103	42.68
2.110	35	200	42.83
1.892	1	113	48.06
1.835	3	004	49.65
1.829	7	202	49.81
1.683	20	104	54.48
1.678	40	212	54.64
1.563	5	114	59.04
1.494	9	213	62.09
1.491	9	220	62.23
1.4684	2	005	63.28
1.3850	2	204	67.58
1.3811	2	222,301	67.80
1.3338	7	310	70.55
1.3153	13	214	71.69
1.3127	12	302,311	71.86
1.2537	4	312	75.82
1.2237	2	006	78.02
1.2054	2	205	79.44
1.1714	<1	313	82.23
1.1590	1	215	83.30
1.1578	1	224	83.41
1.1322	2	116	85.74
1.1160	6	304	87.29
1.1143	5	322	87.46
1.0788	2	314	91.12
1.0585	2	206	93.39
1.0556	3	323	93.72
1.0491	1	007	94.49
1.0465	2	225	94.79
1.0179	1	107	98.35
1.0156	1	305	98.65
0.9943	1	330	101.54
.9894	2	117	102.25
.9868	5	324	102.63

Sample

The sample was prepared by melting an equimolar mixture of $SrCl_2$ and SrF_2. After being ground, the sample was annealed at 500 °C for 75 hours.

Color

Colorless

Optical data

Uniaxial (-), N_o= 1.644, N_e= 1.630

Structure

Tetragonal, P4/nmm (129), Z=2, matlockite type, by analogy. The structure of PbClF (matlockite) was determined by Nieuwenkamp and Bijvoet[1932].

NBS lattice constants:

a= 4.1256(1)Å
c= 6.9598(2)

Density

(calculated) 3.983 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.5

References

Nieuwenkamp, W. and J.M. Bijvoet (1932). Z.Krist. 81, 469.

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

d (Å)	I	hkl	2θ(°)
6.98	20	001	12.67
3.549	90	101	25.07
3.479	30	002	25.58
2.917	90	110	30.62
2.690	12	111	33.28
2.660	100	102	33.67
2.320	1	003	38.78
2.235	75	112	40.32
2.063	50	200	43.85
2.022	25	103	44.79
1.978	3	201	45.83
1.816	12	113	50.20
1.783	20	211	51.18
1.774	19	202	51.47
1.7400	1	004	52.55
1.6298	30	212	56.41
1.6030	18	104	57.44
1.5420	1	203	59.94
1.4947	1	114	62.04
1.4583	12	220	63.77
1.4439	12	213	64.48
1.4276	1	221	65.31
1.3917	3	005	67.21
1.3488	5	301	69.65
1.3453	6	222	69.86
1.3189	1	105	71.47
1.3047	8	310	72.37
1.2790	5	302	74.06
1.2658	13	214	74.97
1.2563	5	115	75.63
1.2348	1	223	77.19
1.2216	10	312	78.18
1.1829	2	303	81.26
1.1602	2	006	83.20
1.1540	6	205	83.75
1.1371	3	313	85.28
1.1290	2	321	86.04
1.1168	1	106	87.22
1.1114	2	215	87.75
1.0869	5	322	90.26
1.0787	4	304	91.13
1.0317	3	400	96.60
1.0262	4	323	97.29
1.0111	1	206	99.25
1.0070	3	225	99.80
0.9941	1	007	101.58
.9888	2	402	102.34
.9821	1	216	103.32
.9725	1	330	104.75
.9665	<1	107	105.69
.9615	3	412	106.47
.9560	4	324	107.37
.9519	4	315	108.04
.9410	3	117	109.89
.9365	2	332	110.68
.9225	3	420	113.23
.9188	3	413	113.94
.9080	1	226	116.06

Strontium manganese oxide, $SrMnO_3$ (hexagonal)

Sample

The sample was prepared at NBS by Negas and Roth [1970].

Color

Dark gray

Structure

Hexagonal, $P6_3/mmc$ (194), Z = 4, isostructural with hexagonal $BaMnO_3$ [Negas and Roth, 1970].

NBS lattice constants:

a = 5.4490(1)Å
c = 9.0804(2)

Density

(calculated) 5.420 g/cm^3

Reference intensity

$I/I_{corundum} = 4.1$

Polymorphism

$SrMnO_3$ exists in a cubic metastable form at ambient conditions. At pressures above 50 k bars and above 850 °C, it forms another hexagonal form with $c \simeq 13.4$Å. [Syono et al., 1969].

Additional patterns

1. Negas and Roth [1970]
2. Syono et al. [1969]

References

Negas, T. and R. S. Roth (1970). J. Solid State Chem. 1, 409.

Syono, Y., S. Skimoto, and K. Koto (1969). J. Phys. Soc. Japan 26, 993.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.719	6	100	18.79
4.539	1	002	19.54
4.187	1	101	21.20
3.272	55	102	27.23
2.725	100	110	32.84
2.548	50	103	35.19
2.360	1	200	38.10
2.336	1	112	38.50
2.284	7	201	39.42
2.270	9	004	39.67
2.093	50	202	43.18
2.047	8	104	44.22
1.8610	30	203	48.90
1.7499	1	211	52.23
1.7440	2	114	52.42
1.6947	7	105	54.07
1.6601	10	212	55.29
1.6356	6	204	56.19
1.5733	14	300	58.63
1.5501	<1	301	59.59
1.5366	17	213	60.17
1.5136	1	006	61.18
1.4411	8	106	64.62
1.4391	7	205	64.72
1.4028	4	214	66.61
1.3622	14	220	68.87
1.3231	1	116	71.21
1.2931	1	304	73.12
1.2740	9	206	74.40
1.2729	6	215	74.48
1.2576	4	312	75.54
1.2012	6	313	79.77
1.1891	<1	305	80.75
1.1680	3	224	82.52
1.1539	4	216	83.76
1.1419	4	402	84.84
1.1351	3	008	85.47
1.1338	2	314	85.59
1.0994	4	403	88.96
1.0908	1	306	89.85

d (Å)	I	hkl	2θ(°)
1.0618	2	315	93.01
1.0531	3	322	94.02
1.0477	4	118	94.65
1.0298	5	410	96.83
1.0193	3	323	98.17
1.0125	1	226	99.07
0.9898	4	316	102.19
.9772	1	324	104.04
.9378	1	414	110.44
.9303	4	406	111.78
.9275	4	209	112.29
.9241	2	502	112.93
.9204	5	308	113.63
.9081	3	330,0·0·10	116.03
.9011	3	503	117.47
.8917	1	420,1·0·10	119.49
.8875	1	421	120.43
.8806	3	326	122.03
.8751	5	422	123.34
.8720	8	228	124.09
.8614	2	1·1·10	126.81
.8555	5	423	128.42
.8514	1	416	129.58
.8474	2	510,2·0·10	130.73
.8432	<1	334	131.99
.8375	1	505	133.79
.8331	2	512	135.21
.8300	2	424	136.25
.8161	3	513	141.40
.8132	3	1·0·11	142.62
.8092	1	2·1·10	144.31
.8005	4	425	148.40
.7991	2	319	149.14
.7940	1	514	151.93

Strontium manganese oxide, $SrMnO_3$ (cubic)

Sample
The sample was prepared at NBS by Negas and Roth [1970].

Color
Dark grey

Structure
Cubic, Pm3m (221), Z = 1, perovskite type [Negas and Roth, 1970].

NBS lattice constant:
a = 3.8060(1)Å

Density
(calculated) 5.739 g/cm^3

Reference intensity
$I/I_{corundum} = 5.6$

Polymorphism
Cubic $SrMnO_3$ is metastable at room temperature and pressure. The stable form is hexagonal. Another hexagonal form exists at pressures above 50 k bars and above 850 °C [Syono et al.,1969].

Additional patterns
1. Negas and Roth [1970]

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

d (Å)	*I*	*hkl*	2θ(°)
3.808	2	100	23.34
2.691	100	110	33.26
2.196	17	111	41.06
1.9031	35	200	47.75
1.7022	1	210	53.81
1.5535	40	211	59.45
1.3455	18	220	69.85
1.2689	1	300	74.75
1.2034	15	310	79.60
1.1476	3	311	84.32
1.0986	6	222	89.04
1.0554	<1	320	93.75
1.0172	15	321	98.44
0.9516	3	400	108.09
.9231	1	410	113.12
.8971	10	411	118.32
.8731	2	331	123.82
.8510	11	420	129.68
.8305	1	421	136.09

References

Negas, T. and R. S. Roth (1970). J. Solid State Chem. 1, 409.

Syono, Y., S. Skimoto, and K. Koto (1969). J. Phys. Soc. Japan 26, 993.

Zinc ammine chloride, $Zn(NH_3)_2Cl_2$

Sample
The sample was precipitated by adding a concentrated NH_4OH solution to a concentrated solution of $ZnCl_2$ and NH_4Cl.

Color
Colorless

Optical data
Biaxial(-), N_α=1.598, N_β=1.618, N_γ=1.624, 2V is large.

Structure
Orthorhombic, Imam (74), Z = 4. The structure was determined by MacGillavry and Bijvoet [1936].

NBS lattice constants:
a = 8.100(1)Å
b = 8.510(1)
c = 7.795(1)

Density
(calculated) 2.106 g/cm^3

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

Additional patterns
1. PDF card 1-165 [New Jersey Zinc Co.]
2. MacGillavry and Bijvoet [1936]

Reference
MacGillavry, C. H. and J. M. Bijvoet (1936). Z. Krist. 94, 249.

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

d (Å)	*I*	*hkl*	2θ(°)
5.86	100	110	15.10
5.745	75	011	15.41
4.257	9	020	20.85
4.051	5	200	21.92
3.895	70	002	22.81
3.392	55	121	26.25
3.310	55	211	26.91
3.245	50	112	27.46
2.933	65	220	30.45
2.874	45	022	31.09
2.807	5	202	31.86
2.677	5	130	33.44
2.483	2	013	36.14
2.345	10	222	38.36
2.226	12	231	40.49
2.207	15	132	40.86
2.188	16	321	41.22
2.140	14	123	42.20
2.118	7	213	42.65
2.026	11	400	44.70
1.990	2	141	45.54
1.956	13	330	46.39
1.950	12	004	46.53
1.916	3	033	47.41
1.910	4	411	47.57
1.883	9	240	48.29
1.850	3	114	49.21
1.796	6	402	50.78
1.771	1	024	51.56
1.7481	9	332	52.29
1.7321	6	233	52.81
1.7137	6	323	53.42
1.6961	19	242	54.02
1.6629	5	051	55.19
1.6552	6	422	55.47
1.6229	5	224	56.67
1.6125	2	143,431	57.06
1.5918	2	510	57.88
1.5338	1	015	60.29

Zinc cobalt oxide, $ZnCo_2O_4$

Sample

Zinc and cobalt in a 1:2 molar ratio were dissolved in nitric acid. The solution was evaporated to dryness. The product was heated to 450 °C for 10 minutes and quenched.

Color

Black

Structure

Cubic, Fd3m (227), Z=8, spinel type. The structure was determined by Natta and Strada [1928] from powder data.

NBS lattice constants:
a = 8.0946(2)Å

Density

(calculated) 6.192 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.3

Additional patterns

1. PDF card 1-1149 [Hanawalt et al.,1938].
2. Holgersson and Karlsson [1929].
3. Natta and Passerini [1929].

References

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

Holgersson, S. and A. Karlsson (1929). Z. Anorg. Allgem. Chem. 183, 384.

Natta, G. and L. Passerini (1929). Gazz. Chim. Ital. 59, 620.

Natta, G. and M. Strada (1928). Atti reale accad. nazl. Lincei 7, 1024.

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.677	10	111	18.96
2.863	35	220	31.22
2.440	100	311	36.80
2.337	9	222	38.49
2.024	18	400	44.73
1.858	1	331	48.99
1.6524	12	422	55.57
1.5575	35	511	59.28
1.4307	35	440	65.15
1.3681	1	531	68.53
1.2799	3	620	74.00
1.2344	8	533	77.22
1.2203	5	622	78.28
1.1684	2	444	82.49
1.1333	1	711	85.63
1.0817	4	642	90.81
1.0538	11	731	93.93
1.0119	4	800	99.15
.9540	2	822	107.69
.9346	7	751	111.01
.9285	2	662	112.12
.9051	2	840	116.66

Zinc manganese oxide (hetaerolite), $ZnMn_2O_4$

Sample

The sample was made by heating equimolar amounts of ZnO and Mn_2O_3 at 900 °C overnight. After grinding, it was reheated at 900 °C for three hours. A small amount of MnO_2 was added and the sample was heated at 1000 °C overnight.

Color

Dark brown

Structure

Tetragonal, $I4_1/amd$ (141), Z=4, distorted spinel type [Frondel and Heinrich, 1942]. Also, it was found to have the cations in the "normal" spinel positions [Sinha et al., 1957].

NBS lattice constants:
a = 5.7204(2)Å
c = 9.245(1)

Density

(calculated) 5.252 g/cm^3

Reference intensity

$I/I_{corundum} = 2.7$

Additional patterns

1. PDF card 18-1484 [Frondel and Klein, 1965], natural mineral.

References

Frondel, C. and C. Klein, Jr. (1965). Am. Mineralogist 50, 1670.

Frondel, C. and E.W. Heinrich (1942). Am. Mineralogist 27, 48.

Sinha, A. P. B., N. R. Sanjana, and A. B. Biswas (1957). Acta Cryst. 10, 439.

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

d (Å)	*I*	*hkl*	2θ(°)
4.87	10	101	18.20
3.047	45	112	29.29
2.862	19	200	31.23
2.715	65	103	32.97
2.466	100	211	36.40
2.432	12	202	36.93
2.311	10	004	38.94
2.022	16	220	44.78
1.798	7	204	50.73
1.760	15	105	51.92
1.684	12	312	54.44
1.621	9	303	56.73
1.564	25	321	59.02
1.522	40	224	60.80
1.439	4	116	64.71
1.4299	17	400	65.19
1.4105	2	323	66.20
1.3721	1	411	68.30
1.3565	2	206	69.20
1.3273	4	305	70.95
1.2944	2	332	73.04
1.2790	2	420	74.06
1.2652	9	413	75.01
1.2328	4	422	77.34
1.2161	3	404	78.60
1.2043	<1	325	79.52
1.1733	5	316,217	82.07
1.1553	3	008	83.60
1.1351	2	431	85.47
1.1192	2	424	86.98
1.1100	5	415	87.89
1.0901	3	512	89.92
1.0725	6	433	91.81
1.0553	2	521	93.76
1.0150	5	327,336	98.73
1.0113	6	440,109	99.22
1.0043	3	523	100.16
1.0031	2	228	100.32
0.9842	2	426	103.01
0.9730	5	435	104.68

Zinc tin oxide, Zn_2SnO_4

Sample

A stoichiometric mixture of ZnO and SnO_2 was heated at 1000 °C overnight.

Color

Colorless

Structure

Cubic, Fd3m(227),Z=8.Isostructural with spinel. The structure was determined by Barth and Posnjak [1932].

NBS lattice constant:

a = 8.6574(3)Å

Density

(calculated) 6.416 g/cm^3

Reference intensity

$I/I_{corundum}$ = 6.8

Additional patterns

1. PDF card 14-381 [Filippova et al., 1960].

References

Barth, T.F.W. and E. Posnjak (1932). Z. Krist.82, 325.

Filippova, N.A., E.V. Savina, and V.A. Korosteleva (1960). Russ. J. Inorg. Chem. 5, 691.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.001	25	111	17.72
3.062	19	220	29.14
2.613	100	311	34.29
2.499	20	222	35.91
2.165	25	400	41.69
1.986	3	331	45.64
1.768	7	422	51.67
1.665	30	511	55.10
1.5304	35	440	60.44
1.4636	4	531	63.51
1.3688	2	620	68.49
1.3203	9	533	71.38
1.3052	8	622	72.34
1.2499	3	444	76.09
1.2121	2	711	78.91
1.1569	2	642	83.49
1.1270	12	731	86.23
1.0820	4	800	90.78
1.0579	<1	733	93.46
1.0202	1	822	98.05
0.9997	8	751	100.80
.9930	4	662	101.74
.9679	4	840	105.46
.9502	1	911	108.32
.9229	1	664	113.16
.9075	6	931	116.16
.8835	12	844	121.34
.8701	1	933	124.56
.8489	2	10·2·0	130.28
.8369	8	951	133.96
.8331	4	10·2·2	135.22
.8073	1	953	145.18
.7903	2	10·4·2	154.14

Barium bromide, $BaBr_2$

Structure

Orthorhombic, Pnam(62), Z=4, isostructural with lead chloride. The structure was determined by Döll and Klemm [1939] and refined by Brackett et al. [1963].

Lattice parameters

a=8.276(8), b=9.919(8), c=4.956(4)Å [Brackett et al., 1963]

Density

(calculated) 4.851 g/cm^3

Thermal parameters

Isotropic [Brackett et al. 1963] Ba 3.37
Br(1) 0.70
Br(2) 0.92

Atomic positions

Brackett et al. [1963]

Scattering factors

Ba^{2+} [Cromer and Waber, 1965]
Br^- [3.3.1A]
Both were modified by the real part of the dispersion correction [3.3.2B]

Scale factors

(integrated intensities) 9.617×10^4

Additional patterns

1. PDF card 2-655 [Döll and Klemm, 1939]

Reference

Brackett, E.B., T.E.Brackett,and R.L. Sass(1963). J. Chem. Phys. 67, 2132.
Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Döll, W. and W.Klemm (1939). Z. anorg. u. allgem. Chem. 241, 239.

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(^\circ)$ $\lambda = 1.54056$ Å
4.96	4	0 2 0	17.88
4.43	16	0 1 1	20.02
4.25	20	1 2 0	20.86
4.14	11	2 0 0	21.46
3.907	17	1 1 1	22.74
3.818	1	2 1 0	23.28
3.227	62	1 2 1	27.62
3.177	42	2 0 1 +	28.06
3.070	20	1 3 0	29.06
3.025	100	2 1 1	29.50
2.751	44	0 3 1	32.52
2.674	5	2 2 1	33.48
2.657	13	3 1 0	33.70
2.609	23	1 3 1	34.34
2.583	9	2 3 0	34.70
2.478	60	0 0 2 +	36.22
2.411	33	3 2 0	37.26
2.342	18	3 1 1	38.40
2.291	26	2 3 1	39.30
2.217	1	0 2 2	40.66
2.142	3	1 2 2	42.16
2.126	5	2 4 0 +	42.48
2.121	3	3 3 0	42.60
2.069	3	4 0 0	43.72
2.026	3	4 1 0	44.70
1.955	5	2 2 2 +	46.42
1.929	9	1 3 2 +	47.08
1.910	2	4 2 0	47.58
1.842	3	0 5 1	49.44
1.812	7	3 1 2	50.30
1.798	2	1 5 1	50.74
1.789	7	2 3 2 +	51.02
1.783	4	4 2 1	51.18
1.753	10	0 4 2 +	52.14
1.728	25	3 2 2 +	52.94
1.683	6	2 5 1	54.48
1.633	1	5 1 0	56.30
1.621	3	1 6 0	56.74
1.614	2	2 4 2	57.02
1.610	2	3 3 2	57.16
1.588	4	4 4 0 +	58.02
1.570	3	5 2 0	58.76
1.568	3	4 1 2	58.84
1.550	12	5 1 1	59.58
1.540	5	1 2 3	60.02
1.535	6	2 6 0 +	60.24
1.532	8	3 5 1	60.38
1.522	2	1 5 2	60.80
1.516	7	2 1 3	61.06
1.512	5	4 2 2	61.24

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
1.478	4	0	3	3		62.84
1.466	1	2	6	1		63.38
1.455	2	1	3	3		63.94
1.451	3	2	5	2		64.14
1.432	1	4	3	2		65.10
1.418	3	5	3	1	+	65.80
1.403	2	3	1	3		66.60
1.397	2	1	7	0		66.94
1.392	3	2	3	3		67.22
1.377	3	5	4	0		68.04
1.366	1	6	1	0		68.64
1.363	3	0	7	1	+	68.84
1.356	3	1	6	2		69.20
1.344	2	1	7	1		69.92
1.337	2	4	4	2		70.34
1.326	2	5	2	2	+	71.00
1.317	1	6	1	1		71.56
1.305	3	2	6	2		72.34
1.292	1	4	6	0		73.22
1.284	1	6	2	1		73.76
1.270	1	0	5	3		74.70
1.250	1	4	6	1		76.10
1.239	2	0	0	4		76.88
1.231	4	3	4	3	+	77.50
1.217	2	1	7	2		78.56
1.214	2	2	5	3		78.80
1.203	3	5	4	2		79.60
1.196	1	6	1	2		80.16
1.161	3	5	1	3		83.10
1.153	1	3	5	3		83.82
1.150	2	7	2	0	+	84.10
1.145	1	4	6	2		84.52
1.138	1	4	7	1		85.22
1.123	1	3	1	4		86.62
1.120	2	7	2	1		86.88
1.117	1	2	3	4		87.18
1.103	1	0	4	4		88.06
1.104	1	6	5	1		88.50
1.102	3	3	2	4	+	88.68
1.076	1	0	7	3		91.46
1.067	1	1	7	3	+	92.46
1.064	1	4	8	0		92.80
1.061	1	7	1	2		93.12
1.043	2	7	2	2		95.18
1.036	1	6	6	1		96.10
1.007	1	5	5	3		99.76
.985	1	1	10	0	+	102.94
.977	1	4	8	2	+	104.04
.966	1	1	10	1		105.80
.965	1	1	2	5		105.86

Calculated Pattern *(Integrated)*

d (Å)	I	hkl			2θ(°) λ = 1.54056 Å
4.96	4	0	2	0	17.87
4.43	14	0	1	1	20.01
4.25	18	1	2	0	20.86
4.14	10	2	0	0	21.46
3.908	16	1	1	1	22.74
3.819	1	2	1	0	23.27
3.228	62	1	2	1	27.61
3.177	9	2	2	0	28.06
3.176	34	2	0	1	28.07
3.070	19	1	3	0	29.06
3.025	100	2	1	1	29.50
2.750	47	0	3	1	32.53
2.675	4	2	2	1	33.47
2.658	13	3	1	0	33.69
2.610	25	1	3	1	34.33
2.583	9	2	3	0	34.70
2.480	21	0	4	0	36.19
2.478	47	0	0	2	36.22
2.411	37	3	2	0	37.27
2.342	19	3	1	1	38.40
2.291	28	2	3	1	39.30
2.217	1	0	2	2	40.67
2.141	4	1	2	2	42.17
2.127	3	2	4	0	42.46
2.126	2	2	0	2	42.49
2.118	2	3	3	0	42.65
2.069	3	4	0	0	43.71
2.025	3	4	1	0	44.71
1.955	2	2	4	1	46.42
1.954	4	2	2	2	46.43
1.929	2	1	5	0	47.07
1.928	9	1	3	2	47.09
1.910	2	4	2	0	47.58
1.842	4	0	5	1	49.45
1.812	8	3	1	2	50.30
1.798	2	1	5	1	50.74
1.789	3	2	5	0	51.01
1.788	5	2	3	2	51.03
1.782	2	4	2	1	51.23
1.754	1	4	3	0	52.10
1.753	12	0	4	2	52.14
1.728	11	3	4	1	52.93
1.728	21	3	2	2	52.95
1.683	7	2	5	1	54.49
1.633	1	5	1	0	56.30
1.621	4	1	6	0	56.74
1.614	2	2	4	2	57.01
1.610	1	3	3	2	57.16
1.589	4	4	4	0	58.01
1.588	2	4	0	2	58.03

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.570	3	5 2 0	58.76
1.568	2	4 1 2	58.84
1.551	16	5 1 1	59.57
1.540	6	1 2 3	60.03
1.535	4	2 6 0	60.23
1.534	3	2 0 3	60.27
1.532	7	3 5 1	60.38
1.522	1	1 5 2	60.80
1.516	8	2 1 3	61.06
1.513	2	4 2 2	61.23
1.478	5	0 3 3	62.83
1.466	1	2 6 1	63.37
1.455	3	1 3 3	63.94
1.450	3	2 5 2	64.16
1.432	1	4 3 2	65.10
1.418	3	5 3 1	65.80
1.418	1	3 6 0	65.80
1.403	2	3 1 3	66.60
1.397	2	1 7 0	66.94
1.392	4	2 3 3	67.21
1.377	3	5 4 0	68.04
1.366	1	6 1 0	68.64
1.363	1	3 6 1	68.80
1.363	1	5 1 2	68.80
1.362	3	0 7 1	68.86
1.357	3	1 6 2	69.19
1.344	3	1 7 1	69.92
1.337	3	4 4 2	70.33
1.326	1	5 4 1	71.00
1.326	3	5 2 2	71.01
1.317	1	6 1 1	71.58
1.305	4	2 6 2	72.35
1.292	1	4 6 0	73.23
1.284	1	6 2 1	73.76
1.269	1	0 5 3	74.71
1.250	2	4 6 1	76.10
1.239	3	0 0 4	76.88
1.231	2	5 5 1	77.47
1.231	1	3 6 2	77.49
1.230	3	3 4 3	77.51
1.217	2	1 7 2	78.56
1.214	2	2 5 3	78.79
1.203	4	5 4 2	79.59
1.196	1	6 1 2	80.16
1.161	5	5 1 3	83.11
1.155	1	2 8 1	83.66
1.153	2	3 5 3	83.82
1.150	2	7 2 0	84.10
1.149	1	1 3 4	84.20
1.145	2	4 6 2	84.53

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.138	2	4 7 1	85.21
1.123	1	3 1 4	86.62
1.120	2	7 2 1	86.88
1.117	1	2 3 4	87.18
1.108	2	0 4 4	88.05
1.104	2	6 5 1	88.49
1.103	1	3 8 1	88.63
1.102	1	5 3 3	88.65
1.102	3	3 2 4	88.69
1.076	1	0 7 3	91.48
1.067	1	1 9 1	92.44
1.067	1	1 7 3	92.47
1.064	1	4 8 0	92.82
1.061	1	7 1 2	93.11
1.043	2	7 2 2	95.19
1.036	2	6 6 1	96.10
1.023	1	3 9 0	97.64
1.019	1	2 5 4	98.27
1.017	1	4 6 3	98.41
1.013	1	8 0 1	99.04
1.007	1	5 5 3	99.76
1.002	1	3 9 1	100.44
.995	1	7 5 1	101.47
.992	1	5 8 0	101.83
.985	1	1 10 0	102.91
.984	1	1 6 4	102.98
.977	1	4 8 2	104.03
.977	1	4 4 4	104.08
.968	1	8 3 1	105.41
.966	1	1 10 1	105.77
.965	1	1 2 5	105.87
.964	1	2 6 4	106.05
.959	1	2 1 5	106.81
.955	1	8 0 2	107.58
.954	1	4 7 3	107.64
.949	1	0 3 5	108.44
.946	1	3 9 2	109.03
.944	1	7 2 3	109.39
.934	1	6 5 3	111.10
.933	1	3 8 3	111.26
.927	1	1 7 4	112.42
.921	2	5 8 2	113.47
.921	2	5 4 4	113.52
.917	1	8 5 0	114.23
.915	2	1 10 2	114.63
.911	1	1 9 3	115.41
.899	1	2 10 2	117.95
.894	1	4 6 4	118.97
.892	2	6 6 3	119.52

Structure

Orthorhombic, Pnam (62), Z=4, isostructural with lead chloride. The structure was determined by Döll and Klemm [1939] and refined by Brackett et al. [1963].

Lattice parameters

a=8.922(8), b=10.695(8), c=5.304(4)Å [Brackett et al., 1963]

Density

(calculated) 5.133 g/cm^3

Thermal parameters

Isotropic [Brackett et al.,1963]

Ba	4.33
I(1)	0.94
I(2)	0.96

Atomic positions

Brackett et al. [1963]

Scattering factors

Ba^{2+} [Cromer and Waber, 1965]
I^- [3.3.1A]
Both were modified by the real part of the dispersion correction [3.3.2B]

Scale factors

(integrated intensities) 18.55×10^4

Additional patterns

1. PDF card 2-497 [Döll and Klemm,1939]

Reference

Brackett, E.B., T.E.Brackett,and R.L. Sass(1963). J. Chem. Phys. 67, 2132.

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

Döll, W. and W.Klemm (1939). Z. anorg. u. allgem. Chem. 241, 239.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
5.35	2	0 2 0	16.56
4.75	5	0 1 1	18.66
4.59	2	1 2 0	19.34
4.46	1	2 0 0	19.88
4.20	1	1 1 1	21.16
4.12	3	2 1 0	21.56
3.469	91	1 2 1	25.66
3.414	61	2 0 1	26.08
3.309	30	1 3 0	26.92
3.252	100	2 1 1	27.40
2.959	41	0 3 1	30.18
2.877	7	2 2 1	31.06
2.866	17	3 1 0	31.18
2.808	24	1 3 1	31.84
2.784	15	2 3 0	32.12
2.674	19	0 4 0	33.48
2.651	46	0 0 2	33.78
2.599	32	3 2 0	34.48
2.562	3	1 4 0	35.00
2.521	12	3 1 1	35.58
2.466	15	2 3 1	36.40
2.334	1	3 2 1	38.54
2.293	1	2 4 0	39.26
2.284	2	3 3 0	39.42
2.230	2	4 0 0 +	40.42
2.183	5	4 1 0	41.32
2.105	4	2 4 1	42.94
2.097	4	2 2 2	43.10
2.080	3	1 5 0	43.48
2.070	13	1 3 2	43.70
2.059	4	4 2 0	43.94
2.019	2	4 1 1	44.86
1.984	5	0 5 1	45.70
1.947	9	3 1 2	46.62
1.929	4	2 5 0	47.08
1.920	9	2 3 2 +	47.30
1.891	2	4 3 0	48.08
1.883	10	0 4 2	48.30
1.862	15	3 4 1	48.88
1.857	22	3 2 2	49.02
1.843	2	1 4 2	49.42
1.812	9	2 5 1	50.30
1.781	1	4 3 1	51.26
1.760	2	5 1 0	51.90
1.748	3	1 6 0	52.30
1.731	2	3 3 2	52.86
1.713	2	4 4 0	53.46
1.708	1	4 0 2	53.62
1.693	1	5 2 0	54.14
1.686	4	4 1 2	54.38

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.670	13	5 1 1	54.92
1.655	3	2 6 0	55.46
1.650	12	1 2 3 +	55.66
1.644	6	2 0 3	55.88
1.637	3	1 5 2	56.14
1.625	8	2 1 3 +	56.60
1.596	1	5 3 0	57.72
1.584	3	0 3 3	58.20
1.580	3	2 6 1	58.36
1.571	1	2 2 3	58.72
1.560	5	2 5 2 +	59.18
1.540	1	4 3 2	60.04
1.528	3	5 3 1 +	60.54
1.506	3	1 7 0 +	61.54
1.493	2	2 3 3	62.14
1.484	3	5 4 0	62.52
1.473	1	6 1 0	63.06
1.468	3	0 7 1 +	63.28
1.467	3	5 1 2	63.36
1.459	2	1 6 2	63.72
1.449	4	1 7 1	64.24
1.439	2	4 4 2	64.74
1.429	2	5 4 1	65.22
1.427	1	5 2 2	65.36
1.419	1	6 1 1	65.74
1.404	3	2 6 2	66.54
1.400	2	2 4 3	66.74
1.392	2	4 6 0	67.18
1.383	1	6 2 1	67.68
1.374	1	4 1 3	68.20
1.367	1	5 3 2	68.58
1.363	2	0 5 3	68.84
1.347	2	4 6 1	69.76
1.326	3	0 0 4 +	71.02
1.321	4	3 4 3	71.32
1.310	3	1 7 2	72.06
1.303	2	2 5 3	72.46
1.295	3	5 4 2	72.98
1.288	1	6 1 2	73.48
1.247	3	5 1 3	76.28
1.244	2	2 8 1	76.48
1.239	1	3 5 3 +	76.88
1.233	3	4 6 2	77.34
1.231	2	1 3 4	77.48
1.226	1	4 7 1	77.82
1.207	2	7 2 1	79.28
1.204	2	3 1 4	79.58
1.197	1	2 3 4	80.10
1.190	2	6 5 1	80.70
1.188	2	3 8 1 +	80.82

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.185	2	5 3 3	81.10
1.181	2	3 2 4	81.40
1.156	1	0 7 3	83.56
1.147	2	1 7 3 +	84.42
1.142	1	7 1 2	84.80
1.133	1	4 1 4	85.62
1.123	1	7 2 2	86.60
1.116	2	6 6 1 +	87.28
1.113	2	6 2 3	87.58
1.094	1	4 6 3	89.52
1.093	1	2 5 4	89.66
1.091	1	8 0 1	89.78
1.054	1	2 9 2	93.94
1.053	1	4 8 2	94.08
1.044	1	8 3 1	95.14
1.041	1	1 10 1	95.44
1.035	1	2 6 4	96.22
1.034	1	1 2 5	96.36
1.032	1	2 0 5	96.54
1.027	1	2 1 5 +	97.16
1.019	1	3 9 2	98.24
1.015	1	7 2 3	98.72
1.012	1	7 5 2	99.12
1.005	1	6 5 3	100.12
1.004	1	3 8 3	100.24
.995	1	1 7 4	101.44
.989	2	5 4 4 +	102.32
.992	1	5 8 2	101.84
.986	2	1 10 2 +	102.72
.960	1	4 6 4	106.68
.959	1	6 6 3	106.84

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.35	2	0 2 0	16.56
4.75	4	0 1 1	18.66
4.59	2	1 2 0	19.34
4.46	1	2 0 0	19.89
4.19	1	1 1 1	21.17
4.12	2	2 1 0	21.57
3.469	89	1 2 1	25.66
3.426	8	2 2 0	25.99
3.414	56	2 0 1	26.08
3.311	30	1 3 0	26.91
3.252	100	2 1 1	27.40
2.959	42	0 3 1	30.18
2.878	6	2 2 1	31.05
2.865	17	3 1 0	31.19
2.808	25	1 3 1	31.84
2.785	15	2 3 0	32.11
2.674	20	0 4 0	33.49
2.652	52	0 0 2	33.77
2.599	35	3 2 0	34.48
2.561	3	1 4 0	35.01
2.521	13	3 1 1	35.58
2.466	17	2 3 1	36.41
2.334	1	3 2 1	38.54
2.293	1	2 4 0	39.25
2.284	2	3 3 0	39.42
2.231	1	4 0 0	40.41
2.230	1	2 1 2	40.42
2.184	6	4 1 0	41.31
2.105	5	2 4 1	42.93
2.097	4	2 2 2	43.10
2.080	3	1 5 0	43.47
2.070	15	1 3 2	43.70
2.059	4	4 2 0	43.95
2.019	3	4 1 1	44.85
1.984	6	0 5 1	45.70
1.946	11	3 1 2	46.63
1.929	4	2 5 0	47.08
1.921	9	2 3 2	47.29
1.919	2	4 2 1	47.33
1.891	2	4 3 0	48.08
1.883	12	0 4 2	48.30
1.862	17	3 4 1	48.88
1.856	21	3 2 2	49.03
1.842	2	1 4 2	49.43
1.813	11	2 5 1	50.30
1.781	1	4 3 1	51.25
1.760	2	5 1 0	51.91
1.748	3	1 6 0	52.29
1.730	2	3 3 2	52.86
1.713	2	4 4 0	53.45
1.707	1	4 0 2	53.65
1.693	2	5 2 0	54.14
1.686	4	4 1 2	54.38
1.670	16	5 1 1	54.92
1.655	4	2 6 0	55.47
1.650	6	3 5 1	55.65
1.650	9	1 2 3	55.67
1.644	5	2 0 3	55.89
1.637	3	1 5 2	56.15
1.626	4	4 2 2	56.55
1.625	9	2 1 3	56.61
1.596	1	5 3 0	57.73
1.584	4	0 3 3	58.20
1.580	1	2 6 1	58.35
1.571	1	2 2 3	58.72
1.560	4	2 5 2	59.18
1.560	3	1 3 3	59.20
1.540	1	4 3 2	60.04
1.529	1	3 6 0	60.50
1.528	4	5 3 1	60.54
1.506	3	1 7 0	61.53
1.505	2	3 1 3	61.59
1.493	2	2 3 3	62.14
1.484	4	5 4 0	62.53
1.473	1	6 1 0	63.07
1.469	1	3 6 1	63.25
1.468	3	0 7 1	63.29
1.466	2	5 1 2	63.37
1.459	3	1 6 2	63.71
1.449	5	1 7 1	64.24
1.439	2	4 4 2	64.74
1.429	2	5 4 1	65.22
1.427	1	5 2 2	65.35
1.419	1	6 1 1	65.75
1.404	4	2 6 2	66.54
1.400	1	2 4 3	66.75
1.392	3	4 6 0	67.17
1.383	2	6 2 1	67.69
1.374	1	4 1 3	68.19
1.367	1	5 3 2	68.58
1.363	2	0 5 3	68.84
1.347	2	4 6 1	69.77
1.327	1	5 5 1	70.99
1.326	4	0 0 4	71.03
1.321	5	3 4 3	71.32
1.310	4	1 7 2	72.06
1.303	3	2 5 3	72.46
1.295	5	5 4 2	72.99
1.288	2	6 1 2	73.49
1.283	1	1 8 1	73.80

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.266	1	7 1 0	74.98
1.247	5	5 1 3	76.27
1.245	1	2 8 1	76.45
1.240	1	7 2 0	76.82
1.239	2	3 5 3	76.89
1.233	4	4 6 2	77.33
1.231	2	1 3 4	77.48
1.226	1	4 7 1	77.82
1.219	1	6 3 2	78.39
1.207	3	7 2 1	79.29
1.203	2	3 1 4	79.60
1.197	2	2 3 4	80.09
1.190	2	6 5 1	80.69
1.188	2	3 8 1	80.81
1.188	2	0 4 4	80.84
1.185	1	5 3 3	81.12
1.181	3	3 2 4	81.41
1.156	1	0 7 3	83.57
1.147	1	4 8 0	84.40
1.146	2	1 7 3	84.43
1.142	1	7 1 2	84.81
1.137	1	5 4 3	85.31
1.133	1	4 1 4	85.63
1.123	2	7 2 2	86.60
1.116	3	6 6 1	87.27
1.115	1	4 2 4	87.42
1.113	1	6 2 3	87.58
1.103	1	3 9 0	88.54
1.094	1	4 6 3	89.52
1.093	1	2 5 4	89.65
1.091	1	8 0 1	89.79
1.070	1	5 8 0	92.10
1.062	1	1 10 0	93.00
1.055	1	7 4 2	93.74
1.054	1	2 9 2	93.94
1.053	1	4 8 2	94.08
1.044	1	8 3 1	95.14
1.041	2	1 10 1	95.42
1.035	1	2 6 4	96.20
1.034	2	1 2 5	96.37
1.032	1	2 0 5	96.56
1.028	1	8 0 2	97.05
1.027	1	2 1 5	97.15
1.019	2	3 9 2	98.23
1.015	2	7 2 3	98.72
1.012	1	7 5 2	99.12
1.005	1	6 5 3	100.12
1.004	1	3 8 3	100.24
.995	2	1 7 4	101.43
.992	2	5 8 2	101.85

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
.989	1	8 5 0	102.32
.989	2	5 4 4	102.33
.986	1	1 10 2	102.77
.985	1	6 1 4	102.82
.975	1	9 2 0	104.42
.972	1	5 9 1	104.79
.960	2	4 6 4	106.67
.959	2	6 6 3	106.84

Structure

Hexagonal, $P3_1$ (144), Z=3. The structure was determined by Gurr et al. [1970].

Lattice parameters

a=4.3360(5), c=8.340 (2)Å; [published values: a=4.3358(5), c=8.3397(18)Å, (ibid.)]

Density

(calculated) 2.554 g/cm^3

Thermal parameters

Isotropic [ibid.]

Polymorphism

A high pressure polymorph, B_2O_3 phase II, is orthorhombic. Its structure was determined by Prewitt and Shannon [1968].

Scattering factors

B^0, O^0 [3.3.1A]

Scale factors

(integrated intensities) 0.1869×10^4.

Additional patterns

1.PDF 6-0634 [Berger, 1953]

Reference

Berger, S. V. (1953). Acta. Chem. Scand. 7, 611.
Gurr, G.E., P.W. Montgomery, C.D. Knutson, and B.T. Gorres (1970). Acta Cryst. B26, 906.
Prewitt, C.T. and R.D.Shannon (1968). Acta Cryst. B24, 869.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ*(°) λ = 1.54056 Å
3.754	1	1 0 0	23.68
3.424	56	1 0 1 +	26.00
2.791	100	1 0 2	32.04
2.783	67	0 0 3	32.14
2.234	37	1 0 3 +	40.34
2.168	2	1 1 0	41.62
2.098	41	1 1 -1 +	43.08
1.923	5	1 1 2 +	47.22
1.8316	2	0 2 1	49.74
1.8226	4	1 0 4 +	50.00
1.7120	9	0 2 2 +	53.48
1.5561	3	2 0 3 +	59.34
1.5245	4	1 0 5 +	60.70
1.4193	2	2 1 0 +	65.74
1.3993	5	1 2 -1 +	66.80
1.3952	8	2 0 4 +	67.02
1.3219	2	1 1 5 +	71.28
1.3036	1	0 1 6	72.44
1.2642	1	1 2 -3	75.08
1.2517	1	3 0 0	75.96
1.2470	1	0 2 5 +	76.30
1.1988	3	3 0 2 +	79.96
1.1732	4	1 2 4 +	82.08
1.1412	2	3 0 3	84.90
1.1356	1	0 1 7	85.42
1.1172	1	2 0 6	87.18
1.0809	2	2 1 5 +	90.90
1.0334	2	1 3 -1 +	96.36
1.0100	1	2 2 3 +	99.40
1.0060	1	0 2 7	99.94
.9395	1	1 1 -8 +	110.14
.9329	1	0 4 1	111.32
.9302	1	3 0 6 +	111.80
.8436	1	2 3 2 +	131.86

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
3.755	1	1 0 0	23.67
3.424	46	1 0 1	26.00
3.424	4	0 1 1	26.00
2.790	100	1 0 2	32.05
2.780	7	0 0 3	32.17
2.234	31	1 0 3	40.33
2.234	8	0 1 3	40.33
2.168	2	1 1 0	41.62
2.098	21	1 1 1	43.07
2.098	23	1 1 -1	43.07
1.924	3	1 1 2	47.21
1.9236	3	1 1 -2	47.21
1.8317	2	0 2 1	49.74
1.8229	3	1 0 4	49.99
1.8229	1	0 1 4	49.99
1.7120	10	0 2 2	53.48
1.7096	1	1 1 3	53.56
1.7096	1	1 1 -3	53.56
1.5559	2	2 0 3	59.35
1.5559	1	0 2 3	59.35
1.5244	3	1 0 5	60.70
1.5244	2	0 1 5	60.70
1.4193	1	2 1 0	65.74
1.4193	1	1 2 0	65.74
1.3992	3	2 1 1	66.81
1.3992	3	1 2 -1	66.81
1.3952	5	2 0 4	67.02
1.3952	3	0 2 4	67.02
1.3220	1	1 1 5	71.28
1.3220	1	1 1 -5	71.28
1.3036	2	0 1 6	72.44
1.2641	1	1 2 -3	75.09
1.2517	2	3 0 0	75.96
1.2470	1	2 0 5	76.30
1.2470	1	0 2 5	76.30
1.2378	1	0 3 1	76.97
1.1989	2	3 0 2	79.96
1.1989	2	0 3 2	79.96
1.1733	1	2 1 4	82.07
1.1733	2	1 2 4	82.07
1.1733	1	1 2 -4	82.07
1.1733	2	2 1 -4	82.07
1.1413	2	3 0 3	84.89
1.1356	2	0 1 7	85.42
1.1172	1	2 0 6	87.18
1.0809	1	2 1 5	90.89
1.0809	1	1 2 5	90.89
1.0809	1	1 2 -5	90.89
1.0809	1	2 1 -5	90.89
1.0335	1	1 3 -1	96.38

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
1.0335	1	3 1 1	96.38
1.0099	1	2 2 3	99.41
1.0099	1	2 2 -3	99.41
1.0060	1	0 2 7	99.94
.9395	1	1 1 -8	110.14
.9395	1	1 1 8	110.14
.9329	2	0 4 1	111.32
.9302	1	3 0 6	111.81
.9302	1	0 3 6	111.81
.9267	1	0 0 9	112.45
.8630	1	3 0 7	126.40
.8437	1	2 3 2	131.85
.8437	1	3 2 -2	131.85
.8142	1	1 0 10	142.21
.7860	1	4 1 -3	157.05

Calcium iron silicate hydroxide, julgoldite, $Ca_2Fe_3Si_3O_{10}(OH,O)_2(OH)_2$

Structure

Monoclinic, C2/m (12), Z=4. The structure was determined by Donnay [1971].

Lattice parameters

a = 19.433(3), b = 6.081(1), c = 8.922(2) Å, β = 97.60(5)° [ibid.]

Density

(calculated) 3.552 g/cm^3

Thermal parameters

Isotropic [Donnay, 1971]

Scattering factors

O^-, Ca^{2+}, Si^0 [3.3.1A]
Fe^{3+} [3.3.1B]

Scale factors

(integrated intensities) 7.619×10^4

Reference

Donnay, G. (1971). private communication.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ Å $\lambda = 1.54056$ Å
9.63	22	2	0	0		9.18
8.84	24	0	0	1		10.00
6.99	9	-2	0	1		12.66
6.12	16	2	0	1		14.46
4.94	11	-1	1	1		17.94
4.81	66	4	0	0		18.42
4.76	45	1	1	1		18.62
4.485	13	-4	0	1		19.78
4.423	20	0	0	2		20.06
4.235	7	-2	0	2		20.96
4.103	6	-3	1	1		21.64
4.012	5	4	0	1		22.14
3.831	90	2	0	2		23.20
3.584	3	-1	1	2		24.82
3.496	16	-4	0	2		25.46
3.450	5	1	1	2		25.80
3.276	1	-3	1	2		27.20
3.171	3	-5	1	1		28.12
3.155	2	-6	0	1		28.26
3.062	16	4	0	2		29.14
3.042	3	0	2	0		29.34
2.992	5	3	1	2		29.84
2.949	100	5	1	1	+	30.28
2.930	25	-2	0	3		30.48
2.899	20	2	2	0	+	30.82
2.875	18	0	2	1		31.08
2.778	69	-6	0	2	+	32.20
2.723	16	2	2	1	+	32.86
2.671	35	-1	1	3	+	33.52
2.586	6	1	1	3		34.66
2.572	76	4	2	0		34.86
2.517	10	-4	2	1		35.64
2.505	21	0	2	2		35.82
2.491	26	-7	1	1	+	36.02
2.470	21	-2	2	2		36.34
2.448	7	6	0	2		36.68
2.424	3	4	2	1		37.06
2.406	9	8	0	0	+	37.34
2.382	51	2	2	2	+	37.74
2.355	12	3	1	3		38.18
2.339	3	7	1	1		38.46
2.331	5	-6	0	3		38.60
2.318	6	-5	1	3		38.82
2.294	1	-4	2	2		39.24
2.242	25	-8	0	2		40.18
2.219	6	-2	0	4		40.62
2.211	17	0	0	4		40.78
2.208	13	6	2	0		40.84
2.189	5	-6	2	1		41.20
2.157	26	4	2	2		41.84

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
2.119	15	-4	0	4	+	42.64
2.097	6	6	2	1	+	43.10
2.093	5	-1	1	4		43.18
2.072	1	5	1	3		43.64
2.034	4	-7	1	3		44.50
2.029	2	2	2	3		44.62
1.9714	1	-1	3	1		46.00
1.9593	3	1	3	1		46.30
1.9450	6	-6	0	4		46.66
1.9317	1	-5	1	4		47.00
1.9164	3	9	1	1	+	47.40
1.9073	17	6	2	2	+	47.64
1.8872	28	8	2	0	+	48.18
1.8733	5	4	2	3	+	48.56
1.8582	2	-10	0	2		48.98
1.8497	4	-6	2	3		49.22
1.8247	1	1	3	2		49.94
1.8078	1	8	2	1		50.44
1.7925	2	-2	2	4		50.90
1.7879	6	0	2	4		51.04
1.7673	4	-7	1	4	+	51.68
1.7546	3	8	0	3		52.08
1.7478	4	-8	0	4		52.30
1.7379	25	-4	2	4	+	52.62
1.7251	3	2	2	4		53.04
1.7197	6	-10	0	3		53.22
1.7179	7	6	0	4		53.28
1.6955	5	-3	1	5		54.04
1.6932	7	-11	1	1		54.12
1.6886	3	10	0	2		54.28
1.6749	9	-1	3	3	+	54.76
1.6274	7	10	2	0	+	56.50
1.6206	45	4	2	4		56.76
1.6169	26	-12	0	1		56.90
1.6050	16	12	0	0		57.36
1.5933	4	-9	1	4	+	57.82
1.5853	22	-10	2	2		58.14
1.5764	4	-5	3	3	+	58.50
1.5696	4	10	2	1	+	58.78
1.5580	1	-10	0	4		59.26
1.5373	2	-2	2	5		60.14
1.5308	10	8	0	4	+	60.42
1.5249	5	-8	0	5		60.68
1.5204	28	0	4	0		60.88
1.5154	29	-8	2	4		61.10
1.5079	5	-4	2	5		61.44
1.4999	1	-1	3	4		61.80
1.4969	2	-10	2	3		61.94
1.4865	1	-2	0	6		62.42
1.4746	13	10	2	2		62.98
1.4705	7	6	0	5		63.18
1.4495	3	4	4	0	+	64.20
1.4395	1	-4	4	1		64.70
1.4375	2	0	4	2		64.80
1.4285	7	2	0	6	+	65.26
1.4196	3	12	2	0		65.72
1.4128	6	2	4	2	+	66.08
1.4000	1	-12	2	2		66.76
1.3941	2	-4	4	2		67.08
1.3894	6	-12	0	4	+	67.34
1.3672	3	8	2	4	+	68.58
1.3644	4	-13	1	3	+	68.74
1.3617	3	4	4	2		68.90
1.3527	2	5	3	4		69.42
1.3510	3	0	4	3		69.52
1.3493	3	-2	4	3		69.62
1.3356	9	-2	2	6		70.44
1.3336	12	-6	4	2	+	70.56
1.3304	8	-11	3	1		70.76
1.3265	3	0	2	6	+	71.00
1.3197	5	-4	2	6		71.42
1.3159	3	-14	0	3		71.66
1.3048	1	-11	1	5		72.36
1.2916	2	6	4	2		73.22
1.2853	2	8	4	0	+	73.64
1.2808	3	-6	2	6	+	73.94
1.2770	3	6	0	6		74.20
1.2740	2	-2	0	7	+	74.40
1.2702	2	-10	2	5		74.66
1.2670	7	14	0	2	+	74.88
1.2585	3	-8	4	2		75.48
1.2551	4	9	1	5		75.72
1.2528	6	0	4	4	+	75.88
1.2495	3	-7	3	5		76.12
1.2461	2	-14	2	2	+	76.36
1.2352	3	-4	4	4		77.16
1.2288	1	8	2	5		77.64
1.2243	2	12	0	4	+	77.98
1.2211	2	14	2	1		78.22

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
9.63	18	2	0	0	9.17
8.84	21	0	0	1	9.99
6.99	9	-2	0	1	12.65
6.12	15	2	0	1	14.45
4.94	10	-1	1	1	17.94
4.82	68	4	0	0	18.41
4.76	44	1	1	1	18.61
4.486	13	-4	0	1	19.78
4.422	21	0	0	2	20.06
4.237	7	-2	0	2	20.95
4.102	7	-3	1	1	21.65
4.012	5	4	0	1	22.14
3.831	98	2	0	2	23.20
3.814	2	3	1	1	23.30
3.586	4	-1	1	2	24.81
3.495	18	-4	0	2	25.46
3.451	5	1	1	2	25.80
3.277	2	-3	1	2	27.19
3.171	3	-5	1	1	28.12
3.154	1	-6	0	1	28.27
3.062	19	4	0	2	29.14
3.040	3	0	2	0	29.35
2.991	5	3	1	2	29.84
2.949	100	5	1	1	30.28
2.948	20	0	0	3	30.29
2.929	24	-2	0	3	30.49
2.899	20	2	2	0	30.81
2.897	3	6	0	1	30.84
2.875	20	0	2	1	31.08
2.788	13	-2	2	1	32.07
2.778	82	-6	0	2	32.19
2.773	5	-5	1	2	32.25
2.723	16	2	2	1	32.86
2.720	7	2	0	3	32.90
2.677	2	-4	0	3	33.45
2.671	41	-1	1	3	33.52
2.587	4	1	1	3	34.65
2.571	99	4	2	0	34.87
2.517	11	-4	2	1	35.64
2.505	24	0	2	2	35.81
2.492	29	-7	1	1	36.01
2.491	3	5	1	2	36.02
2.470	26	-2	2	2	36.34
2.448	7	6	0	2	36.67
2.423	4	4	2	1	37.07
2.408	7	8	0	0	37.32
2.405	7	-8	0	1	37.36
2.382	64	2	2	2	37.74
2.378	1	4	0	3	37.80
2.355	14	3	1	3	38.19
2.339	2	7	1	1	38.45
2.330	5	-6	0	3	38.60
2.317	8	-5	1	3	38.83
2.294	1	-4	2	2	39.24
2.249	2	8	0	1	40.06
2.243	32	-8	0	2	40.17
2.220	6	-2	0	4	40.61
2.211	19	0	0	4	40.78
2.208	7	6	2	0	40.84
2.189	6	-6	2	1	41.20
2.157	33	4	2	2	41.84
2.118	20	-4	0	4	42.65
2.116	1	0	2	3	42.69
2.097	6	6	2	1	43.09
2.095	2	2	0	4	43.14
2.094	3	-1	1	4	43.17
2.073	2	5	1	3	43.63
2.041	1	6	0	3	44.35
2.039	1	1	1	4	44.39
2.035	4	-7	1	3	44.49
2.027	1	2	2	3	44.66
1.9714	1	-1	3	1	46.00
1.9596	4	1	3	1	46.29
1.9450	8	-6	0	4	46.66
1.9319	1	-5	1	4	47.00
1.9170	2	9	1	1	47.38
1.9155	1	4	0	4	47.42
1.9086	4	3	1	4	47.60
1.9070	22	6	2	2	47.65
1.9043	2	-3	3	1	47.72
1.8876	37	8	2	0	48.17
1.8864	6	-8	2	1	48.20
1.8732	5	4	2	3	48.56
1.8729	1	3	3	1	48.57
1.8582	2	-10	0	2	48.98
1.8496	5	-6	2	3	49.22
1.8247	1	1	3	2	49.94
1.8081	1	8	2	1	50.43
1.7929	2	-2	2	4	50.89
1.7881	7	0	2	4	51.03
1.7687	1	0	0	5	51.63
1.7672	4	-7	1	4	51.68
1.7546	4	8	0	3	52.08
1.7477	4	-8	0	4	52.30
1.7406	5	5	1	4	52.53
1.7381	27	-4	2	4	52.61
1.7373	8	5	3	1	52.64
1.7363	1	-4	0	5	52.67
1.7253	3	2	2	4	53.03
1.7200	5	-10	0	3	53.21

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.7178	8	6 0 4	53.28
1.7001	1	2 0 5	53.88
1.6960	5	-3 1 5	54.02
1.6931	7	-11 1 1	54.13
1.6862	1	10 0 2	54.36
1.6748	13	-1 3 3	54.76
1.6745	1	8 2 2	54.78
1.6279	3	-7 3 1	56.48
1.6277	1	5 3 2	56.49
1.6272	5	10 2 0	56.51
1.6207	68	4 2 4	56.76
1.6174	2	-12 0 1	56.88
1.6052	24	12 0 0	57.35
1.5935	2	4 0 5	57.81
1.5931	3	-9 1 4	57.83
1.5877	1	3 3 3	58.04
1.5855	34	-10 2 2	58.13
1.5772	2	-12 0 2	58.47
1.5761	4	-5 3 3	58.51
1.5694	6	10 2 1	58.79
1.5672	1	7 1 4	58.88
1.5580	1	-10 0 4	59.26
1.5374	2	-2 2 5	60.14
1.5350	1	-7 1 5	60.24
1.5308	14	8 0 4	60.42
1.5289	2	0 2 5	60.51
1.5249	2	-8 0 5	60.68
1.5229	2	10 0 3	60.77
1.5202	41	0 4 0	60.89
1.5152	36	-8 2 4	61.11
1.5077	6	-4 2 5	61.45
1.5000	1	-1 3 4	61.80
1.4971	1	-10 2 3	61.93
1.4867	1	-2 0 6	62.41
1.4746	20	10 2 2	62.98
1.4692	1	6 0 5	63.24
1.4508	1	-13 1 1	64.14
1.4497	4	4 4 0	64.19
1.4487	1	12 0 2	64.24
1.4398	1	-4 4 1	64.69
1.4376	1	0 4 2	64.79
1.4309	1	-2 4 2	65.14
1.4290	7	2 0 6	65.24
1.4279	6	-12 2 1	65.29
1.4273	1	3 3 4	65.32
1.4195	4	12 2 0	65.73
1.4131	7	2 4 2	66.07
1.4122	5	-6 0 6	66.11
1.4001	1	-12 2 2	66.76
1.3941	2	-4 4 2	67.08
1.3892	10	-12 0 4	67.35
1.3874	1	11 1 3	67.45
1.3673	4	8 2 4	68.58
1.3660	1	-14 0 2	68.65
1.3652	2	-7 3 4	68.70
1.3646	2	-13 1 3	68.73
1.3631	2	-8 2 5	68.82
1.3616	2	4 4 2	68.90
1.3528	2	5 3 4	69.41
1.3512	3	0 4 3	69.51
1.3494	4	-2 4 3	69.62
1.3374	2	12 0 3	70.33
1.3356	13	-2 2 6	70.44
1.3337	15	-6 4 2	70.56
1.3330	1	14 0 1	70.60
1.3316	4	-3 3 5	70.69
1.3301	3	-11 3 1	70.77
1.3270	1	2 4 3	70.96
1.3263	1	0 2 6	71.01
1.3195	9	-4 2 6	71.43
1.3152	2	-14 0 3	71.70
1.3048	2	-11 1 5	72.37
1.2915	3	6 4 2	73.23
1.2855	3	8 4 0	73.63
1.2851	1	-8 4 1	73.65
1.2808	2	-6 2 6	73.94
1.2800	1	-9 3 4	74.00
1.2798	1	3 3 5	74.01
1.2770	3	6 0 6	74.20
1.2746	2	-2 0 7	74.36
1.2733	1	-6 4 3	74.45
1.2703	2	-10 2 5	74.66
1.2671	9	14 0 2	74.88
1.2670	2	-15 1 1	74.88
1.2584	5	-8 4 2	75.48
1.2550	3	9 1 5	75.72
1.2535	4	14 2 0	75.83
1.2533	1	-10 0 6	75.85
1.2527	6	0 4 4	75.89
1.2493	1	-7 3 5	76.13
1.2460	3	-14 2 2	76.37
1.2448	1	-1 1 7	76.46
1.2351	5	-4 4 4	77.17
1.2287	2	8 2 5	77.65
1.2250	1	-8 2 6	77.93
1.2242	2	12 0 4	77.98
1.2208	2	14 2 1	78.24

Calcium malate hydrate, $CaC_4H_4O_5 \cdot 2H_2O$

Structure

Orthorhombic, $P2_12_12_1$ (19), Z=4. The structure was determined by Brändén and Söderberg [1966].

Lattice parameters

a = 8.448(1), b = 13.414(3), c = 6.728(1)Å, (published value: b = 13.413(3)Å) [ibid.]

Density

(calculated) 1.814 g/cm^3

Thermal parameters

Isotropic:

Ca(1)	1.75	O(7)	3.14
O(2)	2.75	O(8)	2.95
O(3)	3.52	C(9)	2.37
O(4)	3.80	C(10)	2.17
O(5)	2.63	C(11)	2.37
O(6)	2.99	C(12)	2.61

Scattering factors

Ca^{2+}, O^-, C^0 [3.3.1A]

Scale factors

(integrated intensities) 4.668×10^4

Reference

Brändén, C.-I. and B.-O. Söderberg (1966). Acta Chem. Scand. 20, 730.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
7.14	100	1	1	0		12.38
6.01	7	0	1	1		14.72
5.25	15	1	0	1	+	16.86
4.897	29	1	1	1		18.10
4.223	14	2	0	0		21.02
4.141	18	1	2	1		21.44
4.030	20	2	1	0		22.04
3.723	4	0	3	1		23.88
3.576	2	2	2	0	+	24.88
3.456	3	2	1	1		25.76
3.406	5	1	3	1		26.14
3.363	3	0	0	2		26.48
3.356	3	0	4	0		26.54
3.262	2	0	1	2		27.32
3.155	12	2	2	1		28.26
3.125	6	1	0	2		28.54
3.119	5	1	4	0		28.60
3.070	3	2	3	0		29.06
3.044	12	1	1	2		29.32
3.007	5	0	2	2		29.68
2.827	7	1	4	1		31.62
2.793	8	2	3	1		32.02
2.756	4	3	1	0		32.46
2.626	5	2	4	0		34.12
2.596	4	3	2	0		34.52
2.583	1	2	1	2		34.70
2.557	10	1	5	0	+	35.06
2.550	9	3	1	1		35.16
2.491	3	0	5	1		36.02
2.447	2	2	4	1	+	36.70
2.423	1	3	2	1		37.08
2.390	2	1	5	1		37.60
2.383	1	3	3	0		37.72
2.376	2	0	4	2		37.84
2.267	2	2	3	2	+	39.72
2.246	2	3	3	1		40.12
2.236	4	0	6	0		40.30
2.167	1	1	0	3		41.64
2.156	7	3	4	0		41.86
2.146	4	2	5	1		42.06
2.141	3	1	1	3		42.18
2.132	3	3	1	2		42.36
2.127	5	0	2	3		42.46
2.112	3	4	0	0		42.78
2.097	1	0	5	2		43.10
2.086	2	4	1	0		43.34
2.070	1	2	4	2		43.70
2.062	3	1	2	3		43.86
2.055	7	3	2	2	+	44.02
2.036	1	1	5	2		44.46

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
2.015	3	4 0 1	44.94
2.004	2	0 3 3	45.20
1.993	1	4 1 1	45.48
1.976	3	2 6 0	45.88
1.959	2	2 1 3	46.30
1.951	2	1 3 3	46.52
1.945	2	3 3 2	46.66
1.930	1	4 2 1	47.04
1.910	5	4 3 0	47.58
1.900	3	2 2 3	47.84
1.895	2	2 6 1	47.96
1.868	2	1 7 0	48.70
1.864	4	0 4 3	48.82
1.821	1	1 4 3	50.06
1.816	1	3 4 2	50.20
1.811	1	2 3 3	50.34
1.7540	1	3 0 3	52.10
1.7397	1	3 1 3	52.56
1.7281	1	4 2 2	52.94
1.7209	1	0 5 3	53.18
1.6973	1	3 2 3	53.98
1.6857	2	1 5 3	54.38
1.6817	2	3 5 2	54.52
1.6610	1	4 3 2	55.26
1.6386	1	5 2 0	56.08
1.6338	1	1 7 2	56.26
1.5420	1	3 7 1	59.94
1.5181	1	2 8 1	60.98
1.4986	1	4 2 3	61.86
1.4969	1	4 6 1	61.94
1.3739	1	3 3 4	68.20

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
7.15	100	1 1 0	12.37
6.01	8	0 1 1	14.72
5.26	11	1 0 1	16.83
5.253	8	1 2 0	16.86
4.899	33	1 1 1	18.09
4.224	16	2 0 0	21.01
4.140	21	1 2 1	21.44
4.029	23	2 1 0	22.04
3.724	4	0 3 1	23.88
3.577	1	2 0 1	24.87
3.574	1	2 2 0	24.89
3.457	3	2 1 1	25.75
3.408	6	1 3 1	26.13
3.364	4	0 0 2	26.47
3.354	1	0 4 0	26.56
3.263	3	0 1 2	27.31
3.156	16	2 2 1	28.25
3.125	7	1 0 2	28.54
3.117	1	1 4 0	28.62
3.071	4	2 3 0	29.06
3.044	15	1 1 2	29.32
3.007	6	0 2 2	29.69
2.828	10	1 4 1	31.61
2.793	10	2 3 1	32.01
2.756	6	3 1 0	32.46
2.626	6	2 4 0	34.11
2.596	5	3 2 0	34.52
2.582	1	2 1 2	34.71
2.562	2	1 3 2	35.00
2.557	11	1 5 0	35.07
2.550	5	3 1 1	35.16
2.492	5	0 5 1	36.01
2.450	2	2 2 2	36.65
2.447	2	2 4 1	36.70
2.422	1	3 2 1	37.08
2.390	2	1 5 1	37.60
2.383	1	3 3 0	37.72
2.375	2	0 4 2	37.85
2.268	2	2 3 2	39.71
2.265	1	2 5 0	39.77
2.246	2	3 3 1	40.11
2.236	6	0 6 0	40.31
2.168	1	1 0 3	41.63
2.157	9	3 4 0	41.85
2.146	5	2 5 1	42.06
2.140	2	1 1 3	42.20
2.132	3	3 1 2	42.36
2.127	6	0 2 3	42.47
2.112	4	4 0 0	42.78
2.097	1	0 5 2	43.09

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
2.086	3	4 1 0	43.33
2.070	1	2 4 2	43.69
2.063	4	1 2 3	43.86
2.058	1	1 6 1	43.97
2.055	9	3 2 2	44.02
2.036	2	1 5 2	44.47
2.015	5	4 0 1	44.95
2.005	2	0 3 3	45.19
1.993	1	4 1 1	45.48
1.976	5	2 6 0	45.89
1.960	3	2 1 3	46.29
1.950	3	1 3 3	46.52
1.944	2	3 3 2	46.67
1.930	1	4 2 1	47.05
1.910	7	4 3 0	47.58
1.900	3	2 2 3	47.84
1.896	2	2 6 1	47.94
1.869	3	1 7 0	48.68
1.866	2	3 5 1	48.76
1.864	4	0 4 3	48.81
1.862	1	0 6 2	48.87
1.820	2	1 4 3	50.07
1.816	1	3 4 2	50.21
1.811	1	2 3 3	50.34
1.7543	1	3 0 3	52.09
1.7395	2	3 1 3	52.57
1.7283	1	4 2 2	52.93
1.7207	1	0 5 3	53.19
1.6972	1	3 2 3	53.98
1.6860	2	1 5 3	54.37
1.6821	1	3 5 2	54.51
1.6607	1	4 3 2	55.27
1.6496	1	1 0 4	55.67
1.6384	1	5 2 0	56.09
1.6337	2	1 7 2	56.26
1.5782	1	4 4 2	58.43
1.5421	2	3 7 1	59.93
1.5275	1	4 1 3	60.57
1.5183	1	2 8 1	60.97
1.4986	2	4 2 3	61.86
1.4968	1	4 6 1	61.94
1.4683	1	3 5 3	63.29
1.3801	1	3 6 3	67.85
1.3741	1	3 3 4	68.19
1.3340	1	4 5 3	70.54
1.3170	1	6 3 1	71.59
1.2940	1	3 7 3	73.07
1.2454	1	5 7 1	76.41
1.1992	1	4 7 3	79.93

Cesium lithium cobalt cyanide, $Cs_2LiCo(CN)_6$

Structure
Cubic, Fm3m(225),Z=4, isostructural with elpasolite (K_2NaAlF_6). The structure was determined by Wolberg [1969].

Lattice parameters
a=10.54(1)Å [ibid.]

Density
(calculated) 2.767 g/cm^3

Thermal parameters
Isotropic [ibid.]

Scattering factors
Cs^0 [3.3.1B], corrected for dispersion[Wolberg, 1969]
Li^0, Co^0, C^0, N^0 [3.3.1A]

Scale factors
(integrated intensities) 90.96×10^4

Reference
Wolberg, A. (1969). Acta Cryst. B25, 161.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(^\circ)$ $\lambda = 1.54056$ Å
6.09	14	1	1	1		14.54
5.27	19	2	0	0		16.82
3.726	100	2	2	0		23.86
3.177	5	3	1	1		28.06
3.042	36	2	2	2		29.34
2.635	35	4	0	0		34.00
2.417	2	3	3	1		37.16
2.356	13	4	2	0		38.16
2.151	25	4	2	2		41.96
2.028	1	5	1	1		44.64
1.863	14	4	4	0		48.84
1.781	1	5	3	1		51.24
1.757	6	4	4	2		52.02
1.667	14	6	2	0		55.06
1.589	5	6	2	2		58.00
1.521	3	4	4	4		60.84
1.462	1	6	4	0		63.60
1.409	9	6	4	2		66.30
1.317	1	8	0	0		71.56
1.278	2	8	2	0	+	74.12
1.242	3	6	6	0	+	76.64
1.209	1	6	6	2		79.16
1.178	2	8	4	0		81.64
1.150	2	8	4	2		84.10
1.124	2	6	6	4		86.56
1.076	1	8	4	4		91.46
1.034	2	8	6	2	+	96.36
.962	1	10	4	2		106.36
.904	1	10	6	0	+	116.92
.855	1	10	6	4	+	128.58

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
6.09	12	1 1 1	14.54
5.27	17	2 0 0	16.81
3.726	100	2 2 0	23.86
3.178	6	3 1 1	28.05
3.043	41	2 2 2	29.33
2.635	40	4 0 0	33.99
2.418	2	3 3 1	37.15
2.357	16	4 2 0	38.15
2.151	30	4 2 2	41.96
2.028	1	5 1 1	44.64
1.863	18	4 4 0	48.84
1.782	1	5 3 1	51.23
1.757	8	4 4 2	52.02
1.667	19	6 2 0	55.06
1.589	7	6 2 2	57.99
1.521	4	4 4 4	60.84
1.462	1	6 4 0	63.61
1.408	15	6 4 2	66.31
1.372	1	7 3 1	68.30
1.317	2	8 0 0	71.56
1.278	2	8 2 0	74.12
1.278	1	6 4 4	74.12
1.242	3	6 6 0	76.65
1.242	3	8 2 2	76.65
1.209	1	6 6 2	79.15
1.178	4	8 4 0	81.64
1.150	3	8 4 2	84.10
1.124	3	6 6 4	86.56
1.076	2	8 4 4	91.46
1.034	3	8 6 2	96.37
1.034	2	10 2 0	96.37
1.014	1	10 2 2	98.84
.979	1	8 6 4	103.83
.962	3	10 4 2	106.37
.917	1	8 8 2	114.20
.904	2	10 6 0	116.92
.904	1	8 6 6	116.92
.891	1	10 6 2	119.70
.878	1	8 8 4	122.56
.855	1	12 2 2	128.58
.855	3	10 6 4	128.58
.833	2	12 4 0	135.16
.823	1	12 4 2	138.75
.813	2	10 8 2	142.61
.794	2	12 4 4	151.64
.786	1	10 8 4	157.33

Chromium fluoride, CrF_2

Structure

Monoclinic, $P2_1/n$ (14), Z=2, distorted rutile type. The structure was determined by Jack and Maitland [1957].

Lattice parameters

a=4.732(2), b=4.718(2), c=3.505(2)Å, β=96.52(5)° [ibid.]

Density

(calculated) 3.844 g/cm^3

Thermal parameters

Isotropic: overall B = 1.5

Scattering factors

F^-, Cr^{2+} [3.3.1A]

Scale factor

(integrated intensities) 0.2277×10^4

Additional patterns

1. PDF card 11-84 [Insley et al.,1956]

Reference

Insley, H., T.N. McVay, R.E. Thoma and G.D. White (1956). ORNL 2192, 27.

Jack, K.H. and R. Maitland (1957). Proc.Chem.Soc. 1957, 232.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
3.331	100	1 1 0	26.74
2.965	30	-1 0 1	30.12
2.801	32	0 1 1	31.92
2.657	7	1 0 1	33.70
2.510	20	-1 1 1	35.74
2.359	2	0 2 0	38.12
2.350	2	2 0 0	38.26
2.316	11	1 1 1	38.86
2.108	4	1 2 0	42.86
2.104	5	2 1 0	42.96
1.888	17	-2 1 1	48.16
1.845	11	-1 2 1	49.34
1.764	15	1 2 1	51.78
1.741	11	0 0 2	52.52
1.725	10	2 1 1	53.04
1.665	14	2 2 0	55.12
1.633	1	0 1 2	56.28
1.596	5	-1 1 2	57.70
1.494	9	1 1 2 +	62.06
1.491	7	1 3 0	62.22
1.487	5	3 1 0	62.38
1.433	7	0 3 1	65.02
1.424	1	-3 1 1	65.48
1.401	1	0 2 2	66.72
1.372	3	3 0 1	68.32
1.262	1	-3 2 1	75.22
1.255	4	-2 2 2	75.74
1.196	1	-3 1 2	80.16
1.180	1	0 4 0	81.54
1.175	1	4 0 0	81.90
1.158	2	2 2 2 +	83.40
1.153	1	-1 3 2	83.80
1.127	1	0 1 3	86.22
1.121	1	-4 1 1	86.80
1.110	2	3 3 0	87.88
1.096	1	-1 4 1	89.32

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
3.330	100	1	1	0	26.75
2.964	30	-1	0	1	30.13
2.802	32	0	1	1	31.91
2.658	7	1	0	1	33.70
2.510	22	-1	1	1	35.75
2.359	2	0	2	0	38.12
2.351	2	2	0	0	38.26
2.316	11	1	1	1	38.86
2.108	3	1	2	0	42.86
2.104	3	2	1	0	42.95
1.888	20	-2	1	1	48.16
1.846	13	-1	2	1	49.33
1.764	19	1	2	1	51.77
1.741	13	0	0	2	52.51
1.725	13	2	1	1	53.05
1.665	18	2	2	0	55.11
1.633	1	0	1	2	56.27
1.597	6	-1	1	2	57.69
1.494	7	1	1	2	62.05
1.494	5	-3	0	1	62.07
1.491	4	1	3	0	62.19
1.487	4	3	1	0	62.39
1.433	10	0	3	1	65.02
1.424	1	-3	1	1	65.48
1.401	1	0	2	2	66.71
1.372	5	3	0	1	68.31
1.329	1	2	0	2	70.85
1.279	1	2	1	2	74.06
1.262	1	-3	2	1	75.22
1.255	5	-2	2	2	75.73
1.199	1	2	3	1	79.94
1.196	2	-3	1	2	80.16
1.179	1	0	4	0	81.54
1.175	1	4	0	0	81.89
1.158	1	-1	0	3	83.40
1.158	2	2	2	2	83.41
1.153	2	-1	3	2	83.80
1.127	1	0	1	3	86.22
1.121	1	-4	1	1	86.81
1.110	3	3	3	0	87.88
1.096	1	-1	4	1	89.32

Cobalt ammine iodide, $Co(NH_3)_6I_3$

Structure
Cubic, Fm3m(225), Z=4; it is isostructural with $(NH_4)_3FeF_6$. The structure was determined by Kime and Ibers [1969].

Lattice parameters
a=10.82(2)Å [ibid.]

Density
(calculated) 2.841 g/cm^3

Thermal parameters
Isotropic: iodine(1) 2.77, iodine(2) 2.69, cobalt 1.71 [ibid.]; nitrogen 3.02.

Scattering factors
Co^0, I^0 [3.3.1B],corrected for dispersion [Cromer, 1965]
N^0 [3.3.1A]

Scale factors
(integrated intensities) 205.5×10^4

Additional patterns
1. PDF card 2-307 [Natta (1928); Wyckoff and McCutcheon (1927)]

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
6.24	1	1	1	1		14.18
3.82	100	2	2	0		23.24
3.26	3	3	1	1		27.32
3.12	3	2	2	2		28.56
2.21	27	4	2	2		40.82
2.08_2	1	3	3	3		43.42
1.913	10	4	4	0		47.50
1.711	12	6	2	0		53.52
1.562	2	4	4	4		59.10
1.446	9	6	4	2		64.38
1.352	1	8	0	0		69.44
1.275	3	8	2	2	+	74.32
1.210	2	8	4	0		79.10
1.153	1	6	6	4		83.80
1.104	1	8	4	4		88.46
1.061	2	8	6	2	+	93.10
.988	1	10	4	2		102.50
.928	1	10	6	0	+	112.24
.878	1	10	6	4	+	122.74

Reference

Cromer, D.T. (1965). Acta Cryst. 18, 17.
Kime, N.E. and J.A. Ibers(1969). Acta Cryst. B25, 168.
Natta, G. (1928). Gazz. Chim. Ital. 58, 625.
Wyckoff, R.W.G. and T.P. McCutcheon (1927). Am.J. Sci. 13, 223.

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.25	1	1 1 1	14.17
3.83	100	2 2 0	23.23
3.26	4	3 1 1	27.31
3.12	3	2 2 2	28.55
2.21	32	4 2 2	40.82
2.08_2	1	3 3 3	43.42
1.913	12	4 4 0	47.50
1.829	1	5 3 1	49.82
1.803	1	4 4 2	50.57
1.711	16	6 2 0	53.52
1.562	3	4 4 4	59.11
1.446	14	6 4 2	64.38
1.353	1	8 0 0	69.43
1.275	2	6 6 0	74.32
1.275	3	8 2 2	74.32
1.210	3	8 4 0	79.10
1.153	3	6 6 4	83.80
1.104	2	8 4 4	88.46
1.061	3	8 6 2	93.10
1.061	2	10 2 0	93.10
.988	2	10 4 2	102.49
.928	1	10 6 0	112.24
.928	1	8 6 6	112.24
.902	1	8 8 4	117.36
.878	1	12 2 2	122.73
.878	2	10 6 4	122.73
.855	1	12 4 0	128.45
.835	2	10 8 2	134.66
.816	1	12 4 4	141.62
.798	3	12 6 2	149.89

Cobalt fluoride, CoF_2

Structure

Tetragonal, $P4_2mnm$ (136), Z=2, isostructural with rutile [Ferrari, 1926]. The structure was determined by Stout and Reed and refined by Baur [1958].

Lattice parameters

a=4.6953(2), c=3.1797(3)Å, (published as 4.6951 and 3.1796) [Stout and Reed, 1954]

Density

(calculated) 4.592 g/cm^3

Thermal parameters

Isotropic [Baur,1958] Co 0.5
F 0.8

Atomic positions

Baur [1958]

Scattering factors

F^- [Cromer and Waber, 1965]
Co^{2+} [Cromer and Waber,1965], corrected for dispersion using $\Delta f'$=-2.51 and $\Delta f''$=3.95 [Cromer, 1965]

Scale factors

(integrated intensities) 0.2727×10^4

Additional patterns

1. PDF card 3-409 [Dow Chemical Co., Midland, Mich.]
2. Ferrari [1926]

Reference

Baur, W.H. (1958). Acta Cryst. 11, 488.
Cromer, D.T. (1965). Acta Cryst. 18, 17.
Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Ferrari, A. (1926). Atti reale accad. nazl. Lincei 3, 224.
Stout, J.W. and S.A. Reed (1954). J.Am.Chem. Soc. 76, 5279.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
3.3169	100	1 1 0	26.84
2.6331	47	1 0 1	34.02
2.3481	6	2 0 0	38.30
2.2962	21	1 1 1	39.20
2.0998	7	2 1 0	43.04
1.7521	53	2 1 1	52.16
1.6598	14	2 2 0	55.30
1.5898	8	0 0 2	57.96
1.4846	6	3 1 0	62.50
1.4340	9	1 1 2	64.98
1.4041	16	3 0 1	66.54
1.3453	1	3 1 1	69.86
1.3165	2	2 0 2	71.62
1.2676	1	2 1 2	74.84
1.2051	3	3 2 1	79.46
1.1739	2	4 0 0	82.02
1.1483	5	2 2 2	84.26
1.1389	1	4 1 0	85.12
1.1067	2	3 3 0	88.22
1.0852	3	3 1 2	90.44
1.0721	4	4 1 1	91.66
1.0498	2	4 2 0	94.40
1.0339	1	1 0 3	96.32
.9462	3	2 1 3	109.00
.9440	2	4 0 2	109.36
.9209	2	5 1 0	113.54
.9083	2	3 3 2	116.00
.9006	3	4 3 1	117.58
.8776	2	3 0 3	122.74
.8761	2	4 2 2	123.10
.8408	4	5 2 1	132.72
.8220	1	3 2 3	139.12
.7968	3	5 1 2	150.34
.7949	2	0 0 4	151.42
.7825	1	6 0 0	159.68

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
3.3201	100	1	1	0	26.83
2.6328	50	1	0	1	34.02
2.3476	7	2	0	0	38.31
2.2964	23	1	1	1	39.20
2.0998	8	2	1	0	43.04
1.7522	65	2	1	1	52.16
1.6600	18	2	2	0	55.29
1.5898	11	0	0	2	57.96
1.4848	8	3	1	0	62.50
1.4716	1	2	2	1	63.13
1.4339	12	1	1	2	64.98
1.4042	23	3	0	1	66.54
1.3453	1	3	1	1	69.86
1.3164	2	2	0	2	71.63
1.2675	2	2	1	2	74.85
1.2051	4	3	2	1	79.46
1.1738	3	4	0	0	82.02
1.1482	8	2	2	2	84.27
1.1388	1	4	1	0	85.13
1.1067	4	3	3	0	88.22
1.0851	5	3	1	2	90.44
1.0721	7	4	1	1	91.86
1.0499	3	4	2	0	94.39
1.0339	2	1	0	3	96.32
.9462	7	2	1	3	108.99
.9443	3	4	0	2	109.31
.9258	1	4	1	2	112.62
.9208	4	5	1	0	113.55
.9083	5	3	3	2	116.00
.9006	6	4	3	1	117.58
.8776	5	3	0	3	122.74
.8761	5	4	2	2	123.09
.8409	11	5	2	1	132.72
.8300	2	4	4	0	136.26
.8220	3	3	2	3	139.12
.8052	1	5	3	0	146.11
.8031	1	4	4	1	147.12
.7968	12	5	1	2	150.34
.7949	2	0	0	4	151.39
.7825	5	6	0	0	159.68

Copper ammine selenate, $Cu(NH_3)_4SeO_4$

Structure
Monoclinic, $P2_1/n(14)$, Z=4. The structure was determined by Morosin [1969].

Lattice parameters
a=10.3132(4)Å[published value: 10.3128(4)]
b=10.2594(3) [published value: 10.2590(3)]
c= 7.4049(3) [published value: 7.4046(3)]
β= 104.431(3)° [ibid.]

Density
(calculated) 2.404 g/cm^3

Thermal parameters
Isotropic: copper 1.82; selenium 1.53; nitrogen(1) 1.71; nitrogen(2) 2.38;nitrogen(3) 1.95; nitrogen(4) 2.27;oxygen(1) 2.43;oxygen(2) 2.96; oxygen(3) 3.00; oxygen(4) 3.33.

Scattering factors
Cu^{2+}, N^0, H^0, Se^0, O^0 [3.3.1A]
The copper and selenium factors were corrected for dispersion [3.3.2B]

Scale factors
(integrated intensities) 2.767×10^4

Reference
Morosin, B. (1969). Acta Cryst. B25, 19.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
5.878	1	0	1	1		15.06
5.590	5	-1	1	1		15.84
5.236	2	1	0	1		16.92
5.127	79	0	2	0		17.28
4.996	86	2	0	0		17.74
4.667	2	1	1	1		19.00
4.489	8	2	1	0		19.76
4.172	30	0	2	1		21.28
3.6657	3	1	2	1		24.26
3.5786	100	0	0	2	+	24.86
3.4582	28	-2	2	1	+	25.74
3.3858	13	0	1	2		26.30
3.3311	25	-2	0	2		26.74
3.2361	1	1	3	0		27.54
3.1885	3	-3	1	1		27.96
3.1685	1	-2	1	2		28.14
3.0416	1	-1	3	1		29.34
2.9956	3	2	2	1	+	29.80
2.9379	13	0	2	2		30.40
2.8643	4	1	3	1		31.20
2.8220	2	2	3	0		31.68
2.7945	14	-2	2	2		32.00
2.7676	2	3	0	1		32.32
2.7137	2	-3	1	2		32.98
2.6728	2	3	1	1		33.50
2.6196	4	2	0	2		34.20
2.5377	5	2	1	2		35.34
2.5048	4	-1	3	2	+	35.82
2.4981	3	4	0	0		35.92
2.4741	1	0	3	2		36.28
2.4352	2	3	2	1		36.88
2.4263	2	4	1	0		37.02
2.4150	2	0	4	1		37.20
2.4001	1	-1	1	3		37.44
2.3853	4	3	3	0		37.68
2.3329	9	2	2	2		38.56
2.2940	4	-4	2	1		39.24
2.2817	4	2	4	0		39.46
2.2489	14	-2	4	1		40.06
2.2446	17	4	2	0		40.14
2.1752	7	-2	2	3	+	41.48
2.1691	5	0	2	3		41.60
2.1543	1	1	1	3		41.90
2.1291	6	-4	2	2		42.42
2.1064	5	2	4	1		42.90
2.0860	1	0	4	2		43.34
2.0796	4	2	3	2		43.48
2.0171	2	4	3	0	+	44.90
1.9657	1	-2	3	3		46.14
1.9593	2	0	3	3		46.30

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
1.8575	3	-4	2	3		49.00
1.8469	1	4	3	1		49.30
1.8448	2	4	0	2		49.36
1.8399	4	-2	0	4	+	49.50
1.8329	2	2	4	2		49.70
1.8138	10	-4	4	1	+	50.26
1.8105	7	-2	1	4		50.36
1.7932	3	0	0	4	+	50.88
1.7892	3	4	4	0		51.00
1.7660	2	0	1	4		51.72
1.7534	5	-2	4	3		52.12
1.7490	4	0	4	3		52.26
1.7360	2	4	2	2		52.68
1.7318	3	-2	2	4	+	52.82
1.7090	2	2	3	3	+	53.58
1.6926	1	0	2	4		54.14
1.6778	1	-6	0	2		54.66
1.6671	4	4	4	1	+	55.04
1.6632	5	0	6	1	+	55.18
1.6434	2	6	1	0		55.90
1.6295	1	-6	2	1		56.42
1.6237	2	4	3	2		56.64
1.6060	3	-2	6	1		57.32
1.5949	2	-6	2	2		57.76
1.5878	1	0	3	4		58.04
1.5848	3	-4	2	4	+	58.16
1.5735	5	-4	4	3		58.62
1.5638	2	2	4	3		59.02
1.5599	2	-2	5	3		59.18
1.5571	2	0	5	3		59.30
1.5514	2	2	6	1	+	59.54
1.4986	2	4	5	1		61.86
1.4278	2	-6	4	1		65.30
1.4223	3	-4	6	1	+	65.58
1.4075	2	-6	0	4	+	66.36
1.4041	2	-6	4	2		66.54
1.3930	2	-2	6	3		67.14
1.3908	2	0	6	3		67.26
1.3715	2	6	1	2		68.34
1.3572	1	-6	2	4		69.16
1.3333	1	-6	4	3		70.58

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
5.878	1	0	1	1	15.06
5.589	6	-1	1	1	15.84
5.239	1	1	0	1	16.91
5.130	87	0	2	0	17.27
4.994	100	2	0	0	17.75
4.666	2	1	1	1	19.00
4.490	9	2	1	0	19.76
4.172	35	0	2	1	21.28
3.6654	3	1	2	1	24.26
3.5856	74	0	0	2	24.81
3.5783	74	2	2	0	24.86
3.4630	1	-1	1	2	25.70
3.4580	34	-2	2	1	25.74
3.3849	17	0	1	2	26.31
3.3325	33	-2	0	2	26.73
3.2354	1	1	3	0	27.55
3.1897	5	-3	1	1	27.95
3.1695	1	-2	1	2	28.13
3.0427	1	-1	3	1	29.33
2.9985	2	1	1	2	29.77
2.9953	2	2	2	1	29.80
2.9895	1	-1	2	2	29.86
2.9388	18	0	2	2	30.39
2.8638	5	1	3	1	31.21
2.8216	2	2	3	0	31.68
2.7946	18	-2	2	2	32.00
2.7677	2	3	0	1	32.32
2.7142	2	-3	1	2	32.97
2.6722	3	3	1	1	33.51
2.6197	5	2	0	2	34.20
2.5382	6	2	1	2	35.33
2.5081	1	2	3	1	35.77
2.5048	5	-1	3	2	35.82
2.4970	2	4	0	0	35.94
2.4747	2	0	3	2	36.27
2.4358	2	3	2	1	36.87
2.4261	2	4	1	0	37.02
2.4150	3	0	4	1	37.20
2.3997	2	-1	1	3	37.45
2.3855	6	3	3	0	37.68
2.3408	1	-4	0	2	38.42
2.3331	11	2	2	2	38.56
2.2941	5	-4	2	1	39.24
2.2815	5	2	4	0	39.46
2.2494	17	-2	4	1	40.05
2.2451	16	4	2	0	40.13
2.1752	10	-2	2	3	41.48
2.1714	1	-3	1	3	41.56
2.1667	3	0	2	3	41.65
2.1546	1	1	1	3	41.89

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.1296	9	-4 2 2	42.41
2.1060	8	2 4 1	42.91
2.0861	1	0 4 2	43.34
2.0796	6	2 3 2	43.48
2.0326	1	-2 4 2	44.54
2.0175	1	4 2 1	44.89
2.0166	3	4 3 0	44.91
1.9655	2	-2 3 3	46.15
1.9592	2	0 3 3	46.30
1.8573	5	-4 2 3	49.00
1.8469	1	4 3 1	49.30
1.8448	1	4 0 2	49.36
1.8416	1	2 2 3	49.45
1.8403	1	3 3 2	49.49
1.8394	4	-2 0 4	49.51
1.8327	2	2 4 2	49.71
1.8157	5	4 1 2	50.21
1.8136	14	-4 4 1	50.26
1.8106	3	-2 1 4	50.36
1.7932	2	2 5 1	50.88
1.7928	2	0 0 4	50.89
1.7891	3	4 4 0	51.00
1.7660	3	0 1 4	51.72
1.7531	7	-2 4 3	52.13
1.7487	3	0 4 3	52.27
1.7359	3	4 2 2	52.68
1.7315	3	-2 2 4	52.83
1.7290	2	-4 4 2	52.91
1.7091	2	2 3 3	53.58
1.7078	1	5 2 1	53.62
1.6924	1	0 2 4	54.15
1.6780	2	-6 0 2	54.65
1.6674	4	4 4 1	55.03
1.6663	2	-4 0 4	55.07
1.6646	2	6 0 0	55.13
1.6633	5	0 6 1	55.18
1.6432	2	6 1 0	55.91
1.6296	1	-6 2 1	56.42
1.6236	3	4 3 2	56.64
1.6061	4	-2 6 1	57.32
1.5948	3	-6 2 2	57.76
1.5879	1	0 3 4	58.04
1.5848	4	-4 2 4	58.16
1.5834	2	6 2 0	58.22
1.5735	8	-4 4 3	58.62
1.5639	3	2 4 3	59.02
1.5601	1	-2 5 3	59.17
1.5570	2	0 5 3	59.30
1.5514	3	2 6 1	59.54
1.5497	1	2 1 4	59.61

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.4987	2	4 5 1	61.85
1.4277	2	-6 4 1	65.30
1.4251	1	2 3 4	65.44
1.4227	3	-4 6 1	65.56
1.4222	3	2 5 3	65.58
1.4080	2	4 3 3	66.33
1.4072	2	-6 0 4	66.37
1.4042	1	-6 4 2	66.54
1.3930	2	-2 6 3	67.14
1.3907	3	0 6 3	67.27
1.3715	4	6 1 2	68.34
1.3571	2	-6 2 4	69.17
1.3488	1	4 6 1	69.65
1.3332	1	-6 4 3	70.59

Copper ammine sulfate hydrate, $Cu(NH_3)_4SO_4 \cdot H_2O$

Structure

Orthorhombic, Pnam(62), Z=4. The structure was determined by Mazzi [1955], and refined by Morosin [1969].

Lattice parameters

a=10.651(1), b=11.986(2), c=7.0690(3)Å [ibid.]

Density

(calculated) 1.809 g/cm^3

Thermal parameters

Isotropic: copper 2.32; sulfur 1.84; nitrogen(1) 2.99; nitrogen(2) 3.07; oxygen(1) 5.34; oxygen(2) 3.93; oxygen(3) 4.08; oxygen(4) 4.12.

Scattering factors

Cu^{2+}, N^0, H^0, S^0, O^0 [3.3.1A]. The copper factor was corrected for dispersion using $\Delta f'=-2.1$ and $\Delta f''=0.7$.

Scale factors

(integrated intensities) 8.801×10^4

Additional patterns

1. PDF card 20-349 [Givens, Noranda Research Centre, Point Clare, Quebec, Canada]

Reference

Mazzi, F. (1955). Acta Cryst. 8, 137.
Morosin, B. (1969). Acta Cryst. B25, 19.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl			$2\theta(°)$ $\lambda = 1.54056$ Å
7.96	2	1	1	0	11.10
6.09	15	0	1	1	14.54
5.99	33	0	2	0	14.78
5.29	51	1	1	1	16.76
5.22	43	1	2	0	16.96
4.865	1	2	1	0	18.22
4.008	100	2	1	1	22.16
3.980	33	2	2	0	22.32
3.742	1	1	3	0	23.76
3.534	8	0	0	2	25.18
3.477	26	0	3	1 +	25.60
3.229	3	1	1	2	27.60
3.054	26	3	2	0	29.22
3.046	21	0	2	2	29.30
2.996	2	0	4	0	29.80
2.944	2	2	0	2	30.34
2.927	19	1	2	2	30.52
2.912	8	2	3	1	30.68
2.884	4	1	4	0	30.98
2.859	3	2	1	2	31.26
2.664	7	4	0	0	33.62
2.644	2	2	2	2	33.88
2.611	4	2	4	0	34.32
2.452	1	3	1	2	36.62
2.439	3	4	1	1	36.82
2.434	7	4	2	0	36.90
2.371	1	2	3	2	37.92
2.2851	4	0	4	2	39.40
2.2350	1	1	4	2	40.32
2.2202	2	1	5	1	40.60
2.1262	7	4	0	2	42.48
2.1215	8	2	1	3	42.58
2.1148	7	4	3	1	42.72
2.1008	14	2	4	2	43.02
2.0888	6	2	5	1	43.28
2.0291	3	0	3	3 +	44.62
2.0044	6	4	2	2	45.20
1.9985	4	0	6	0	45.34
1.9911	1	4	4	0	45.52
1.9310	1	5	2	1	47.02
1.8968	4	2	3	3	47.92
1.8247	1	1	4	3	49.94
1.7673	3	0	0	4	51.68
1.7622	2	3	3	3	51.84
1.7453	3	5	2	2 +	52.38
1.7391	3	0	6	2 +	52.58
1.7348	3	4	4	2	52.72
1.7275	2	4	5	1	52.96
1.7227	1	6	0	1	53.12
1.7167	1	1	6	2	53.32

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
1.7043	3	6	1	1		53.74
1.6949	2	0	2	4		54.06
1.6806	2	0	5	3		54.56
1.6744	1	1	2	4		54.78
1.6532	2	2	6	2		55.54
1.6143	2	4	3	3	+	57.00
1.6025	2	2	5	3		57.46
1.5984	2	4	6	0		57.62
1.5883	3	2	7	1		58.02
1.5814	1	6	3	1		58.30
1.5336	1	6	2	2		60.30
1.5295	1	3	2	4		60.48
1.5272	2	6	4	0		60.58
1.4638	1	2	4	4	+	63.50
1.4560	1	4	6	2		63.88
1.4301	1	4	2	4		65.18
1.4212	1	4	5	3		65.64
1.4079	2	6	1	3		66.34
1.4019	1	6	4	2		66.66
1.3986	1	6	5	1		66.84
1.3575	2	2	1	5		69.14
1.3406	1	2	7	3		70.14
1.2459	1	8	0	2		76.38
1.2431	1	8	3	1		76.58
1.2248	1	4	8	2		77.94

Calculated Pattern *(Integrated)*					
d (Å)	I	hkl			2θ(°) λ = 1.54056 Å
7.96	2	1	1	0	11.10
6.09	13	0	1	1	14.54
5.99	30	0	2	0	14.77
5.33	1	2	0	0	16.63
5.29	46	1	1	1	16.76
5.22	39	1	2	0	16.96
4.867	1	2	1	0	18.21
4.009	100	2	1	1	22.16
3.981	26	2	2	0	22.31
3.741	1	1	3	0	23.77
3.535	8	0	0	2	25.18
3.478	29	0	3	1	25.59
3.469	1	2	2	1	25.66
3.230	3	1	1	2	27.59
3.055	28	3	2	0	29.21
3.044	10	0	2	2	29.31
2.996	2	0	4	0	29.79
2.945	2	2	0	2	30.33
2.927	21	1	2	2	30.51
2.912	7	2	3	1	30.68
2.885	5	1	4	0	30.98
2.860	3	2	1	2	31.25
2.671	1	1	4	1	33.53
2.663	7	4	0	0	33.63
2.643	2	2	2	2	33.89
2.611	5	2	4	0	34.31
2.452	1	3	1	2	36.62
2.440	3	4	1	1	36.81
2.433	7	4	2	0	36.91
2.371	1	2	3	2	37.92
2.2857	4	0	4	2	39.39
2.2348	1	1	4	2	40.32
2.2203	3	1	5	1	40.60
2.1268	8	4	0	2	42.47
2.1208	6	2	1	3	42.59
2.1143	6	4	3	1	42.73
2.1004	18	2	4	2	43.03
2.0884	7	2	5	1	43.29
2.0296	3	0	3	3	44.61
2.0277	1	2	2	3	44.65
2.0043	8	4	2	2	45.20
1.9977	2	0	6	0	45.36
1.9904	1	4	4	0	45.53
1.9308	1	5	2	1	47.02
1.8966	6	2	3	3	47.93
1.8249	1	1	4	3	49.94
1.7816	1	4	5	0	51.23
1.7673	4	0	0	4	51.68
1.7620	2	3	3	3	51.84
1.7458	1	4	1	3	52.36

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
1.7454	3	5 2 2	52.38
1.7410	1	3 6 0	52.52
1.7391	4	0 6 2	52.58
1.7343	1	4 4 2	52.74
1.7276	3	4 5 1	52.96
1.7217	1	6 0 1	53.15
1.7164	1	1 6 2	53.33
1.7042	5	6 1 1	53.74
1.6951	2	0 2 4	54.06
1.6804	2	0 5 3	54.57
1.6740	1	1 2 4	54.79
1.6532	3	2 6 2	55.54
1.6152	1	2 2 4	56.96
1.6142	1	4 3 3	57.00
1.6025	2	2 5 3	57.46
1.5980	1	4 6 0	57.64
1.5884	4	2 7 1	58.02
1.5811	1	6 3 1	58.31
1.5335	2	6 2 2	60.30
1.5297	1	3 2 4	60.47
1.5273	2	6 4 0	60.58
1.4725	1	4 0 4	63.08
1.4636	2	2 4 4	63.51
1.4561	1	4 6 2	63.88
1.4299	1	4 2 4	65.19
1.4211	1	4 5 3	65.64
1.4080	4	6 1 3	66.33
1.4020	1	6 4 2	66.65
1.3984	1	6 5 1	66.85
1.3794	1	0 8 2	67.89
1.3577	3	2 1 5	69.13
1.3406	2	2 7 3	70.14
1.3328	1	0 3 5	70.61
1.3057	1	4 8 0	72.30
1.2459	1	8 0 2	76.38
1.2434	1	8 3 1	76.56
1.2248	1	4 8 2	77.94
1.2141	1	6 7 1	78.76
1.1556	1	6 4 4	83.61

Structure

Monoclinic, $P2_1/a$ (14), Z=2. The structure was determined by Siegel and Hoekstra [1968] who published data in terms of the $P2_1/n$ cell with a=5.475, b=4.957, c=6.569, β=118.87°.

Lattice parameters

a=6.197(6),b=4.957(6),c=5.457(6),β=111.82(.15)°

Density

(calculated) 7.776 g/cm^3

Thermal parameters

Isotropic: O(1) 1.40 [Siegel and Hoekstra,1968]
O(2) 2.01 [ibid.]
Cu 1.11
U 0.54

Scattering factors

Cu^0 [3.3.1A]
O^{2-} [Tokonami, 1965]
U^0 [Cromer and Waber,1965], corrected for dispersion using Δf'=-9.19 [Cromer, 1965]

Scale factor

(integrated intensities) 5.968×10^4

Additional patterns

1. PDF card 16-236 [Brisi, 1963]

Reference

Brisi, C. (1963). Ann. Chim. Rome 53, 325.
Cromer, D.T. (1965). Acta Cryst. 18, 17.
Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Siegel, S. and H.R. Hoekstra (1968). Acta Cryst. B24, 967.
Tokonami, M. (1965). Acta Cryst. 19, 486.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				*2θ*(°) λ = 1.54056 Å
5.08	37	0	0	1		17.44
3.75	31	1	1	0		23.68
3.45	100	-1	1	1		25.84
3.03	6	-2	0	1		29.42
2.877	27	2	0	0		31.06
2.722	38	1	1	1		32.88
2.542	13	0	0	2		35.28
2.487	3	2	1	0		36.08
2.478	12	0	2	0		36.22
2.398	11	-2	0	2		37.48
2.391	15	-1	1	2		37.58
2.262	1	0	1	2		39.82
2.228	6	0	2	1		40.46
2.180	2	2	0	1		41.38
1.919	4	-2	2	1		47.32
1.907	16	-3	1	1		47.66
1.902	12	1	1	2		47.78
1.878	13	2	2	0		48.44
1.789	4	3	1	0		51.02
1.782	4	-3	1	2		51.22
1.774	14	0	2	2	+	51.46
1.723	12	-2	2	2		53.10
1.707	10	-1	1	3		53.64
1.694	1	0	0	3		54.08
1.637	3	2	2	1		56.14
1.628	5	2	0	2		56.48
1.588	2	1	3	0		58.02
1.562	6	-1	3	1		59.08
1.542	1	-4	0	1		59.94
1.529	6	3	1	1		60.50
1.521	5	-3	1	3		60.84
1.516	5	-4	0	2		61.06
1.473	6	1	3	1		63.04
1.444	1	-2	2	3		64.46
1.438	2	4	0	0		64.76
1.420	4	1	1	3		65.68
1.414	1	-1	3	2		66.04
1.399	1	0	2	3		66.84
1.365	2	-2	0	4		68.72
1.361	4	2	2	2		68.96
1.304	1	-1	1	4		72.44
1.293	3	-4	2	2		73.10
1.290	4	-3	3	1	+	73.32
1.271	2	0	0	4	+	74.64
1.268	1	2	0	3		74.84
1.263	1	-3	1	4		75.16
1.249	1	-3	3	2		76.12
1.244	3	4	2	0		76.52
1.239	1	0	4	0		76.86
1.223	2	-1	3	3		78.08

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.204	1	-4 2 3 +	79.54
1.199	2	-4 0 4 +	79.98
1.196	2	-2 2 4	80.22
1.189	2	-5 1 1	80.78
1.152	2	3 3 1	83.90
1.149	2	-3 3 3	84.22
1.147	1	-2 4 1	84.36
1.145	2	-5 1 3	84.58
1.138	2	2 4 0	85.18
1.131	2	0 2 4	85.88
1.128	1	4 2 1	86.18
1.121	1	5 1 0	86.82
1.114	1	0 4 2	87.50
1.103	1	1 3 3	88.54
1.101	2	-2 4 2	88.80
1.090	1	4 0 2	89.94

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.08	32	0 0 1	17.43
3.76	29	1 1 0	23.67
3.45	100	-1 1 1	25.83
3.03	7	-2 0 1	29.43
2.876	29	2 0 0	31.07
2.721	41	1 1 1	32.89
2.541	15	0 0 2	35.29
2.488	2	2 1 0	36.07
2.479	12	0 2 0	36.21
2.397	11	-2 0 2	37.48
2.391	9	-1 1 2	37.58
2.261	1	0 1 2	39.83
2.228	7	0 2 1	40.46
2.180	3	2 0 1	41.38
1.919	5	-2 2 1	47.33
1.907	19	-3 1 1	47.66
1.901	4	1 1 2	47.80
1.878	16	2 2 0	48.44
1.788	4	3 1 0	51.03
1.782	3	-3 1 2	51.22
1.777	2	-2 0 3	51.38
1.774	16	0 2 2	51.46
1.723	15	-2 2 2	53.11
1.707	12	-1 1 3	53.63
1.694	1	0 0 3	54.08

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.637	3	2 2 1	56.14
1.628	6	2 0 2	56.49
1.588	2	1 3 0	58.03
1.562	8	-1 3 1	59.09
1.542	2	-4 0 1	59.93
1.529	8	3 1 1	60.49
1.521	7	-3 1 3	60.85
1.516	4	-4 0 2	61.06
1.473	9	1 3 1	63.04
1.444	2	-2 2 3	64.47
1.438	3	4 0 0	64.77
1.421	6	1 1 3	65.67
1.414	2	-1 3 2	66.04
1.399	2	0 2 3	66.83
1.378	1	-4 0 3	67.98
1.365	3	-2 0 4	68.72
1.361	4	2 2 2	68.96
1.309	1	-4 2 1	72.07
1.303	1	-1 1 4	72.45
1.293	4	-4 2 2	73.10
1.290	3	-3 3 1	73.31
1.289	1	1 3 2	73.42
1.271	2	0 0 4	74.63
1.270	1	3 1 2	74.68
1.268	1	2 0 3	74.80
1.263	1	-3 1 4	75.16
1.252	1	3 3 0	75.96
1.249	1	-3 3 2	76.12
1.244	4	4 2 0	76.52
1.239	2	0 4 0	76.86
1.223	3	-1 3 3	78.08
1.204	1	-4 2 3	79.53
1.204	1	0 4 1	79.55
1.199	2	-4 0 4	79.98
1.198	1	-5 1 2	80.03
1.196	3	-2 2 4	80.22
1.189	3	-5 1 1	80.78
1.152	3	3 3 1	83.91
1.149	3	-3 3 3	84.22
1.147	1	-2 4 1	84.36
1.145	3	-5 1 3	84.58
1.138	3	2 4 0	85.19
1.131	3	0 2 4	85.88
1.127	1	4 2 1	86.19
1.124	1	1 1 4	86.55
1.121	1	5 1 0	86.83
1.114	2	0 4 2	87.50
1.104	2	1 3 3	88.53
1.101	2	-2 4 2	88.81
1.090	1	4 0 2	89.93

Iron sulfate hydroxide, butlerite, $FeSO_4(OH)\cdot 2H_2O$

Structure

Monoclinic, $P2_1/m$ (11), Z=2. The structure was determined by Fanfani et al. [1971].

Lattice parameters

a = 6.50(1), b = 7.37(1), c = 5.84(1)Å ,
β = 108.38(8)° [ibid.]

Density

(calculated) 2.564 g/cm^3

Thermal parameters

Isotropic [Fanfani et al., 1971]

Polymorphism

Butlerite is often found with its orthorhombic polymorph called parabutlerite [ibid.]. A pattern for the latter appears on PDF card 16-939.

Scattering factors

Fe^{3+}, O^0, S^0 [Cromer and Waber, 1965]

Scale factors

(integrated intensities 1.412×10^4

Additional patterns

1. PDF card 16-819 [Cesbron, 1964]

Reference

Cesbron, F. (1964). Bull. Soc. Franc. Mineral. Crist. 87, 125.

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

Fanfani, L., A. Nunzi, and P.F. Zanazzi (1971). Am. Mineralogist 56, 751.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
6.16	7	1 0 0	14.36
5.54	10	0 0 1	15.98
4.97	100	-1 0 1	17.82
4.73	14	1 1 0	18.74
4.43	17	0 1 1	20.04
3.68	1	0 2 0	24.14
3.60	18	1 0 1	24.74
3.23	15	1 1 1	27.58
3.16	50	1 2 0	28.18
3.08	4	2 0 0	28.94
3.07	23	0 2 1	29.08
2.89	5	-1 0 2 +	30.90
2.84	6	2 1 0	31.42
2.69	1	-1 1 2	33.26
2.59	3	0 1 2	34.56
2.57	5	1 2 1	34.82
2.49	16	-2 0 2	36.08
2.39	8	2 0 1 +	37.54
2.36	1	-2 1 2	38.14
2.28	1	1 3 0	39.46
2.27	6	1 0 2 +	39.60
2.215	1	0 2 2	40.70
2.173	1	1 1 2	41.52
2.163	1	-3 0 1	41.72
2.075	3	-3 1 1	43.58
2.062	3	-2 2 2	43.88
2.028	2	1 3 1	44.64
2.007	6	2 2 1	45.14
1.976	3	-3 0 2	45.88
1.922	2	2 3 0	47.26
1.909	1	-3 1 2	47.60
1.872	1	-1 3 2	48.60
1.865	4	-2 0 3 +	48.78
1.848	3	0 0 3	49.28
1.843	7	0 4 0	49.42
1.798	1	2 0 2	50.72
1.794	1	3 2 0	50.84
1.792	1	0 1 3	50.92
1.756	1	3 0 1	52.04
1.748	1	0 4 1	52.28
1.742	4	-3 2 2	52.50
1.728	2	-1 4 1	52.96
1.721	3	-1 2 3	53.18
1.716	2	2 3 1	53.34
1.664	2	-2 2 3	55.14
1.659	3	-3 0 3	55.34
1.640	5	1 4 1	56.04
1.624	3	-4 0 1 +	56.64
1.616	6	2 2 2	56.92
1.585	2	3 2 1	58.16

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
1.581	3	2 4 0	58.30
1.577	2	3 3 0	58.46
1.554	1	-1 4 2	59.44
1.540	1	-4 1 2	60.02
1.493	2	1 2 3	62.10
1.486	1	-4 2 1	62.44
1.481	2	-2 4 2	62.70
1.460	1	2 4 1	63.68
1.453	2	-1 0 4	64.02
1.448	1	-4 2 2 +	64.28
1.432	1	1 4 2	65.10
1.423	2	4 2 0	65.56
1.419	2	-2 1 4	65.76
1.403	1	-3 4 1	66.62
1.347	1	3 2 2 +	69.74
1.338	1	-1 4 3	70.30
1.329	1	-4 2 3	70.82
1.326	1	-4 3 2	71.02
1.311	1	-2 4 3	71.98
1.305	1	0 4 3	72.38
1.297	2	0 2 4	72.88
1.233	1	-3 4 3	77.34
1.221	2	-5 2 1	78.24
1.218	2	-4 4 1	78.46
1.205	1	1 6 0	79.50
1.199	1	0 6 1	79.92
1.197	1	-4 4 2	80.10
1.141	1	-1 4 4	84.92

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
6.17	7	1 0 0	14.35
5.54	10	0 0 1	15.98
4.98	100	-1 0 1	17.81
4.73	14	1 1 0	18.74
4.43	18	0 1 1	20.03
3.69	1	0 2 0	24.13
3.60	20	1 0 1	24.73
3.23	18	1 1 1	27.57
3.16	58	1 2 0	28.19
3.15	1	-2 0 1	28.31
3.08	2	2 0 0	28.93
3.07	26	0 2 1	29.08
2.90	2	-2 1 1	30.85
2.89	4	-1 0 2	30.90
2.85	7	2 1 0	31.42
2.69	1	-1 1 2	33.26
2.59	4	0 1 2	34.55
2.57	6	1 2 1	34.83
2.49	20	-2 0 2	36.07
2.39	5	-2 2 1	37.53
2.39	6	2 0 1	37.55
2.36	1	-2 1 2	38.15
2.28	1	1 3 0	39.45
2.27	1	-1 2 2	39.59
2.27	7	1 0 2	39.60
2.215	1	0 2 2	40.71
2.173	1	1 1 2	41.53
2.163	1	-3 0 1	41.72
2.075	4	-3 1 1	43.57
2.062	4	-2 2 2	43.87
2.029	2	1 3 1	44.63
2.007	8	2 2 1	45.13
1.976	4	-3 0 2	45.88
1.922	2	2 3 0	47.26
1.909	1	-3 1 2	47.60
1.872	1	-1 3 2	48.59
1.865	2	-3 2 1	48.78
1.865	3	-2 0 3	48.79
1.847	4	0 0 3	49.29
1.843	8	0 4 0	49.42
1.799	2	2 0 2	50.72
1.796	1	3 2 0	50.81
1.792	1	0 1 3	50.92
1.756	1	3 0 1	52.05
1.748	1	0 4 1	52.28
1.742	5	-3 2 2	52.50
1.728	3	-1 4 1	52.95
1.721	4	-1 2 3	53.17
1.714	1	2 3 1	53.40
1.664	2	-2 2 3	55.15

d (Å)	I	hkl	2θ(°) $\lambda = 1.54056$ Å
1.659	4	-3 0 3	55.35
1.640	7	1 4 1	56.03
1.624	3	-4 0 1	56.64
1.623	1	-3 3 1	56.65
1.616	8	2 2 2	56.92
1.585	3	3 2 1	58.16
1.582	3	2 4 0	58.28
1.577	1	3 3 0	58.49
1.554	2	-1 4 2	59.44
1.540	1	-4 1 2	60.02
1.534	1	0 4 2	60.27
1.494	3	1 2 3	62.09
1.486	1	-4 2 1	62.45
1.481	2	-2 4 2	62.70
1.460	2	2 4 1	63.69
1.453	2	-1 0 4	64.01
1.448	1	-4 2 2	64.27
1.447	1	3 0 2	64.31
1.432	2	1 4 2	65.11
1.423	3	4 2 0	65.57
1.419	1	-2 1 4	65.77
1.403	2	-3 4 1	66.62
1.348	1	-3 4 2	69.72
1.347	1	3 2 2	69.75
1.346	1	-2 2 4	69.83
1.338	1	-1 4 3	70.29
1.329	1	-4 2 3	70.82
1.326	1	-4 3 2	71.04
1.311	2	-2 4 3	71.98
1.305	1	0 4 3	72.38
1.297	3	0 2 4	72.88
1.244	1	-4 0 4	76.52
1.233	1	-3 4 3	77.35
1.221	3	-5 2 1	78.24
1.218	2	-4 4 1	78.44
1.205	1	1 6 0	79.50
1.199	1	0 6 1	79.93
1.197	1	-4 4 2	80.09
1.162	1	1 6 1	83.00
1.141	1	-1 4 4	84.91
1.103	1	-1 2 5	88.57
1.064	1	-5 2 4	92.72
1.039	1	-1 6 3	95.72
1.038	1	-6 2 2	95.85
.996	1	4 2 3	101.35

Structure

Monoclinic, I2/m (12), Z=2. The structure was determined by Hansen and Smith [1968] who published data in terms of the B2/m cell with constants a=19.1551,b=5.4288,c=4.4988, β=107.671°.

Lattice parameters

a=18.2559(5), b=4.4990(1), c=5.4290(1)Å, β=91.211(2)°

Density

(calculated) 1.269 g/cm^3

Thermal parameters

Isotropic: Li(1) 3.0, Li(2) 2.6, Li(3) 2.6, Li(4) 2.2, Li(5) 2.8 [Hansen and Smith 1968] Al(1) 1.48, Al(2) 1.63.

Scattering factors

Li^0, Al^0 [3.3.1A]

Scale factor

(integrated intensities) 0.5617 × 10^4

Reference

Hansen, D.A. and J.F. Smith (1968). Acta Cryst. B24, 913.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ Å, λ = 1.54056 Å
9.13	5	2	0	0		9.68
5.23	42	-1	0	1		16.94
5.18	12	1	0	1		17.12
4.562	72	4	0	0		19.44
4.367	1	1	1	0		20.32
4.092	4	-3	0	1		21.70
4.008	45	3	0	1		22.16
3.616	3	3	1	0		24.60
3.463	4	0	1	1		25.70
3.252	34	-2	1	1		27.40
3.225	13	2	1	1		27.64
3.060	1	-5	0	1		29.16
3.042	1	6	0	0		29.34
2.8342	7	5	1	0		31.54
2.7776	1	-4	1	1		32.20
2.7412	1	4	1	1		32.64
2.3540	2	-4	0	2		38.20
2.3305	28	7	0	1		38.60
2.3008	100	1	1	2	+	39.12
2.2817	6	8	0	0		39.46
2.2500	25	0	2	0		40.04
2.1842	17	-3	1	2		41.30
2.0670	4	-1	2	1		43.76
2.0625	3	1	2	1		43.86
2.0179	9	4	2	0		44.88
2.0044	2	6	0	2		45.20
1.9763	1	-5	1	2		45.88
1.9714	1	-3	2	1		46.00
1.9617	8	3	2	1		46.24
1.9442	6	5	1	2		46.68
1.8490	4	9	1	0		49.24
1.8044	1	-1	0	3		50.54
1.7647	1	-8	0	2		51.76
1.7509	3	-7	1	2		52.20
1.6783	2	0	1	3		54.64
1.6451	1	2	1	3		55.84
1.6348	6	-5	0	3		56.22
1.6237	6	-10	1	1		56.64
1.6190	14	7	2	1		56.82
1.6020	2	8	2	0		57.48
1.5774	2	11	0	1		58.46
1.5652	4	4	1	3		58.96
1.5141	1	9	1	2		61.16
1.4999	1	10	0	2		61.80
1.4965	2	6	2	2		61.96
1.4289	1	-2	3	1		65.24
1.4258	1	2	3	1		65.40
1.4075	1	-1	2	3		66.36
1.3883	1	-8	2	2		67.40
1.3872	1	5	3	0		67.46

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.3857	1	12 1 1	67.54
1.3644	1	-9 0 3	68.74
1.3463	1	-2 0 4	69.80
1.3396	9	8 1 3 +	70.20
1.3226	4	-5 2 3	71.24
1.3083	8	1 3 2 +	72.14
1.2916	1	11 2 1	73.22
1.2859	2	-3 3 2	73.60

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
9.13	6	2 0 0	9.68
5.23	56	-1 0 1	16.93
5.17	14	1 0 1	17.13
4.563	100	4 0 0	19.44
4.368	2	1 1 0	20.31
4.093	5	-3 0 1	21.69
4.008	64	3 0 1	22.16
3.617	5	3 1 0	24.59
3.464	7	0 1 1	25.70
3.253	51	-2 1 1	27.39
3.224	19	2 1 1	27.65
3.059	1	-5 0 1	29.17
3.042	1	6 0 0	29.34
2.9999	1	5 0 1	29.76
2.8347	12	5 1 0	31.53
2.7770	1	-4 1 1	32.21
2.7412	1	4 1 1	32.64
2.5864	1	2 0 2	34.65
2.3545	2	-4 0 2	38.19
2.3312	49	7 0 1	38.59
2.3112	2	-4 0 2	38.94
2.3011	91	-6 1 1	39.11
2.3000	92	1 1 2	39.13
2.2815	6	8 0 0	39.46
2.2559	4	7 1 0	39.93
2.2495	44	0 2 0	40.05
2.1841	29	-3 1 2	41.30
2.0666	7	-1 2 1	43.77
2.0629	2	1 2 1	43.85
2.0467	1	-6 0 2	44.22
2.0176	17	4 2 0	44.89
2.0042	3	6 0 2	45.20
1.9766	1	-5 1 2	45.87
1.9714	1	-3 2 1	46.00
1.9617	14	3 2 1	46.24
1.9445	11	5 1 2	46.67
1.8488	8	9 1 0	49.24
1.8042	2	-1 0 3	50.55
1.7648	2	-8 0 2	51.76
1.7506	7	-7 1 2	52.21
1.7285	1	8 0 2	52.93
1.6786	5	0 1 3	54.63
1.6567	1	-2 1 3	55.41
1.6452	1	2 1 3	55.84
1.6349	12	-5 0 3	56.22
1.6265	1	-4 2 2	56.53
1.6238	10	-10 1 1	56.64
1.6187	26	7 2 1	56.83
1.6120	1	4 2 2	57.09
1.6018	3	8 2 0	57.49
1.5855	1	-4 1 3	58.13
1.5775	4	11 0 1	58.46
1.5655	8	4 1 3	58.95
1.5145	2	9 1 2	61.14
1.4999	2	10 0 2	61.80
1.4964	2	6 2 2	61.96
1.4289	3	-2 3 1	65.24
1.4265	1	2 3 1	65.37
1.4074	2	-1 2 3	66.36
1.3885	2	-8 2 2	67.39
1.3872	1	5 3 0	67.46
1.3858	1	12 1 1	67.54
1.3706	1	8 2 2	68.39
1.3645	3	-9 0 3	68.74
1.3463	3	-2 0 4	69.80
1.3403	11	13 1 0	70.16
1.3396	11	8 1 3	70.20
1.3389	5	-12 0 2	70.24
1.3381	5	2 0 4	70.29
1.3225	10	-5 2 3	71.25
1.3085	10	-6 3 1	72.13
1.3083	10	1 3 2	72.14
1.2916	3	11 2 1	73.22
1.2858	4	-3 3 2	73.61

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a=6.002(1)Å [Johnston and Heikes, 1958]

Density

(calculated) 2.852 g/cm^3

Thermal parameters

Isotropic: Li 1.0
Se 0.6

Scattering factors

Li^+ [3.3.1A]
Se^0 [3.3.1B]

Scale factors

(integrated intensities) 3.971×10^4

Additional patterns

1. Zintl et al. [1934]

Reference

Johnston,W.D. and R.R.Heikes (1958). J. Am. Chem. Soc. 80, 5904.
Zintl,E., A.Harder, and B.Dauth (1934). Z. Electrochem. 40, 588.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ*(°) λ = 1.54056 Å
3.466	100	1 1 1	25.68
3.002	37	2 0 0	29.74
2.122	38	2 2 0	42.56
1.810	34	3 1 1	50.38
1.732	7	2 2 2	52.80
1.500	5	4 0 0	61.78
1.377	10	3 3 1	68.04
1.342	7	4 2 0	70.06
1.225	8	4 2 2	77.92
1.155	6	5 1 1 +	83.66
1.061	2	4 4 0	93.10
1.015	6	5 3 1	98.80
1.000	3	4 4 2 +	100.72
.949	3	6 2 0	108.52
.915	2	5 3 3	114.62
.905	2	6 2 2	116.70
.866	1	4 4 4	125.54
.840	4	7 1 1 +	132.84
.832	2	6 4 0	135.48
.802	5	6 4 2	147.64

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	*2θ*(°) λ = 1.54056 Å
3.465	100	1 1 1	25.69
3.001	38	2 0 0	29.75
2.122	45	2 2 0	42.57
1.810	41	3 1 1	50.38
1.733	9	2 2 2	52.79
1.500	7	4 0 0	61.77
1.377	15	3 3 1	68.03
1.342	10	4 2 0	70.05
1.225	12	4 2 2	77.91
1.155	8	5 1 1	83.65
1.155	3	3 3 3	83.65
1.061	4	4 4 0	93.10
1.015	11	5 3 1	98.80
1.000	4	4 4 2	100.71
1.000	1	6 0 0	100.71
.949	6	6 2 0	108.52
.915	5	5 3 3	114.61
.905	4	6 2 2	116.71
.866	2	4 4 4	125.53
.840	6	5 5 1	132.84
.840	6	7 1 1	132.84
.832	5	6 4 0	135.47
.802	20	6 4 2	147.64

Lithium sulfide, Li_2S

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a=5.720(3)Å [ibid.]

Density

(calculated) 1.630 g/cm^3

Thermal parameters

Isotropic: Li 1.0
S 0.6

Scattering factors

Li^+, S^{2-} [3.3.1A]

Scale factors

(integrated intensities) 0.6784×10^4

Additional patterns

1. Zintl et al. [1934]

Reference

Zintl,E., A.Harder, and B.Dauth (1934). Z. Electrochem. 40, 588.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.302	100	1 1 1	26.98
2.861	20	2 0 0	31.24
2.022	40	2 2 0	44.78
1.725	23	3 1 1	53.06
1.651	3	2 2 2	55.62
1.430	5	4 0 0	65.18
1.312	8	3 3 1	71.88
1.279	3	4 2 0	74.06
1.168	8	4 2 2	82.56
1.101	5	5 1 1 +	88.82
1.011	2	4 4 0	99.24
.967	5	5 3 1	105.62
.953	2	4 4 2 +	107.80
.904	4	6 2 0	116.80
.872	2	5 3 3	124.02
.862	1	6 2 2	126.58
.826	1	4 4 4	137.80
.801	5	7 1 1 +	148.18
.793	2	6 4 0	152.38

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.302	100	1 1 1	26.98
2.860	23	2 0 0	31.25
2.022	48	2 2 0	44.78
1.725	30	3 1 1	53.06
1.651	4	2 2 2	55.61
1.430	7	4 0 0	65.18
1.312	12	3 3 1	71.89
1.279	5	4 2 0	74.06
1.168	14	4 2 2	82.56
1.101	7	5 1 1	88.81
1.101	2	3 3 3	88.81
1.011	5	4 4 0	99.24
.967	12	5 3 1	105.63
.953	3	4 4 2	107.80
.953	1	6 0 0	107.80
.904	9	6 2 0	116.79
.872	6	5 3 3	124.03
.862	4	6 2 2	126.57
.826	4	4 4 4	137.81
.801	10	5 5 1	148.18
.801	10	7 1 1	148.18
.793	7	6 4 0	152.37

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a=6.517Å [ibid.]

Density

(calculated) 3.395 g/cm^3

Thermal parameters

Isotropic: Li 1.0
Te 0.6

Scattering factors

Li^+ [3.3.1A]
Te^0 [3.3.1B]

Scale factors

(integrated intensities) 12.02×10^4

Additional patterns

1. Zintl et al. [1934]

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
3.764	100	1	1	1		23.62
3.259	41	2	0	0		27.34
2.304	40	2	2	0		39.06
1.965	39	3	1	1		46.16
1.881	9	2	2	2		48.34
1.629	5	4	0	0		56.44
1.495	13	3	3	1		62.02
1.457	10	4	2	0		63.82
1.330	9	4	2	2		70.76
1.254	8	5	1	1	+	75.78
1.152	2	4	4	0		83.92
1.102	7	5	3	1		88.74
1.086	4	4	4	2	+	90.34
1.030	3	6	2	0		96.76
.994	2	5	3	3		101.62
.982	2	6	2	2		103.26
.941	1	4	4	4		109.94
.913	4	7	1	1	+	115.14
.904	2	6	4	0		116.92
.871	4	6	4	2		124.38
.848	6	7	3	1	+	130.42
.796	2	7	3	3		150.70
.790	4	8	2	0	+	154.16

Calculated Pattern *(Integrated)*

d (Å)	I	hkl			2θ(°) λ = 1.54056 Å
3.763	100	1	1	1	23.63
3.259	44	2	0	0	27.35
2.304	45	2	2	0	39.06
1.965	47	3	1	1	46.16
1.881	11	2	2	2	48.34
1.629	7	4	0	0	56.43
1.495	18	3	3	1	62.02
1.457	14	4	2	0	63.82
1.330	14	4	2	2	70.77
1.254	9	5	1	1	75.78
1.254	3	3	3	3	75.78
1.152	4	4	4	0	83.92
1.102	13	5	3	1	88.73
1.086	1	6	0	0	90.34
1.086	5	4	4	2	90.34
1.030	6	6	2	0	96.75
.994	5	5	3	3	101.62
.982	4	6	2	2	103.26
.941	2	4	4	4	109.95
.913	5	5	5	1	115.15
.913	5	7	1	1	115.15
.904	4	6	4	0	116.93
.871	11	6	4	2	124.38
.848	11	7	3	1	130.43
.848	5	5	5	3	130.43
.815	2	8	0	0	142.02
.796	9	7	3	3	150.69
.790	9	8	2	0	154.15
.790	9	6	4	4	154.15

Reference

Zintl,E., A.Harder, and B.Dauth (1934). Z. Electrochem. 40, 588.

Magnesium iron carbonate hydroxide hydrate, sjögrenite, $Mg_6Fe_2CO_3(OH)_{16}\cdot 4H_2O$, phase I

Structure
Hexagonal, $P6_3/mmc$ (194), $Z=\frac{1}{4}$. The structure was determined by Allmann and Lohse [1966]

Lattice parameters
a=3.113(3), c=15.61(1)Å [ibid.]

Density
(calculated) 2.097 g/cm^3

Thermal parameters
Isotropic: magnesium B=0.66, iron B=0.66, hydroxyl B=0.65 [ibid.]
Anisotropic oxygen: B_{11}=31.8, B_{33}=1.56 [ibid.]

Polymorphism
A rhombohedral polymorph called pyroaurite has very similar physical properties, and the two phases occur as intergrowths. Their structures differ only in the stacking sequence [Allmann, 1968].

Scattering factors
$\frac{1}{4}$ ($3Mg^{2+}$ + Fe^{3+}) [3.3.1A]
O^- [3.3.1A]

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.80	100	0 0 2	11.34
3.900	25	0 0 4	22.78
2.696	2	1 0 0	33.20
2.656	6	1 0 1	33.72
2.547	11	1 0 2	35.20
2.394	7	1 0 3	37.54
2.218	12	1 0 4	40.64
2.040	7	1 0 5	44.36
1.872	13	1 0 6	48.60
1.581	6	1 0 8	58.32
1.557	5	1 1 0	59.32
1.526	7	1 1 2	60.62
1.446	2	1 1 4	64.38
1.351	3	1 0 10	69.52
1.328	1	2 0 2	70.88
1.274	1	2 0 4	74.40
1.197	1	2 0 6	80.12
1.109	1	2 0 8	87.98
.986	1	2 1 4	102.76
.949	1	2 1 6	108.56
.906	1	1 1 14	116.38
.903	1	2 1 8	117.04

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.81	100	0 0 2	11.33
3.903	32	0 0 4	22.77
2.696	3	1 0 0	33.20
2.657	8	1 0 1	33.71
2.548	15	1 0 2	35.19
2.394	10	1 0 3	37.54
2.218	17	1 0 4	40.64
2.040	10	1 0 5	44.36
1.872	21	1 0 6	48.59
1.581	10	1 0 8	58.33
1.557	9	1 1 0	59.32
1.526	12	1 1 2	60.61
1.446	4	1 1 4	64.39
1.351	5	1 0 10	69.53
1.328	2	2 0 2	70.89
1.305	1	2 0 3	72.36
1.301	1	0 0 12	72.62
1.274	2	2 0 4	74.40
1.256	1	1 0 11	75.67
1.197	3	2 0 6	80.12
1.172	1	1 0 12	82.21
1.109	3	2 0 8	87.98
1.020	2	2 0 10	98.05
1.010	1	2 1 2	99.34
.998	1	1 1 12	101.02
.986	2	2 1 4	102.76
.949	3	2 1 6	108.55
.936	1	2 0 12	110.75
.906	2	1 1 14	116.38
.903	3	2 1 8	117.04
.899	1	3 0 0	118.00
.893	2	3 0 2	119.27

Scale factors
(integrated intensities) 0.4158×10^4

Additional patterns
1. PDF card 14-281 [Neumann and Bergstol, Mineral Museum, Oslo, Norway]

Reference

Allmann, R. (1968). Acta Cryst. B24, 972.
Allmann, R. and H.-H. Lohse (1966). Neues Jahr. Mineral. Monatsh. 1966, 161.

Structure

Hexagonal, $R\bar{3}m$ (166), Z=3/8. The structure was determined by Allmann [1968].

Lattice parameters

a=3.1095(2), c=23.4126(9)Å, [published values: a=3.1094(2), c=23.4117(9)Å, (ibid.)]

Density

(calculated) 2.102 g/cm^3

Thermal parameters

Isotropic: magnesium B=0.769, iron B=0.769, hydroxyl B=1.005 [ibid.]
Anisotropic oxygen: B_{11}=30.8, B_{33}=2.29 [ibid.]

Polymorphism

Sjögrenite,a hexagonal polymorph, has very similar physical properties, and the two phases occur as intergrowths. Their structures differ only in the stacking sequence [ibid.].

Scattering factors

$\frac{1}{4}(3Mg^{2+} + Fe^{3+})$ [3.3.1A]
O^- [3.3.1A]

Scale factors

(integrated intensities) 0.9321×10^4

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.796	100	0 0 3	11.34
3.9004	25	0 0 6	22.78
2.6241	16	0 1 2	34.14
2.3340	18	0 1 5	38.54
1.9820	17	0 1 8	45.74
1.7666	4	1 0 10	51.70
1.6699	4	0 1 11	54.94
1.5547	5	1 1 0	59.40
1.5249	6	1 1 3	60.68
1.4969	3	1 0 13	61.94
1.4443	2	1 1 6	64.46
1.4208	1	0 1 14	65.66
1.3376	1	2 0 2	70.32
1.2941	1	2 0 5	73.06
1.2856	2	1 0 16	73.62
1.2232	1	2 0 8	78.06
.9947	1	1 2 5	101.50
.9613	1	1 2 8	106.50

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.804	100	0 0 3	11.33
3.9021	31	0 0 6	22.77
2.6244	22	0 1 2	34.14
2.3344	26	0 1 5	38.53
1.9816	27	0 1 8	45.75
1.7669	7	1 0 10	51.69
1.6698	6	0 1 11	54.94
1.5547	9	1 1 0	59.40
1.5248	11	1 1 3	60.69
1.4970	5	1 0 13	61.93
1.4443	4	1 1 6	64.46
1.4207	2	0 1 14	65.67
1.3376	1	2 0 2	70.32
1.3007	1	0 0 18	72.63
1.2940	3	2 0 5	73.06
1.2857	4	1 0 16	73.61
1.2232	3	2 0 8	78.06
1.1672	1	0 2 10	82.59
1.1379	1	2 0 11	85.21
1.1205	1	1 0 19	86.86
1.0784	1	0 2 13	91.17
1.0140	1	1 2 2	98.87
.9976	1	1 1 18	101.09
.9946	2	1 2 5	101.51
.9908	1	0 2 16	102.05
.9613	2	1 2 8	106.50
.9334	1	2 1 10	111.22
.9182	2	1 2 11	114.04
.9090	1	0 2 19	115.85
.9060	2	1 1 21	116.46
.8976	1	3 0 0	118.21
.8918	1	3 0 3	119.49
.8918	1	0 3 3	119.49

Additional patterns

1. PDF card 14-293 [Neumann and Bergstol,Mineral Museum, Oslo, Norway]

Reference

Allmann, R. (1968). Acta Cryst. B24, 972.

Manganese fluoride, MnF_2

Structure

Tetragonal, $P4_2mnm$ (136), Z=2, isostructural with rutile [Ferrari, 1926]. The structure was determined by Stout and Reed and refined by Baur [1958].

Lattice parameters

a=4.8736(2), c=3.3100(5)Å (published as 4.8734 and 3.3099) [Stout and Reed, 1954]

Density

(calculated) 3.926 g/cm^3

Thermal parameters

Isotropic [Baur 1958] : Mn 0.9
F 1.1

Scattering factors

F^- [Cromer and Waber, 1965]
Mn^{2+} [Cromer and Waber,1965],corrected for dispersion using $\Delta f'=-0.5$ and $\Delta f''=3.00$ [Cromer, 1965]

Scale factors

(integrated intensities) 0.0688×10^4

Additional patterns

1. PDF card 1-601 [Hanawalt et al., 1938]
2. Ferrari [1926]

Reference

Baur, W.H. (1958). Acta Cryst. 11, 488.
Cromer, D.T. (1965). Acta Cryst. 18, 17.
Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Ferrari, A. (1926). Atti reale accad. nazl. Lincei 3, 224.
Griffel, M. and J.W. Stout (1950). J. Am. Chem. Soc. 72, 4351.
Hanawalt, J.D.,H.W. Rinn, and L.K. Frevel (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Stout, J.W. and S.A. Reed (1954). J.Am.Chem. Soc. 76, 5279.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
3.445	100	1	1	0		25.84
2.738	48	1	0	1		32.68
2.4365	6	2	0	0		36.86
2.3877	21	1	1	1		37.64
2.1792	7	2	1	0		41.40
1.8206	51	2	1	1		50.06
1.7233	14	2	2	0		53.10
1.6549	9	0	0	2		55.48
1.5410	6	3	1	0		59.98
1.4917	9	1	1	2		62.18
1.4585	16	3	0	1		63.76
1.3971	1	3	1	1		66.92
1.3690	1	2	0	2		68.48
1.3181	1	2	1	2		71.52
1.2514	2	3	2	1		75.98
1.2185	2	4	0	0		78.42
1.1936	5	2	2	2		80.38
1.1820	1	4	1	0		81.34
1.1487	2	3	3	0		84.22
1.1280	3	3	1	2		86.14
1.1131	3	4	1	1		87.56
1.0897	1	4	2	0		89.96
1.0761	1	1	0	3		91.42
.9844	3	2	1	3		102.98
.9813	2	4	0	2		103.44
.9558	1	5	1	0		107.40
.9437	2	3	3	2		109.42
.9356	2	4	3	1		110.94
.9127	2	3	0	3		115.12
.9102	2	4	2	2		115.62
.8730	3	5	2	1		123.86
.8548	1	3	2	3		128.62
.8277	2	5	1	2	+	137.08
.8066	2	4	1	3		145.50
.8046	2	1	1	4		146.42

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.446	100	1 1 0	25.83
2.738	50	1 0 1	32.68
2.4368	6	2 0 0	36.85
2.3872	25	1 1 1	37.65
2.1795	8	2 1 0	41.39
1.8203	65	2 1 1	50.07
1.7231	19	2 2 0	53.11
1.6550	11	0 0 2	55.48
1.5412	8	3 1 0	59.97
1.5284	1	2 2 1	60.53
1.4919	12	1 1 2	62.17
1.4584	23	3 0 1	63.77
1.3971	1	3 1 1	66.92
1.3691	2	2 0 2	68.47
1.3181	2	2 1 2	71.52
1.2514	4	3 2 1	75.98
1.2184	3	4 0 0	78.43
1.1936	8	2 2 2	80.38
1.1820	1	4 1 0	81.33
1.1487	4	3 3 0	84.22
1.1279	5	3 1 2	86.15
1.1132	6	4 1 1	87.57
1.0898	3	4 2 0	89.95
1.0761	2	1 0 3	91.42
.9844	6	2 1 3	102.98
.9812	3	4 0 2	103.45
.9619	1	4 1 2	106.41
.9558	3	5 1 0	107.40
.9437	4	3 3 2	109.42
.9350	5	4 3 1	110.94
.9127	4	3 0 3	115.12
.9102	4	4 2 2	115.62
.8730	8	5 2 1	123.86
.8615	1	4 4 0	126.78
.8547	2	3 2 3	128.63
.8358	1	5 3 0	134.32
.8277	7	5 1 2	137.07
.8275	1	0 0 4	137.14
.8123	2	6 0 0	142.99
.8066	5	4 1 3	145.50
.8046	3	1 1 4	146.40
.7836	2	2 0 4	158.88

Structure

Monoclinic, I2/c (15), Z=4. The structure was determined by Dorm [1967], who published his data in terms of the C2/c cell with a=18.806, b=4.470, c=8.595Å, β=107.19°.

Lattice parameters

a=18.222(7),b=4.470(1), c=8.595(2)Å,β=99.59(3)°

Density

(calculated) 6.321 g/cm^3

Thermal parameters

Isotropic:	Hg	3.73	
	Br	2.4	[Dorm, 1967]
	O(1)	2.4	[ibid.]
	O(2)	1.3	[ibid.]
	O(3)	4.3	[ibid.]

Scattering factors

O^- [3.3.1A]
Br^0[3.3.1B]
Hg^+[Cromer and Waber, 1965]

Scale factor

(integrated intensities) 52.50×10^4

Reference

Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Dorm, E. (1967). Acta Chem. Scand. 21, 2834.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
8.98	66	2	0	0		9.84
4.49	8	4	0	0		19.76
4.34	74	1	1	0		20.46
4.24	7	0	0	2		20.94
4.10	37	-2	0	2		21.64
3.952	6	0	1	1		22.48
3.581	47	3	1	0		24.84
3.376	58	-4	0	2		26.38
3.093	100	-1	1	2	+	28.84
2.994	2	6	0	0		29.82
2.881	33	-3	1	2		31.02
2.854	26	4	0	2	+	31.32
2.801	15	5	1	0		31.92
2.611	15	3	1	2		34.32
2.490	2	-5	1	2		36.04
2.393	1	-2	1	3		37.56
2.388	1	0	1	3		37.64
2.302	1	6	1	1		39.10
2.273	10	6	0	2		39.62
2.246	22	8	0	0		40.12
2.235	17	0	2	0	+	40.32
2.225	19	7	1	0		40.50
2.208	9	5	1	2		40.84
2.169	5	2	2	0		41.60
2.144	5	-2	0	4		42.12
2.138	7	-8	0	2	+	42.24
2.119	2	0	0	4		42.64
2.053	3	-4	0	4		44.08
2.006	3	3	2	1		45.16
1.989	8	2	0	4		45.56
1.977	1	0	2	2		45.86
1.963	6	-2	2	2		46.20
1.935	1	-1	1	4		46.92
1.909	2	-3	1	4		47.60
1.887	2	-5	2	1		48.18
1.883	4	-6	0	4		48.28
1.863	20	7	1	2	+	48.84
1.823	3	9	1	0		50.00
1.806	16	-5	1	4	+	50.48
1.797	2	10	0	0		50.76
1.791	2	6	2	0		50.94
1.776	9	-9	1	2		51.42
1.760	8	4	2	2	+	51.92
1.749	10	3	1	4		52.26
1.689	2	-7	2	1	+	54.28
1.644	1	-5	2	3		55.88
1.608	1	6	0	4		57.26
1.593	6	6	2	2	+	57.82
1.584	5	8	2	0		58.18
1.547	2	-2	2	4		59.72

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
1.545	2	-8	2	2		59.82
1.538	1	0	2	4		60.12
1.534	2	11	1	0		60.28
1.521	3	-11	1	2		60.86
1.512	2	-4	2	4		61.26
1.4991	1	-10	0	4		61.84
1.4973	1	12	0	0		61.92
1.4921	2	-12	0	2		62.16
1.4857	3	2	2	4	+	62.46
1.4675	1	0	3	1		63.32
1.4459	1	3	3	0		64.38
1.4403	1	-6	2	4		64.66
1.4344	1	7	1	4		64.96
1.4324	1	-2	0	6		65.06
1.4071	3	-1	3	2	+	66.38
1.4038	2	4	2	4		66.56
1.4004	1	10	2	0		66.74
1.3825	2	7	2	3		67.72
1.3753	2	11	1	2		68.12
1.3686	2	-6	0	6		68.50
1.3610	2	2	0	6		68.94
1.3592	2	-1	1	6		69.04
1.3521	1	3	3	2		69.46
1.3470	1	-8	2	4		69.76
1.3433	1	12	0	2		69.98
1.3317	1	-12	0	4		70.68
1.3274	2	1	1	6		70.94
1.3181	1	0	3	3		71.52
1.2886	1	7	3	0	+	73.42
1.2790	1	-7	1	6		74.06
1.2700	1	10	0	4		74.68
1.2450	1	-10	2	4		76.44
1.2409	1	-12	2	2		76.74
1.2105	2	-13	1	4		79.04
1.2092	2	-9	1	6		79.14
1.2059	1	7	3	2		79.40
1.1895	1	-5	3	4		80.72
1.1805	1	-9	3	2		81.46
1.1774	1	-8	3	3		81.72
1.1751	1	14	0	2		81.92
1.1725	1	3	3	4		82.14
1.1671	1	-6	2	6		82.60
1.1595	1	11	1	4		83.26
1.1570	1	15	1	0		83.48
1.1441	1	-12	2	4		84.64
1.1041	1	10	2	4		88.48

Calculated Pattern *(Integrated)*

d (Å)	I	hkl			2θ(°) λ = 1.54056 Å
8.98	49	2	0	0	9.84
4.49	8	4	0	0	19.75
4.34	67	1	1	0	20.46
4.24	6	0	0	2	20.95
4.11	36	-2	0	2	21.63
3.954	6	0	1	1	22.47
3.607	1	2	0	2	24.66
3.582	45	3	1	0	24.83
3.376	56	-4	0	2	26.38
3.094	100	-1	1	2	28.83
3.089	8	-4	1	1	28.88
2.994	2	6	0	0	29.81
2.881	33	-3	1	2	31.02
2.860	4	4	1	1	31.25
2.854	23	4	0	2	31.32
2.801	16	5	1	0	31.93
2.610	16	3	1	2	34.33
2.490	2	-5	1	2	36.04
2.393	1	-2	1	3	37.55
2.388	1	0	1	3	37.64
2.303	1	6	1	1	39.09
2.273	11	6	0	2	39.61
2.246	24	8	0	0	40.12
2.235	15	0	2	0	40.32
2.231	1	2	1	3	40.39
2.226	19	7	1	0	40.49
2.208	9	5	1	2	40.83
2.169	5	2	2	0	41.61
2.143	6	-2	0	4	42.12
2.137	4	-8	0	2	42.25
2.135	4	1	2	1	42.30
2.119	2	0	0	4	42.64
2.053	4	-4	0	4	44.08
2.010	1	-6	1	3	45.06
2.006	3	3	2	1	45.17
1.989	9	2	0	4	45.56
1.977	1	0	2	2	45.86
1.963	8	-2	2	2	46.21
1.935	1	-1	1	4	46.92
1.909	3	-3	1	4	47.60
1.891	1	8	1	1	48.08
1.888	2	-5	2	1	48.16
1.884	4	-6	0	4	48.27
1.864	13	-4	2	2	48.83
1.863	13	7	1	2	48.95
1.823	3	9	1	0	50.01
1.806	19	-5	1	4	50.48
1.804	2	4	0	4	50.56
1.797	2	10	0	0	50.77
1.791	2	6	2	0	50.94

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.775	11	-9 1 2	51.43
1.763	2	-10 0 2	51.81
1.762	2	-1 2 3	51.84
1.760	8	4 2 2	51.92
1.749	12	3 1 4	52.27
1.689	2	-7 2 1	54.27
1.688	1	-8 0 4	54.30
1.659	1	-7 1 4	55.33
1.644	1	-5 2 3	55.89
1.608	1	6 0 4	57.25
1.594	5	6 2 2	57.80
1.593	3	5 1 4	57.83
1.584	6	8 2 0	58.19
1.547	3	-2 2 4	59.72
1.545	1	-8 2 2	59.82
1.538	2	0 2 4	60.13
1.534	2	11 1 0	60.28
1.521	4	-11 1 2	60.87
1.512	2	-4 2 4	61.26
1.4991	1	-10 0 4	61.84
1.4972	1	12 0 0	61.92
1.4920	3	-12 0 2	62.17
1.4860	3	2 2 4	62.44
1.4849	2	1 3 0	62.50
1.4675	1	0 3 1	63.32
1.4459	1	3 3 0	64.38
1.4405	1	-6 2 4	64.65
1.4346	1	7 1 4	64.95
1.4324	1	-2 0 6	65.06
1.4074	3	-1 3 2	66.36
1.4070	1	-4 3 1	66.39
1.4037	1	4 2 4	66.57
1.4003	1	10 2 0	66.74
1.3856	1	-3 3 2	67.55
1.3842	1	-10 2 2	67.62
1.3824	1	7 2 3	67.72
1.3752	3	11 1 2	68.13
1.3685	2	-6 0 6	68.51
1.3610	2	2 0 6	68.94
1.3593	2	-1 1 6	69.04
1.3519	1	3 3 2	69.47
1.3470	1	-8 2 4	69.76
1.3431	1	12 0 2	69.99
1.3318	1	-12 0 4	70.67
1.3274	3	1 1 6	70.94
1.3179	1	0 3 3	71.53
1.3052	1	6 2 4	72.34
1.2896	1	2 3 3	73.35
1.2886	1	7 3 0	73.42
1.2792	1	-7 1 6	74.05
1.2699	2	10 0 4	74.68
1.2450	1	-10 2 4	76.44
1.2409	2	-12 2 2	76.74
1.2104	3	-13 1 4	79.04
1.2091	2	-9 1 6	79.15
1.2051	1	7 3 2	79.46
1.1894	1	-5 3 4	80.72
1.1804	1	-9 3 2	81.47
1.1773	1	-8 3 3	81.73
1.1751	1	14 0 2	81.91
1.1725	1	3 3 4	82.13
1.1671	1	-6 2 6	82.60
1.1624	1	2 2 6	83.01
1.1594	1	11 1 4	83.27
1.1570	2	15 1 0	83.48
1.1441	1	-12 2 4	84.64
1.1041	1	10 2 4	88.48

Structure

Orthorhombic, Bb2m (36), Z=4, The structure was determined by Verweel and Bijvoet [1931] and by Braekken [1932].

Lattice parameters

a=6.812(1), b=12.470(1), c=4.633(1)Å, [Braekken 1932]

Density

(calculated) 6.082 g/cm^3

Thermal parameters

Isotropic: overall B=1.5

Atomic positions

Braekken [1932]

Scattering factors

Hg^0, Br^0 [3.3.1B]

Scale factors

(integrated intensities) 19.63×10^4

Additional patterns

1. PDF card 3-327 [Verweel and Bijvoet, 1931]

Reference

Braekken, H. (1932). Z. Krist. **81**, 152.
Verweel, H.J., and J.M. Bijvoet (1931). Z. Krist. 77, 122.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
6.23	100	0 2 0	14.20
3.83	13	1 0 1	23.20
3.663	85	1 1 1	24.28
3.285	10	2 1 0	27.12
3.264	65	1 2 1	27.30
3.116	1	0 4 0	28.62
2.990	11	2 2 0	29.86
2.817	51	1 3 1	31.74
2.635	44	2 3 0	34.00
2.417	10	1 4 1	37.16
2.317	23	0 0 2	38.84
2.300	12	2 4 0	39.14
2.171	9	0 2 2	41.56
2.090	18	1 5 1	43.26
2.079	8	0 6 0	43.50
2.039	15	3 0 1	44.40
2.012	17	2 5 0 +	45.02
1.938	13	3 2 1	46.84
1.893	2	2 1 2	48.02
1.8309	7	2 2 2 +	49.76
1.8267	11	1 6 1	49.88
1.7743	1	2 6 0	51.46
1.7397	18	2 3 2	52.56
1.7066	4	3 4 1	53.66
1.7025	4	4 0 0	53.80
1.6875	7	4 1 0	54.32
1.6429	1	4 2 0	55.92
1.6322	5	2 4 2	56.32
1.6153	4	1 7 1	56.96
1.5784	3	3 5 1	58.42
1.5750	2	4 3 0	58.56
1.5590	4	0 8 0	59.22
1.5471	4	0 6 2	59.72
1.5190	7	2 5 2	60.94
1.4951	4	1 1 3	62.02
1.4638	3	1 2 3	63.50
1.4556	5	3 6 1	63.90
1.4439	1	1 8 1	64.48
1.4162	3	1 3 3	65.90
1.4086	1	2 6 2	66.30
1.4064	1	4 5 0	66.42
1.3722	1	4 0 2	68.30
1.3637	5	4 1 2	68.78
1.3562	1	1 4 3	69.22
1.3399	1	4 2 2	70.18
1.3030	3	1 9 1 +	72.48
1.2999	2	5 1 1	72.68
1.2931	4	0 8 2	73.12
1.2895	3	1 5 3	73.36
1.2835	1	2 9 0	73.76

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.2793	2	5 2 1	74.04
1.2770	2	3 0 3	74.20
1.2702	1	3 1 3	74.66
1.2509	2	3 2 3	76.02
1.2470	4	5 3 1	76.30
1.2385	3	3 8 1	76.92
1.2309	2	4 7 0	77.48
1.2195	1	1 6 3	78.34
1.2054	1	5 4 1	79.44
1.2024	1	4 5 2	79.68
1.1858	1	1 10 1	81.02
1.1817	1	3 4 3	81.36
1.1579	2	5 5 1 +	83.40
1.1500	1	1 7 3 +	84.10
1.1458	1	3 9 1	84.48
1.1452	1	4 6 2	84.54
1.0871	3	4 7 2 +	90.24
1.0755	1	2 11 0 +	91.48
1.0669	1	6 4 0	92.44
1.0639	1	3 10 1	92.78
1.0603	2	2 3 4	93.18
1.0197	1	1 9 3	98.12
1.0061	1	6 2 2	99.92
1.0038	2	2 5 4 +	100.24
.9922	1	5 3 3	101.66
.9878	1	3 8 3	102.48
.9755	2	2 11 2 +	104.30
.9690	2	6 4 2	105.30
.9549	1	4 1 4	107.54
.9496	1	7 1 1	108.42
.9455	1	5 5 3	109.12
.9304	1	1 13 1	111.76
.9297	1	0 8 4	111.90
.9155	1	1 1 5 +	114.58
.9134	1	2 12 2	114.98

Calculated Pattern *(Integrated)*			
d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
6.24	98	0 2 0	14.19
3.83	15	1 0 1	23.20
3.662	100	1 1 1	24.28
3.286	9	2 1 0	27.12
3.264	77	1 2 1	27.30
3.118	1	0 4 0	28.61
2.989	13	2 2 0	29.87
2.817	64	1 3 1	31.74
2.635	56	2 3 0	34.00
2.418	14	1 4 1	37.15
2.317	31	0 0 2	38.84
2.300	14	2 4 0	39.14
2.171	13	0 2 2	41.55
2.090	26	1 5 1	43.25
2.078	11	0 6 0	43.51
2.039	22	3 0 1	44.39
2.012	7	3 1 1	45.01
2.012	17	2 5 0	45.01
1.938	19	3 2 1	46.84
1.893	4	2 1 2	48.01
1.8310	6	2 2 2	49.76
1.8306	3	3 3 1	49.77
1.8266	11	1 6 1	49.88
1.7741	1	2 6 0	51.47
1.7396	28	2 3 2	52.56
1.7064	6	3 4 1	53.67
1.7030	2	4 0 0	53.78
1.6873	10	4 1 0	54.32
1.6428	2	4 2 0	55.92
1.6320	9	2 4 2	56.33
1.6153	7	1 7 1	56.96
1.5786	4	3 5 1	58.41
1.5759	1	4 3 0	58.52
1.5588	7	0 8 0	59.23
1.5470	7	0 6 2	59.73
1.5191	12	2 5 2	60.94
1.5061	1	1 0 3	61.52
1.4953	6	1 1 3	62.02
1.4640	5	1 2 3	63.49
1.4555	9	3 6 1	63.91
1.4438	2	1 8 1	64.49
1.4160	6	1 3 3	65.91
1.4085	1	2 6 2	66.31
1.4064	1	4 5 0	66.42
1.3721	2	4 0 2	68.30
1.3639	9	4 1 2	68.77
1.3561	2	1 4 3	69.22
1.3400	2	4 2 2	70.17
1.3173	1	4 6 0	71.57
1.3030	1	4 3 2	72.48

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
1.3029	4	1 9 1	72.48
1.2999	2	5 1 1	72.68
1.2932	6	0 8 2	73.11
1.2893	4	1 5 3	73.38
1.2834	1	2 9 0	73.76
1.2792	2	5 2 1	74.05
1.2770	4	3 0 3	74.20
1.2703	1	3 1 3	74.65
1.2510	4	3 2 3	76.01
1.2469	6	5 3 1	76.31
1.2383	6	3 8 1	76.93
1.2310	4	4 7 0	77.47
1.2195	2	1 6 3	78.34
1.2054	2	5 4 1	79.44
1.2022	1	4 5 2	79.69
1.1858	2	1 10 1	81.02
1.1817	2	3 4 3	81.36
1.1710	1	2 10 0	82.27
1.1583	2	0 0 4	83.37
1.1577	3	5 5 1	83.42
1.1501	2	1 7 3	84.09
1.1498	1	4 8 0	84.12
1.1460	1	3 9 1	84.47
1.1451	1	4 6 2	84.55
1.1388	1	0 2 4	85.13
1.1366	1	3 5 3	85.32
1.1226	1	2 9 2	86.65
1.1170	1	6 2 0	87.20
1.1064	1	5 6 1	88.24
1.0880	3	3 6 3	90.14
1.0870	4	4 7 2	90.24
1.0870	2	1 11 1	90.24
1.0800	1	2 2 4	91.00
1.0756	2	2 11 0	91.47
1.0748	1	4 9 0	91.56
1.0668	2	6 4 0	92.45
1.0638	2	3 10 1	92.78
1.0603	4	2 3 4	93.18
1.0450	1	2 10 2	94.97
1.0344	1	2 4 4	96.25
1.0299	1	4 8 2	96.82
1.0197	2	1 9 3	98.12
1.0183	1	5 1 3	98.31
1.0117	1	0 6 4	99.16
1.0082	1	5 2 3	99.64
1.0061	2	6 2 2	99.92
1.0038	2	2 5 4	100.23
1.0029	1	1 12 1	100.36
.9921	3	5 3 3	101.86
.9878	3	3 8 3	102.48

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
.9756	4	2 11 2	104.29
.9750	2	4 9 2	104.38
.9709	1	5 4 3	105.01
.9690	4	6 4 2	105.30
.9605	1	1 10 3	106.63
.9549	3	4 1 4	107.54
.9508	1	5 9 1	108.22
.9496	3	7 1 1	108.42
.9454	2	5 5 3	109.13
.9305	1	1 13 1	111.75
.9297	2	0 8 4	111.90
.9258	1	3 12 1	112.60
.9157	1	1 1 5	114.54
.9153	1	6 6 2	114.61
.9134	1	2 12 2	114.98
.9083	1	1 2 5	115.99
.9057	1	1 11 3	116.52
.9022	1	5 10 1	117.24
.8965	1	1 3 5	118.45
.8922	1	3 10 3	119.40
.8907	1	0 14 0	119.72

Structure

Monoclinic, I2/c (15), Z=8. The structure was determined by Lindh [1967], who published data in terms of the C2/c cell with a=26.33,b=6.254, c=12.90, β=116.94°.

Lattice parameters

a=23.49(2), b=6.254(2), c=12.90(1)Å, β=92.36°

Density

(calculated) 3.966 g/cm^3

Thermal parameters

Isotropic: O(1) 5.2,O(2) 5.9,O(3) 5.6,O(4) 7.6, C(1) 3.2, C(2) 4.5, C(3) 6.2,C(4) 5.3,C(5) 1.6, C(6) 5.3, C(7) 4.7, C(8) 3.6 [Lindh,1967] Hg(1) 4.44, Hg(2) 4.50

Scattering factors

C^0, O^0 [Hanson et al., 1964]
Hg^0 [Cromer and Waber,1965], corrected for dispersion using Δf'=-4.8,Δf"=7.04 [Cromer, 1965]

Scale factor

(integrated intensities) 617.4 × 10^4

Reference

Cromer, D.T. (1965). Acta Cryst. 18, 17.
Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Hanson,H.P., F. Herman, J.D. Lea, and S. Skillman (1964). Acta Cryst. 17, 1040.
Lindh, B. (1967). Acta Chem. Scand. 21, 2743.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
11.72	100	2	0	0		7.54
6.04	15	1	1	0		14.66
5.75	1	-2	0	2		15.40
5.63	16	0	1	1		15.74
5.56	2	2	0	2		15.94
5.11	15	-2	1	1		17.34
5.04	1	2	1	1		17.58
4.43	9	-1	1	2	+	20.02
4.38	4	1	1	2		20.24
4.25	7	4	0	2		20.88
4.10	2	-4	1	1		21.66
3.844	2	3	1	2		23.12
3.754	2	5	1	0		23.68
3.542	2	0	1	3		25.12
3.422	1	-2	1	3		26.02
3.406	1	-6	0	2		26.14
3.358	5	2	1	3		26.52
3.285	8	6	0	2	+	27.12
3.238	1	-6	1	1		27.52
3.197	5	5	1	2		27.88
3.188	4	6	1	1		27.96
3.079	2	-4	1	3	+	28.98
3.017	4	-1	2	1	+	29.58
2.988	7	4	1	3		29.88
2.955	1	7	1	0		30.22
2.855	1	-1	1	4		31.30
2.841	2	-3	2	1		31.46
2.813	2	0	2	2		31.78
2.776	2	4	0	4		32.22
2.759	4	4	2	0		32.42
2.748	2	-2	2	2		32.56
2.723	2	-7	1	2		32.86
2.671	2	-6	1	3		33.52
2.659	2	3	1	4		33.68
2.630	1	8	0	2		34.06
2.621	1	-8	1	1		34.18
2.582	3	6	1	3		34.72
2.539	2	-6	0	4	+	35.32
2.443	2	6	2	0		36.76
2.406	1	5	1	4		37.34
2.389	1	3	2	3		37.62
2.347	1	10	0	0		38.32
2.303	1	-6	2	2		39.08
2.299	1	-8	1	3		39.16
2.249	1	-5	2	3		40.06
2.244	2	0	2	4		40.16
2.216	4	-8	0	4	+	40.68
2.204	1	5	2	3		40.92
2.180	2	-10	1	1		41.38
2.140	1	8	2	0		42.20

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
2.128	1	-2 0 6	42.44
2.117	1	-4 2 4	42.68
2.043	2	-7 2 3 +	44.30
1.985	1	-3 1 6	45.66
1.946	1	-4 3 1	46.64
1.936	1	-10 0 4	46.90
1.894	1	-12 0 2	48.00
1.875	1	0 3 3	48.50
1.857	2	-2 3 3 +	49.00
1.826	1	-6 3 1	49.90
1.817	1	8 1 5	50.18
1.787	1	10 2 2	51.08

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
11.74	100	2 0 0	7.53
6.04	17	1 1 0	14.65
5.75	1	-2 0 2	15.40
5.63	18	0 1 1	15.74
5.55	2	2 0 2	15.95
5.11	18	-2 1 1	17.34
5.04	1	2 1 1	17.59
4.43	9	-1 1 2	20.02
4.43	1	-4 0 2	20.02
4.38	5	1 1 2	20.23
4.25	8	4 0 2	20.87
4.10	3	-4 1 1	21.67
3.846	3	3 1 2	23.11
3.754	3	5 1 0	23.68
3.541	3	0 1 3	25.13
3.423	1	-2 1 3	26.01
3.407	1	-6 0 2	26.13
3.359	6	2 1 3	26.52
3.292	2	-5 1 2	27.07
3.284	10	6 0 2	27.13
3.240	1	-6 1 1	27.51
3.198	7	5 1 2	27.87
3.185	1	6 1 1	27.99
3.079	3	-4 1 3	28.98
3.075	1	2 0 4	29.01
3.022	2	2 2 0	29.54
3.017	4	-1 2 1	29.58
2.987	9	4 1 3	29.89
2.955	1	7 1 0	30.22
2.856	1	-1 1 4	31.29
2.842	2	-3 2 1	31.45
2.813	3	0 2 2	31.78
2.776	3	4 0 4	32.21
2.760	5	4 2 0	32.42
2.747	2	-2 2 2	32.57
2.724	2	-7 1 2	32.85
2.671	3	-6 1 3	33.52
2.658	2	3 1 4	33.69
2.630	1	8 0 2	34.07
2.621	1	-8 1 1	34.19
2.582	4	6 1 3	34.71
2.540	1	5 2 1	35.31
2.539	2	-6 0 4	35.32
2.520	1	-1 2 3	35.59
2.443	3	6 2 0	36.76
2.406	1	5 1 4	37.34
2.389	2	3 2 3	37.62
2.347	1	10 0 0	38.31
2.304	1	-6 2 2	39.07
2.298	2	-8 1 3	39.17
2.249	1	-5 2 3	40.06
2.244	2	0 2 4	40.15
2.219	2	-7 1 4	40.63
2.216	2	-2 2 4	40.68
2.216	3	-8 0 4	40.69
2.204	2	5 2 3	40.92
2.180	2	-10 1 1	41.38
2.140	1	8 2 0	42.20
2.129	2	-2 0 6	42.43
2.116	1	-4 2 4	42.69
2.045	2	-4 0 6	44.26
2.043	2	-7 2 3	44.31
2.031	1	-1 1 6	44.58
2.020	1	11 1 0	44.84
1.985	1	-3 1 6	45.66
1.946	1	-4 3 1	46.64
1.936	1	-10 0 4	46.90
1.894	1	-12 0 2	48.01
1.876	2	0 3 3	48.50
1.858	1	-12 1 1	48.98
1.857	2	-2 3 3	49.01
1.826	2	-6 3 1	49.89
1.816	1	8 1 5	50.19
1.787	1	10 2 2	51.08
1.742	1	2 2 6	52.48
1.710	1	-4 1 7	53.54
1.700	1	8 0 6	53.88
1.690	1	-8 3 1	54.23
1.679	1	4 2 6	54.60
1.641	1	10 1 5	55.98

Structure

Monoclinic, I2/m (12), Z=4. The structure was determined by Jensen et al. [1966].

Lattice parameters

a = 11.197(2), b = 3.2350(4), c = 9.643(1)Å, β = 100.57(2)° (published value: b = 3.2349Å, [ibid.]

Density

(calculated) 8.058 g/cm^3

Thermal parameters

Isotropic [Jensen et al., 1966]

Scattering factors

As^0, Mo^0 [3.3.1A]

Scale factors

(integrated intensities) 6.441×10^4

Reference

Jensen, P., A. Kjekshus, and T. Skansen (1966). Acta Chem. Scand. 20, 1003.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
7.94	5	-1	0	1		11.14
6.60	6	1	0	1		13.40
5.50	51	2	0	0		16.10
4.741	14	0	0	2		18.70
3.654	10	-3	0	1		24.34
3.304	1	2	0	2		26.96
3.227	9	3	0	1		27.62
3.197	9	-1	0	3		27.88
3.062	20	0	1	1		29.14
2.751	38	4	0	0		32.52
2.746	39	-2	1	1		32.58
2.660	77	-1	1	2		33.66
2.647	40	-3	0	3		33.84
2.611	34	2	1	1		34.32
2.538	96	1	1	2		35.34
2.370	3	0	0	4		37.94
2.338	50	-2	0	4		38.48
2.261	34	0	1	3		39.84
2.2371	26	-5	0	1		40.28
2.2026	35	3	0	3		40.94
2.1944	54	-2	1	3		41.10
2.1101	33	-4	1	1		42.82
2.0607	100	3	1	2	+	43.90
2.0002	2	2	1	3		45.30
1.9844	27	-4	0	4	+	45.68
1.9325	12	-1	1	4		46.98
1.8711	3	-4	1	3		48.62
1.8343	7	6	0	0		49.66
1.8267	6	-3	0	5	+	49.88
1.8213	4	5	1	0		50.04
1.8138	16	1	0	5		50.26
1.7925	64	-5	1	2		50.90
1.6682	2	5	0	3		55.00
1.6521	6	4	0	4		55.58
1.6440	5	4	1	3		55.88
1.6402	8	-2	1	5		56.02
1.6359	11	0	1	5		56.18
1.6174	31	0	2	0		56.88
1.6009	7	3	1	4		57.52
1.5984	9	-2	0	6	+	57.62
1.5799	2	0	0	6		58.36
1.5711	5	3	0	5		58.72
1.5518	2	2	2	0		59.52
1.5308	1	0	2	2		60.42
1.5258	3	-6	1	3		60.64
1.5154	2	-4	1	5		61.10
1.5074	1	7	0	1		61.46
1.5043	2	2	1	5		61.60
1.4793	1	-3	2	1		62.76
1.4495	4	2	0	6		64.20

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.4459	3	3 2 1	64.38
1.4431	2	-1 2 3	64.52
1.4384	10	-1 1 6	64.76
1.4208	3	-7 1 2	65.66
1.3945	5	4 2 0	67.06
1.3912	3	-8 0 2	67.24
1.3800	7	-3 2 3 +	67.86
1.3761	7	8 0 0	68.08
1.3409	5	6 1 3	70.12
1.3370	8	-7 0 5 +	70.36
1.3300	13	-2 2 4 +	70.78
1.3232	1	-6 0 6	71.20
1.3219	1	5 0 5	71.28
1.3175	3	4 1 5	71.56
1.3149	5	1 0 7 +	71.72
1.3108	6	-5 2 1	71.98
1.3039	7	3 2 3	72.42
1.2729	8	5 2 1 +	74.48
1.2613	4	-5 0 7	75.28
1.2539	7	-4 2 4	75.80
1.2506	4	0 1 7	76.04
1.2282	7	8 1 1	77.68
1.2177	6	-4 1 7 +	78.48
1.2133	3	6 2 0	78.82
1.2110	3	-3 2 5 +	79.00
1.2071	5	1 2 5	79.30
1.1856	1	9 0 1	81.04
1.1613	1	5 2 3	83.10
1.1559	2	4 2 4	83.58
1.1525	2	-7 1 6	83.88
1.1461	5	-8 1 5	84.46
1.1439	3	9 1 0	84.66
1.1369	4	-2 2 6 +	85.30
1.1348	6	6 1 5	85.50
1.1303	1	0 2 6	85.92
1.1267	5	-1 1 8 +	86.26
1.1248	4	-6 1 7	86.44
1.1196	3	-3 1 8	86.94
1.1184	2	-10 0 2	87.06
1.1123	4	8 1 3	87.66
1.1073	1	-9 1 4	88.16
1.1051	1	8 0 4	88.38
1.0884	1	1 1 8	90.10
1.0796	2	2 2 6	91.04
1.0766	2	-10 0 4	91.36
1.0712	3	4 1 7	91.96
1.0701	2	-5 1 8	92.08
1.0672	2	-1 0 9	92.40
1.0656	1	-3 0 9	92.58
1.0560	3	-10 1 1	93.68

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.0508	2	-1 3 2	94.28
1.0479	3	8 2 0 +	94.62
1.0451	3	-10 1 3	94.96
1.0426	3	1 3 2	95.26
1.0304	4	-7 2 5 +	96.76
1.0234	1	-6 2 6	97.64
1.0222	1	4 0 8	97.80
1.0205	4	1 2 7 +	98.02
1.0172	4	3 1 8 +	98.44
1.0143	3	-2 3 3 +	98.82
1.0128	2	-9 1 6	99.02
1.0055	1	-4 3 1	100.00
1.0038	1	-9 0 7	100.24
1.0001	4	3 3 2	100.74
.9947	3	-5 2 7	101.50
.9731	3	-9 2 3	104.66
.9642	6	-5 3 2 +	106.04
.9597	1	6 1 7	106.76
.9564	2	2 1 9 +	107.30
.9514	1	9 0 5	108.12
.9459	1	-11 1 4	109.04
.9440	1	7 0 7	109.36
.9374	1	0 3 5	110.52
.9307	1	3 3 4	111.72
.9214	1	6 0 8 +	113.44
.9199	1	-10 2 2	113.72
.9125	1	8 2 4 +	115.16
.9072	2	11 0 3 +	116.22
.9044	1	-6 2 8	116.80
.8962	1	-10 2 4	118.52
.8953	2	-1 3 6	118.72
.8931	1	-12 1 1	119.20
.8916	1	-12 1 3	119.52
.8910	1	-7 3 2 +	119.66
.8899	1	-3 2 9 +	119.90

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
7.94	3	-1	0	1	11.14
6.61	5	1	0	1	13.39
5.50	40	2	0	0	16.09
4.740	12	0	0	2	18.71
3.655	9	-3	0	1	24.33
3.304	1	2	0	2	26.96
3.228	8	3	0	1	27.61
3.197	9	-1	0	3	27.89
3.062	18	0	1	1	29.14
2.752	34	4	0	0	32.51
2.746	18	-2	1	1	32.59
2.660	72	-1	1	2	33.66
2.646	31	-3	0	3	33.84
2.611	33	2	1	1	34.32
2.537	100	1	1	2	35.35
2.370	3	0	0	4	37.94
2.338	52	-2	0	4	38.47
2.260	36	0	1	3	39.85
2.2367	26	-5	0	1	40.29
2.2028	33	3	0	3	40.94
2.1946	50	-2	1	3	41.10
2.1097	36	-4	1	1	42.83
2.0627	32	5	0	1	43.86
2.0609	90	3	1	2	43.90
2.0007	1	2	1	3	45.29
1.9889	4	4	1	1	45.57
1.9852	2	-5	0	3	45.66
1.9848	27	-4	0	4	45.67
1.9324	13	-1	1	4	46.98
1.8713	3	-4	1	3	48.61
1.8346	7	6	0	0	49.65
1.8275	2	-6	0	2	49.86
1.8265	4	-3	0	5	49.89
1.8200	2	5	1	0	50.08
1.8135	18	1	0	5	50.27
1.7925	72	-5	1	2	50.90
1.6684	3	5	0	3	54.99
1.6521	7	4	0	4	55.58
1.6441	5	4	1	3	55.88
1.6404	6	-2	1	5	56.01
1.6357	10	0	1	5	56.19
1.6175	37	0	2	0	56.88
1.6011	6	3	1	4	57.51
1.5994	3	-7	0	1	57.58
1.5983	6	-2	0	6	57.62
1.5799	2	0	0	6	58.36
1.5709	6	3	0	5	58.73
1.5519	2	2	2	0	59.52
1.5308	1	0	2	2	60.42
1.5258	4	-6	1	3	60.64
1.5153	2	-4	1	5	61.10
1.5073	1	7	0	1	61.47
1.5042	2	2	1	5	61.60
1.4791	1	-3	2	1	62.77
1.4497	5	2	0	6	64.19
1.4461	1	3	2	1	64.37
1.4433	1	-1	2	3	64.51
1.4384	13	-1	1	6	64.76
1.4210	4	-7	1	2	65.65
1.4042	1	-3	1	6	66.54
1.3944	6	4	2	0	67.06
1.3915	1	-8	0	2	67.22
1.3801	6	-3	2	3	67.85
1.3794	4	1	1	6	67.89
1.3759	5	8	0	0	68.09
1.3410	7	6	1	3	70.12
1.3368	6	-7	0	5	70.37
1.3368	2	6	0	4	70.37
1.3302	13	-2	2	4	70.77
1.3299	6	-6	1	5	70.79
1.3232	1	-6	0	6	71.20
1.3217	1	5	0	5	71.30
1.3175	2	4	1	5	71.56
1.3151	3	1	0	7	71.71
1.3149	3	7	0	3	71.72
1.3107	7	-5	2	1	71.99
1.3038	9	3	2	3	72.43
1.2730	1	4	0	6	74.47
1.2728	10	5	2	1	74.48
1.2613	5	-5	0	7	75.28
1.2561	1	3	1	6	75.64
1.2539	9	-4	2	4	75.81
1.2492	1	0	1	7	76.14
1.2423	1	-9	0	1	76.64
1.2281	10	8	1	1	77.69
1.2183	5	-9	0	3	78.43
1.2176	6	-4	1	7	78.48
1.2133	3	6	2	0	78.82
1.2112	1	-6	2	2	78.98
1.2109	2	-3	2	5	79.00
1.2071	7	1	2	5	79.30
1.1857	1	9	0	1	81.03
1.1613	1	5	2	3	83.10
1.1558	3	4	2	4	83.59
1.1525	2	-7	1	6	83.88
1.1461	7	-8	1	5	84.46
1.1440	3	9	1	0	84.65
1.1373	2	-7	2	1	85.27
1.1369	3	-2	2	6	85.30
1.1349	8	6	1	5	85.49

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.1302	1	0 2 6	85.93
1.1269	3	3 2 5	86.24
1.1266	5	-1 1 8	86.27
1.1262	1	-9 0 5	86.31
1.1249	4	-6 1 7	86.43
1.1197	4	-3 1 8	86.94
1.1184	1	-10 0 2	87.06
1.1123	6	8 1 3	87.66
1.1073	1	-9 1 4	88.15
1.1051	2	8 0 4	88.37
1.0907	1	-6 0 8	89.86
1.0884	2	1 1 8	90.10
1.0795	3	2 2 6	91.04
1.0766	1	-10 0 4	91.36
1.0713	4	4 1 7	91.95
1.0700	3	-5 1 8	92.09
1.0672	1	-1 0 9	92.40
1.0655	1	-3 0 9	92.59
1.0559	4	-10 1 1	93.68
1.0508	2	-1 3 2	94.29
1.0480	4	8 2 0	94.61
1.0476	1	2 3 1	94.66
1.0451	3	-10 1 3	94.96
1.0427	4	1 3 2	95.25
1.0305	5	-7 2 5	96.75
1.0304	1	6 2 4	96.75
1.0242	1	-6 2 6	97.55
1.0223	1	4 0 8	97.78
1.0205	2	0 3 3	98.01
1.0204	2	1 2 7	98.03
1.0203	2	7 2 3	98.04
1.0172	3	3 1 8	98.45
1.0168	2	10 1 1	98.49
1.0143	3	-2 3 3	98.83
1.0142	1	-8 1 7	98.84
1.0128	2	-9 1 6	99.02
1.0055	2	-4 3 1	100.01
1.0039	1	-9 0 7	100.23
1.0001	6	3 3 2	100.75
.9988	1	-4 1 9	100.93
.9946	4	-5 2 7	101.51
.9843	1	-1 3 4	103.00
.9731	5	-9 2 3	104.66
.9642	3	-2 0 10	106.04
.9642	8	-5 3 2	106.05
.9597	2	6 1 7	106.76
.9564	3	2 1 9	107.30
.9563	1	9 2 1	107.32
.9513	2	9 0 5	108.13
.9460	1	-11 1 4	109.04
.9441	2	7 0 7	109.36
.9382	1	-2 3 5	110.37
.9373	1	0 3 5	110.53
.9307	1	3 3 4	111.72
.9242	1	-9 2 5	112.91
.9217	1	-3 1 10	113.39
.9213	1	6 0 8	113.46
.9199	2	-10 2 2	113.72
.9132	1	-6 0 10	115.01
.9125	2	8 2 4	115.16
.9073	2	11 0 3	116.21
.9068	2	2 0 10	116.31
.9043	1	-6 2 8	116.81
.8984	1	-5 1 10	118.05
.8962	2	-10 2 4	118.51
.8952	3	-1 3 6	118.73
.8934	1	-12 1 1	119.13
.8917	1	-12 1 3	119.49
.8910	1	-7 3 2	119.66
.8908	1	-1 2 9	119.70
.8899	1	-11 1 6	119.90
.8898	1	-3 2 9	119.92

Nickel bromide, $NiBr_2$

Structure

Hexagonal, $R\bar{3}m$ (166), Z=3, isostructural with cadmium chloride. The structure was determined by Ketelaar [1934].

Lattice parameters

a= 3.72(1), c= 18.34(4)Å [ibid.]

Density

(calculated) 4.945 g/cm^3

Thermal parameters

Isotropic; overall B= 2.0

Polymorphism

Ketelaar [1934] described an alternate hexagonal form which had a smaller cell and a structure like the form of $CdBr_2$ discussed by Bijvoet and Nieuwenkamp [1933].

Scattering factors

Ni^{2+} [3.3.1A]
Br^- [Cromer and Waber, 1965]

Scale factors

(integrated intensities) 6.079×10^4

Additional patterns

1. PDF card 3-0580 [Ketelaar, 1934]

Reference

Bijvoet, J.M. and W. Nieuwenkamp (1933). Z. Krist. 86, 466.
Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Ketelaar, J.A.A. (1934). Z. Krist. 88, 26.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
6.11	46	0 0 3	14.48
3.18	13	1 0 1	28.08
3.06	12	0 0 6	29.20
3.04	33	0 1 2	29.34
2.64	100	1 0 4	33.96
2.42	2	0 1 5	37.10
2.03	7	1 0 7	44.52
1.87	27	0 1 8	48.70
1.86	31	1 1 0	48.88
1.78	5	1 1 3	51.26
1.61	1	0 2 1	57.32
1.59	3	1 0 10	57.80
1.59	6	1 1 6	57.96
1.59	4	2 0 2	58.04
1.53	3	0 0 12	60.54
1.52	10	0 2 4	60.86
1.48	3	0 1 11	62.68
1.373	1	0 2 7	68.26
1.319	5	2 0 8	71.48
1.211	1	0 2 10	79.02
1.208	2	1 2 2	79.24
1.181	5	1 1 12	81.40
1.178	7	2 1 4	81.68
1.080	1	1 0 16	91.00
1.076	4	1 2 8	91.42
1.075	2	3 0 0	91.56
1.022	1	1 1 15	97.84
.934	1	0 2 16	111.08
.931	1	2 2 0	111.70
.890	1	3 1 2 +	119.86
.879	1	3 0 12 +	122.38
.878	2	1 3 4	122.72
.835	1	2 1 16	134.60
.833	2	3 1 8	135.22
.795	1	2 2 12	151.38
.794	1	4 0 4	151.98

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.11	35	0 0 3	14.48
3.18	12	1 0 1	28.08
3.06	10	0 0 6	29.19
3.04	30	0 1 2	29.34
2.64	100	1 0 4	33.96
2.42	2	0 1 5	37.09
2.03	8	1 0 7	44.52
1.87	29	0 1 8	48.70
1.86	30	1 1 0	48.89
1.78	6	1 1 3	51.26
1.61	1	0 2 1	57.33
1.59	3	1 0 10	57.79
1.59	6	1 1 6	57.96
1.59	3	2 0 2	58.04
1.53	4	0 0 12	60.53
1.52	13	0 2 4	60.86
1.48	3	0 1 11	62.68
1.373	2	0 2 7	68.25
1.319	7	2 0 8	71.48
1.214	1	0 1 14	78.79
1.211	1	0 2 10	79.01
1.208	2	1 2 2	79.23
1.181	8	1 1 12	81.40
1.178	8	2 1 4	81.69
1.159	1	2 0 11	83.31
1.105	1	2 1 7	88.39
1.080	2	1 0 16	90.99
1.076	6	1 2 8	91.42
1.075	3	3 0 0	91.57
1.022	2	1 1 15	97.83
1.015	1	2 1 10	98.73
.984	1	1 2 11	103.06
.934	2	0 2 16	111.09
.931	2	2 2 0	111.70
.925	1	1 0 19	112.82
.890	1	2 2 6	119.79
.890	1	3 1 2	119.87
.882	1	0 1 20	121.69
.879	2	3 0 12	122.37
.879	2	0 3 12	122.37
.878	3	1 3 4	122.71
.835	3	2 1 16	134.61
.833	3	3 1 8	135.22
.828	1	0 2 19	136.90
.807	1	3 0 15	145.20
.807	1	0 3 15	145.20
.804	1	1 3 10	146.80
.797	2	2 0 20	150.20
.795	4	2 2 12	151.38
.794	2	4 0 4	151.99
.788	1	3 1 11	155.62

Structure

Tetragonal, $P4_2mnm$ (136), Z=2, isostructural with rutile [Ferrari, 1926]. The structure was determined by Stout and Reed and refined by Baur [1958].

Lattice parameters

a=4.6508(2), c=3.0837(4)Å, (published as 4.6506 and 3.0836) [Stout and Reed, 1954]

Density

(calculated) 4.815 g/cm^3

Thermal parameters

Isotropic [Baur, 1958] Ni 0.3
F 0.7

Atomic positions

Baur [1958]

Scattering factors

F^- [Cromer and Waber, 1965]
Ni^{2+} [Cromer and Waber,1965];corrected for dispersion using $\Delta f'=-3.20$ and $\Delta f''=0.67$ [Cromer, 1965]

Scale factors

(integrated intensities) 0.2613×10^4

Additional patterns

1. PDF card 1-672 [Dow Chemical Co., Midland, Mich.]
2. Ferrari [1926]

Reference

Baur, W.H. (1958). Acta Cryst. 11, 488.
Cromer, D.T. (1965). Acta Cryst. 18, 17.
Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Ferrari, A. (1926). Atti reale accad. nazl. Lincei 3, 224.
Stout, J.W. and S.A. Reed (1954). J.Am.Chem. Soc. 76, 5279.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
3.2877	100	1 1 0	27.10
2.5701	49	1 0 1	34.88
2.3259	5	2 0 0	38.68
2.2489	20	1 1 1	40.06
2.0796	6	2 1 0	43.48
1.7245	50	2 1 1	53.06
1.6445	15	2 2 0	55.86
1.5420	7	0 0 2	59.94
1.4709	6	3 1 0	63.16
1.3960	8	1 1 2	66.98
1.3850	15	3 0 1	67.58
1.3274	1	3 1 1	70.94
1.2850	1	2 0 2	73.66
1.2387	1	2 1 2	76.90
1.1900	3	3 2 1	80.66
1.1627	2	4 0 0	82.98
1.1280	1	4 1 0	86.14
1.1248	5	2 2 2	86.44
1.0962	2	3 3 0	89.28
1.0642	3	3 1 2	92.74
1.0593	3	4 1 1	93.30
1.0399	1	4 2 0	95.56
1.0036	1	1 0 3	100.26
.9284	2	4 0 2	112.14
.9215	3	2 1 3	113.42
.9121	2	5 1 0	115.24
.9099	1	4 1 2	115.68
.8934	2	3 3 2	119.12
.8905	3	4 3 1	119.76
.8621	2	4 2 2	126.62
.8567	2	3 0 3	128.06
.8317	4	5 2 1	135.70
.8039	1	3 2 3	146.76
.7850	3	5 1 2	157.76

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
3.2886	100	1 1 0	27.09
2.5701	51	1 0 1	34.88
2.3254	6	2 0 0	38.69
2.2495	23	1 1 1	40.05
2.0799	7	2 1 0	43.47
1.7243	64	2 1 1	53.07
1.6443	19	2 2 0	55.87
1.5419	10	0 0 2	59.94
1.4707	9	3 1 0	63.17
1.3960	12	1 1 2	66.98
1.3851	22	3 0 1	67.58
1.3275	2	3 1 1	70.94
1.2850	2	2 0 2	73.66
1.2386	1	2 1 2	76.91
1.1900	4	3 2 1	80.68
1.1627	3	4 0 0	82.98
1.1280	1	4 1 0	86.14
1.1247	8	2 2 2	86.45
1.0962	4	3 3 0	89.28
1.0642	5	3 1 2	92.74
1.0593	6	4 1 1	93.29
1.0399	3	4 2 0	95.58
1.0037	2	1 0 3	100.25
.9283	3	4 0 2	112.15
.9215	7	2 1 3	113.42
.9121	4	5 1 0	115.24
.9104	1	4 1 2	115.58
.8934	5	3 3 2	119.12
.8905	6	4 3 1	119.76
.8622	4	4 2 2	126.61
.8567	6	3 0 3	128.09
.8316	12	5 2 1	135.71
.8221	2	4 4 0	139.08
.8039	3	3 2 3	146.75
.7976	1	5 3 0	149.92
.7944	1	4 4 1	151.69
.7850	14	5 1 2	157.76

Structure

Hexagonal, R$\bar{3}$m (166), Z=9, isostructural with $NbBe_3$. The structure was determined by Smith and Hansen [1965].

Lattice parameters

a=4.9781(4), c=24.450(3)Å, [published values: a=4.9779(4), c=24.449(3)Å, (ibid.)]

Density

(calculated) 7.548 g/cm^3 [ibid.]

Thermal parameters

Isotropic [ibid.]

Polymorphism

Data on PDF card 20-644 is for another hexagonal phase with space group $P6_3/mmc$ [Bartram and Chase, private communication to the PDF].

Scattering factors

Y^0, Ni^0 [3.3.1A]

Scale factors

(integrated intensities) 33.32×10^4

Additional patterns

1. PDF card 15-118 [Beaudry and Daane, 1961]

Reference

Beaudry, B.J. and A.H.Daane (1961). Am.Soc.Metals Trans. Quart. 53, 899.

Smith, J.F., and D.A. Hansen (1965). Acta Cryst. 19, 1019.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ λ = 1.54056 Å
4.247	1	1	0	1		20.90
2.7137	29	1	0	7	+	32.98
2.4927	42	0	1	8		36.00
2.4887	53	1	1	0		36.06
2.1475	33	0	2	1		42.04
2.1243	100	1	1	6	+	42.52
2.0378	18	0	0	12		44.42
2.0326	20	0	2	4		44.54
1.9754	20	0	1	11		45.90
1.9722	30	2	0	5		45.98
1.8350	9	1	1	9	+	49.64
1.7239	1	1	0	13		53.08
1.6301	3	0	0	15		56.40
1.6185	2	0	1	14	+	56.84
1.4768	6	2	1	7		62.88
1.4375	11	1	2	8	+	64.80
1.4173	5	0	2	13		65.84
1.3637	6	1	1	15		68.78
1.3566	12	2	0	14	+	69.18
1.3551	18	3	0	6	+	69.26
1.3143	6	1	2	11		71.76
1.2702	1	0	3	9	+	74.66
1.2445	15	2	2	0		76.46
1.1963	3	2	0	17		80.16
1.1924	3	1	1	18	+	80.46
1.1762	1	0	1	20		81.82
1.1313	2	1	3	7		85.82
1.1135	3	3	1	8	+	87.54
1.1049	4	0	2	19		88.40
1.0779	3	3	0	15	+	91.22
1.0766	3	4	0	1	+	91.36
1.0737	2	0	4	2		91.68
1.0621	7	2	2	12	+	92.98
1.0546	3	1	1	21		93.84
1.0527	4	3	1	11	+	94.06
1.0188	1	0	0	24		98.24
.9892	3	2	2	15		102.28
.9877	2	0	2	22		102.50
.9867	3	3	1	14	+	102.64
.9779	1	1	2	20		103.94
.9536	2	1	0	25	+	107.76
.9515	2	3	2	7		108.10
.9408	4	4	1	0	+	109.92
.9351	1	4	0	13		110.92
.9167	9	1	4	6	+	114.34
.9047	2	0	3	21	+	116.74
.9036	2	2	3	11		116.96
.8890	1	4	1	9	+	120.10
.8624	2	0	4	17	+	126.54
.8604	1	2	3	14		127.08
.8548	1	3	1	20		128.62
.8503	1	2	2	21		129.90
.8386	2	2	1	25		133.44
.8370	1	0	5	7		133.92
.8297	2	3	3	0	+	136.36
.8276	1	0	1	29		137.12
.8263	2	4	0	19		137.58

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
4.246	1	1 0 1	20.91
2.7167	2	0 0 9	32.94
2.7139	27	1 0 7	32.98
2.4933	32	0 1 8	35.99
2.4891	37	1 1 0	36.05
2.1472	36	0 2 1	42.04
2.1268	2	1 0 10	42.47
2.1242	100	1 1 6	42.52
2.1228	13	2 0 2	42.55
2.0375	19	0 0 12	44.43
2.0329	12	0 2 4	44.53
1.9756	16	0 1 11	45.90
1.9724	28	2 0 5	45.97
1.8352	7	1 1 9	49.63
1.8344	5	0 2 7	49.66
1.7239	1	1 0 13	53.08
1.6300	4	0 0 15	56.40
1.6187	3	0 1 14	56.83
1.6169	1	0 2 10	56.90
1.4767	8	2 1 7	62.88
1.4403	2	1 0 16	64.66
1.4379	10	1 2 8	64.78
1.4370	6	3 0 0	64.83
1.4172	7	0 2 13	65.85
1.3636	8	1 1 15	68.79
1.3583	1	0 0 18	69.09
1.3570	11	2 0 14	69.17
1.3559	1	2 1 10	69.23
1.3553	11	3 0 6	69.27
1.3553	11	0 3 6	69.27
1.3142	8	1 2 11	71.77
1.2703	1	0 3 9	74.66
1.2703	1	3 0 9	74.66
1.2445	23	2 2 0	76.48
1.1964	5	2 0 17	80.16
1.1923	3	1 1 18	80.48
1.1914	2	1 2 14	80.56
1.1761	1	0 1 20	81.83
1.1312	3	1 3 7	85.83
1.1146	1	2 1 16	87.43
1.1135	5	3 1 8	87.54
1.1049	6	0 2 19	88.39
1.0779	2	3 0 15	91.22
1.0779	2	0 3 15	91.22
1.0767	4	4 0 1	91.35
1.0762	1	1 0 22	91.41
1.0736	1	0 4 2	91.69
1.0621	12	2 2 12	92.98
1.0614	1	4 0 4	93.06
1.0546	5	1 1 21	93.84
1.0530	4	3 1 11	94.03
1.0525	3	0 4 5	94.08
1.0187	2	0 0 24	98.24
.9892	5	2 2 15	102.29
.9878	3	0 2 22	102.48
.9871	1	0 3 18	102.58
.9871	1	3 0 18	102.58
.9866	1	3 1 14	102.65
.9779	1	1 2 20	103.94
.9538	2	1 0 25	107.73
.9534	2	2 0 23	107.79
.9516	2	3 2 7	108.08
.9417	1	1 3 16	109.77
.9410	4	2 3 8	109.88
.9408	4	4 1 0	109.92
.9351	2	4 0 13	110.92
.9181	2	2 1 22	114.06
.9176	3	2 2 18	114.16
.9172	5	0 4 14	114.24
.9167	9	4 1 6	114.35
.9167	9	1 4 6	114.35
.9046	2	3 0 21	116.75
.9046	2	0 3 21	116.75
.9036	3	2 3 11	116.95
.8890	1	4 1 9	120.10
.8890	1	1 4 9	120.10
.8625	4	0 4 17	126.53
.8619	1	2 0 26	126.67
.8606	1	2 3 14	127.02
.8558	1	1 0 28	128.32
.8548	2	3 1 20	128.61
.8502	2	2 2 21	129.91
.8386	5	2 1 25	133.44
.8371	2	0 5 7	133.90
.8303	2	3 2 16	136.16
.8298	2	5 0 8	136.32
.8297	3	3 3 0	136.37
.8274	1	0 1 29	137.16
.8263	6	4 0 19	137.57

Potassium oxide, K_2O

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a= 6.449Å [ibid.]

Density

(calculated) 2.333 g/cm^3

Thermal parameters

Isotropic; overall B = 2.0

Scattering factors

K^+ [3.3.1A]
O^{2-} [Suzuki, 1960]

Scale factors

(integrated intensities) 2.390×10^4

Additional patterns

1. Zintl et al. [1934]

Reference

Suzuki, T. (1960). Acta Cryst. 13, 279.
Zintl. E., A. Harder, and B. Dauth (1934). Z. Electrochem. 40, 588.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
3.723	16	1 1 1	23.88
3.225	75	2 0 0	27.64
2.280	100	2 2 0	39.50
1.9442	3	3 1 1	46.68
1.8618	13	2 2 2	48.88
1.6122	10	4 0 0	57.08
1.4419	11	4 2 0	64.58
1.3165	13	4 2 2	71.62
1.1399	3	4 4 0	85.02
1.0748	3	4 4 2 +	91.56
1.0197	3	6 2 0	98.12
.9722	2	6 2 2	104.80
.9309	1	4 4 4	111.68
.8943	1	6 4 0	118.92
.8618	4	6 4 2	126.72

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
3.723	13	1 1 1	23.88
3.225	64	2 0 0	27.64
2.280	100	2 2 0	39.49
1.9445	3	3 1 1	46.67
1.8617	13	2 2 2	48.88
1.6123	11	4 0 0	57.08
1.4420	13	4 2 0	64.57
1.3164	17	4 2 2	71.63
1.1400	4	4 4 0	85.01
1.0748	1	6 0 0	91.56
1.0748	4	4 4 2	91.56
1.0197	6	6 2 0	98.12
.9722	3	6 2 2	104.80
.9308	2	4 4 4	111.69
.8943	2	6 4 0	118.93
.8618	9	6 4 2	126.71
.8061	1	8 0 0	145.70

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a=7.692Å [ibid.]

Density

(calculated) 2.294 g/cm^3

Thermal parameters

Isotropic: K 1.0
Se 0.6

Scattering factors

K^+ [3.3.1A]
Se^0 [3.3.1B]

Scale factors

(integrated intensities) 12.50×10^4

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
4.440	74	1 1 1	19.98
2.720	100	2 2 0	32.90
2.319	29	3 1 1	38.80
1.923	14	4 0 0	47.22
1.765	10	3 3 1	51.76
1.570	24	4 2 2	58.76
1.480	6	5 1 1 +	62.72
1.360	6	4 4 0	69.02
1.300	5	5 3 1	72.66
1.216	7	6 2 0	78.60
1.173	2	5 3 3	82.10
1.110	2	4 4 4	87.86
1.077	2	7 1 1 +	91.32
1.028	7	6 4 2	97.08
1.001	3	7 3 1 +	100.56
.961	1	8 0 0	106.48
.940	1	7 3 3	110.10
.907	4	8 2 2 +	116.36
.888	2	7 5 1	120.28
.860	2	8 4 0	127.20
.844	2	7 5 3 +	131.66
.820	3	6 6 4	139.90
.806	2	9 3 1	145.60
.785	3	8 4 4	157.72

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
4.441	60	1 1 1	19.98
2.720	100	2 2 0	32.91
2.319	30	3 1 1	38.80
1.923	16	4 0 0	47.23
1.765	12	3 3 1	51.76
1.570	29	4 2 2	58.76
1.480	6	5 1 1	62.71
1.480	2	3 3 3	62.71
1.360	8	4 4 0	69.01
1.300	8	5 3 1	72.66
1.216	11	6 2 0	78.59
1.173	3	5 3 3	82.09
1.110	3	4 4 4	87.86
1.077	2	5 5 1	91.31
1.077	2	7 1 1	91.31
1.028	13	6 4 2	97.07
1.001	4	7 3 1	100.56
1.001	2	5 5 3	100.56
.961	1	8 0 0	106.47
.940	2	7 3 3	110.11
.907	6	8 2 2	116.36
.907	3	6 6 0	116.36
.888	3	7 5 1	120.28
.860	6	8 4 0	127.19
.844	4	7 5 3	131.66
.844	2	9 1 1	131.66
.820	7	6 6 4	139.90
.806	5	9 3 1	145.60
.785	13	8 4 4	157.72

Additional patterns

1. Zintl et al. [1934]

Reference

Zintl,E., A.Harder, and B.Dauth (1934). Z. Electrochem. 40, 588.

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a=7.406(1)Å [ibid.]

Density

(calculated) 1.803 g/cm^3

Thermal parameters

Isotropic: K 1.0
S 0.6

Scattering factors

K^+, S^{2-} [3.3.1A]

Scale factors

(integrated intensities) 5.624×10^4

Additional patterns

1. PDF card 2-989 [Zintl et al., 1934]

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
4.275	32	1 1 1	20.76
3.702	25	2 0 0	24.02
2.618	100	2 2 0	34.22
2.233	9	3 1 1	40.36
2.138	6	2 2 2	42.24
1.852	12	4 0 0	49.16
1.699	3	3 3 1	53.92
1.656	5	4 2 0	55.44
1.512	20	4 2 2	61.26
1.425	2	5 1 1	65.42
1.309	5	4 4 0	72.08
1.252	2	5 3 1	75.96
1.234	1	4 4 2	77.22
1.171	6	6 2 0	82.26
1.069	1	4 4 4	92.20
1.037	1	7 1 1 +	95.94
.990	6	6 4 2	102.22
.964	1	7 3 1	106.06
.873	4	8 2 2 +	123.90
.855	1	7 5 1	128.50
.828	3	8 4 0	136.96
.813	1	7 5 3 +	142.72
.789	3	6 6 4	154.68

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
4.276	27	1 1 1	20.76
3.703	23	2 0 0	24.01
2.618	100	2 2 0	34.22
2.233	9	3 1 1	40.36
2.138	6	2 2 2	42.24
1.852	14	4 0 0	49.17
1.699	3	3 3 1	53.92
1.656	7	4 2 0	55.44
1.512	26	4 2 2	61.27
1.425	2	5 1 1	65.43
1.309	7	4 4 0	72.08
1.252	2	5 3 1	75.95
1.234	2	4 4 2	77.22
1.171	10	6 2 0	82.26
1.129	1	5 3 3	86.00
1.117	1	6 2 2	87.25
1.069	2	4 4 4	92.21
1.037	1	5 5 1	95.93
1.037	1	7 1 1	95.93
1.027	1	6 4 0	97.18
.990	13	6 4 2	102.21
.964	1	7 3 1	106.05
.926	1	8 0 0	112.62
.873	3	6 6 0	123.90
.873	6	8 2 2	123.90
.855	2	7 5 1	128.51
.828	7	8 4 0	136.95
.813	2	7 5 3	142.72
.813	1	9 1 1	142.72
.808	2	8 4 2	144.82
.789	12	6 6 4	154.67

Reference

Zintl,E., A.Harder, and B.Dauth (1934). Z. Electrochem. 40, 588.

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a=8.168(3)Å [ibid.]

Density

(calculated) 2.508 g/cm^3

Thermal parameters

Isotropic: K 1.0
Te 0.6

Scattering factors

K^+ [3.3.1A]
Te^0 [3.3.1B]

Scale factors

(integrated intensities) 24.62×10^4

Additional patterns

1. Zintl et al. [1934]

Reference

Zintl,E., A.Harder, and B.Dauth (1934). Z. Electrochem. 40, 588.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
4.716	98	1	1	1		18.80
4.085	5	2	0	0		21.74
2.888	100	2	2	0		30.94
2.462	42	3	1	1		36.46
2.358	2	2	2	2		38.14
2.042	15	4	0	0		44.32
1.874	16	3	3	1		48.54
1.827	2	4	2	0		49.88
1.667	25	4	2	2		55.04
1.572	11	5	1	1	+	58.68
1.444	7	4	4	0		64.48
1.381	9	5	3	1		67.82
1.361	1	4	4	2		68.92
1.291	8	6	2	0		73.24
1.246	3	5	3	3		76.40
1.179	2	4	4	4		81.60
1.144	4	7	1	1	+	84.68
1.091	8	6	4	2		89.78
1.063	5	7	3	1	+	92.84
1.021	1	8	0	0		97.96
.998	1	7	3	3		101.06
.963	4	8	2	2	+	106.30
.943	2	7	5	1	+	109.52
.913	2	8	4	0		115.02
.897	3	7	5	3	+	118.44
.871	2	6	6	4		124.42
.856	2	9	3	1		128.22
.834	2	8	4	4		135.04
.821	3	9	3	3	+	139.54
.801	7	8	6	2	+	148.20
.790	3	9	5	1	+	154.58

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
4.716	85	1 1 1	18.80
4.084	5	2 0 0	21.74
2.888	100	2 2 0	30.94
2.463	46	3 1 1	36.45
2.358	2	2 2 2	38.13
2.042	17	4 0 0	44.32
1.874	19	3 3 1	48.54
1.826	3	4 2 0	49.89
1.667	32	4 2 2	55.03
1.572	11	5 1 1	58.68
1.572	4	3 3 3	58.68
1.444	9	4 4 0	64.48
1.381	13	5 3 1	67.82
1.361	1	4 4 2	68.92
1.291	12	6 2 0	73.23
1.246	5	5 3 3	76.40
1.231	1	6 2 2	77.44
1.179	3	4 4 4	81.59
1.144	3	5 5 1	84.67
1.144	3	7 1 1	84.67
1.133	1	6 4 0	85.69
1.091	14	6 4 2	89.77
1.063	6	7 3 1	92.63
1.063	3	5 5 3	92.83
1.021	1	8 0 0	97.95
.998	2	7 3 3	101.05
.963	5	8 2 2	106.30
.963	3	6 6 0	106.30
.943	5	7 5 1	109.51
.943	1	5 5 5	109.51
.913	5	8 4 0	115.02
.897	2	9 1 1	118.44
.897	5	7 5 3	118.44
.891	1	8 4 2	119.61
.871	6	6 6 4	124.42
.856	5	9 3 1	128.21
.834	6	8 4 4	135.03
.821	3	9 3 3	139.54
.821	3	7 7 1	139.54
.821	3	7 5 5	139.54
.817	1	8 6 0	141.14
.801	17	8 6 2	148.19
.801	9	10 2 0	148.19
.790	5	7 7 3	154.58
.790	10	9 5 1	154.58
.786	1	10 2 2	157.07

Sodium hydrogen phosphate, $Na_3H(PO_3)_4$

Structure
Monoclinic, $P2_1/n(14)$, Z=4. The structure was determined by Jost [1968].

Lattice parameters
a=11.32(3), b=9.95(2), c=8.73(2)Å, β=90.1(2)° [ibid.]

Density
(calculated) 2.606 g/cm^3

Thermal parameters
Isotropic [ibid.]

Scattering factors
Na^+, O^0, P^0 [3.3.1A]

Scale factors
(integrated intensities) 4.976×10^4

Additional patterns
1. PDF card 9-90 [Research Dept.,R and E Div., Monsanto Chemical Co., Dayton, Ohio]

Reference
Jost, K.H. (1968). Acta Cryst. B24, 992.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
7.47	2	1	1	0		11.84
6.91	6	-1	0	1	+	12.80
6.56	1	0	1	1		13.48
5.68	38	-1	1	1	+	15.60
4.97	84	0	2	0		17.82
4.92	12	2	1	0		18.02
4.55	1	1	2	0		19.48
4.28	8	2	1	1	+	20.72
4.04	21	1	2	1	+	22.00
4.00	23	0	1	2		22.22
3.77	1	1	1	2		23.60
3.74	10	2	2	0		23.80
3.46	33	3	0	1	+	25.72
3.45	35	2	0	2		25.78
3.44	16	-2	2	1		25.90
3.27	100	-2	1	2	+	27.26
3.18	44	1	3	0		28.02
3.15	15	-1	2	2		28.28
3.01	3	3	2	0		29.70
2.99	8	-1	3	1		29.86
2.86	6	2	3	0		31.24
2.84	91	3	2	1	+	31.46
2.75	8	-3	1	2		32.58
2.71	19	1	1	3	+	33.02
2.64	1	0	3	2		33.92
2.60	5	4	1	1		34.50
2.50	3	2	1	3	+	35.84
2.48	9	-3	2	2		36.22
2.45	12	1	2	3	+	36.62
2.39	4	-2	3	2	+	37.54
2.37	9	4	2	1		37.98
2.34	2	1	4	1	+	38.42
2.31	6	-3	0	3		39.02
2.30	5	3	0	3		39.10
2.30	6	2	2	3		39.22
2.25	5	-3	1	3	+	40.10
2.21	2	5	1	0		40.84
2.20	3	2	4	1	+	40.92
2.19	6	-5	0	1	+	41.14
2.19	4	0	0	4		41.26
2.16	1	-3	3	2		41.70
2.14	3	5	1	1		42.20
2.13	4	0	1	4		42.36
2.12	5	-1	4	2		42.54
2.09	8	3	2	3	+	43.26
2.04	2	-2	0	4	+	44.42
2.02	6	-2	4	2		44.84
1.99	2	2	1	4		45.46
1.99	3	4	1	3		45.64
1.97	4	-1	2	4	+	46.06

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
1.96	4	1	5	0		46.28
1.91	1	-1	5	1		47.50
1.89	2	3	3	3	+	48.08
1.88	2	-4	2	3		48.38
1.87	3	3	4	2		48.52
1.87	3	4	4	0	+	48.68
1.86	6	1	4	3	+	48.80
1.85	1	6	1	0		49.10
1.83	6	5	3	1	+	49.84
1.81	5	-6	1	1		50.26
1.80	1	1	3	4		50.68
1.79	1	-2	4	3		50.84
1.79	5	5	0	3		51.12
1.77	1	-3	2	4		51.68
1.76	2	-5	1	3		51.90
1.74	1	-2	3	4	+	52.70
1.73	7	-1	0	5	+	53.02
1.70	4	-4	1	4	+	53.74
1.69	4	3	4	3	+	54.24
1.68	1	5	2	3		54.56
1.67	2	5	4	0		54.78
1.66	1	0	6	0		55.36
1.645	4	-5	4	1	+	55.86
1.641	5	0	4	4	+	56.00
1.636	3	-6	2	2		56.16
1.633	6	-3	5	2	+	56.30
1.630	5	1	2	5	+	56.42
1.623	3	1	4	4		56.66
1.612	1	-6	3	1	+	57.10
1.600	4	4	5	1		57.56
1.590	3	-7	0	1		57.94
1.583	1	3	0	5		58.22
1.577	3	2	5	3	+	58.46
1.573	4	-4	4	3		58.64
1.566	3	-2	6	1	+	58.94
1.564	3	3	1	5		59.02
1.562	3	6	1	3		59.08
1.553	1	-5	1	4		59.46
1.551	2	5	1	4		59.56
1.536	2	-1	6	2		60.20
1.509	1	3	2	5		61.38
1.506	2	3	5	3	+	61.54
1.500	1	-7	1	2		61.80
1.496	2	-2	6	2	+	62.00
1.473	2	-5	5	1	+	63.04
1.470	2	0	5	4		63.18
1.455	1	0	0	6		63.94
1.451	1	5	4	3		64.14
1.434	1	-3	6	2		64.98
1.428	2	6	3	3		65.30
1.426	3	6	0	4		65.38

Calculated Pattern *(Integrated)*

d (Å)	I	hkl			2θ(°) λ = 1.54056 Å
7.47	2	1	1	0	11.83
6.92	5	-1	0	1	12.78
6.91	2	1	0	1	12.81
6.56	1	0	1	1	13.48
5.68	42	-1	1	1	15.59
5.67	1	1	1	1	15.60
5.66	4	2	0	0	15.64
4.98	100	0	2	0	17.81
4.92	10	2	1	0	18.02
4.55	2	1	2	0	19.47
4.36	1	0	0	2	20.33
4.29	3	-2	1	1	20.69
4.28	8	2	1	1	20.72
4.04	12	-1	2	1	21.99
4.04	14	1	2	1	22.00
4.00	29	0	1	2	22.22
3.77	1	1	1	2	23.60
3.74	13	2	2	0	23.79
3.47	2	-3	0	1	25.68
3.46	28	3	0	1	25.72
3.46	8	-2	0	2	25.73
3.45	21	2	0	2	25.78
3.44	15	-2	2	1	25.90
3.28	4	0	2	2	27.16
3.27	16	-3	1	1	27.22
3.27	39	3	1	1	27.26
3.27	89	-2	1	2	27.27
3.26	12	2	1	2	27.31
3.18	62	1	3	0	28.01
3.15	19	-1	2	2	28.29
3.01	3	3	2	0	29.69
2.99	10	-1	3	1	29.85
2.86	4	2	3	0	31.23
2.84	78	3	2	1	31.46
2.84	38	-2	2	2	31.47
2.84	45	2	2	2	31.51
2.83	1	4	0	0	31.59
2.82	1	-1	0	3	31.71
2.75	11	-3	1	2	32.58
2.72	2	2	3	1	32.92
2.71	3	-1	1	3	32.99
2.71	24	1	1	3	33.02
2.64	1	0	3	2	33.92
2.60	7	4	1	1	34.50
2.51	2	-2	1	3	35.80
2.50	4	2	1	3	35.85
2.48	13	-3	2	2	36.23
2.46	1	4	2	0	36.50
2.45	1	-1	2	3	36.60
2.45	17	1	2	3	36.63

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.39	4	-2 3 2	37.54
2.39	2	0 4 1	37.57
2.37	13	4 2 1	37.99
2.34	1	-1 4 1	38.42
2.34	1	1 4 1	38.43
2.31	2	-4 1 2	38.93
2.31	6	-3 0 3	39.02
2.30	3	3 0 3	39.09
2.29	7	2 2 3	39.23
2.25	7	-3 1 3	40.10
2.24	1	3 1 3	40.17
2.21	2	5 1 0	40.84
2.20	1	-2 4 1	40.91
2.20	1	2 4 1	40.93
2.19	8	-5 0 1	41.14
2.19	2	5 0 1	41.17
2.18	1	0 0 4	41.33
2.16	2	-3 3 2	41.69
2.14	1	-4 2 2	42.10
2.14	3	5 1 1	42.21
2.13	6	0 1 4	42.36
2.12	7	-1 4 2	42.54
2.10	2	-1 1 4	43.13
2.09	3	1 1 4	43.16
2.09	3	-3 2 3	43.20
2.09	1	-4 3 1	43.23
2.09	2	4 3 1	43.26
2.09	5	3 2 3	43.26
2.04	2	2 3 3	44.38
2.04	2	-2 0 4	44.43
2.02	8	-2 4 2	44.84
1.99	3	2 1 4	45.45
1.99	4	4 1 3	45.64
1.97	3	-5 1 2	46.00
1.97	5	-1 2 4	46.07
1.96	5	1 5 0	46.28
1.91	2	-1 5 1	47.50
1.89	1	-3 3 3	48.01
1.89	2	3 3 3	48.07
1.89	1	0 4 3	48.08
1.88	3	-4 2 3	48.37
1.87	3	3 4 2	48.52
1.87	1	5 3 0	48.65
1.87	2	4 4 0	48.70
1.86	7	1 4 3	48.80
1.86	1	-5 2 2	48.80
1.85	1	6 1 0	49.11
1.83	1	-5 3 1	49.82
1.83	8	5 3 1	49.85
1.83	1	4 4 1	49.89

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.81	8	-6 1 1	50.26
1.80	1	1 3 4	50.69
1.79	1	-2 4 3	50.85
1.79	1	-1 5 2	51.03
1.79	8	5 0 3	51.12
1.77	1	-3 2 4	51.68
1.76	3	-5 1 3	51.90
1.74	1	-2 3 4	52.68
1.73	1	2 3 4	52.73
1.73	1	4 3 3	52.89
1.73	1	6 2 1	52.93
1.73	2	4 0 4	52.98
1.73	8	-1 0 5	53.01
1.73	1	3 5 1	53.04
1.71	1	-6 1 2	53.64
1.71	2	6 1 2	53.71
1.70	4	-4 1 4	53.74
1.69	4	-3 4 3	54.19
1.69	6	3 4 3	54.24
1.68	2	5 2 3	54.56
1.67	3	5 4 0	54.78
1.66	2	0 6 0	55.35
1.64_6	3	-2 1 5	55.80
1.645	4	-5 4 1	55.85
1.644	1	5 4 1	55.88
1.643	1	0 5 3	55.93
1.643	1	-3 3 4	55.93
1.641	4	0 4 4	56.01
1.636	1	-6 2 2	56.16
1.634	3	-4 2 4	56.26
1.633	5	-3 5 2	56.29
1.632	3	3 5 2	56.33
1.631	1	-1 2 5	56.38
1.630	2	1 2 5	56.40
1.629	1	0 6 1	56.43
1.623	4	1 4 4	56.66
1.612	1	-6 3 1	57.08
1.611	1	6 3 1	57.12
1.600	6	4 5 1	57.56
1.591	4	-7 0 1	57.93
1.584	1	3 0 5	58.21
1.578	1	-2 5 3	58.44
1.577	3	2 5 3	58.47
1.573	5	-4 4 3	58.64
1.566	1	-3 1 5	58.93
1.566	4	-2 6 1	58.94
1.564	3	3 1 5	59.02
1.562	1	6 1 3	59.09
1.553	1	-5 1 4	59.46
1.551	3	5 1 4	59.57

d (Å)	I	hkl	$2\theta(^\circ)$ $\lambda = 1.54056$ Å
1.536	4	-1 6 2	60.20
1.509	1	3 2 5	61.39
1.506	1	3 5 3	61.54
1.505	1	-3 4 4	61.56
1.500	1	-7 1 2	61.80
1.496	1	3 6 1	62.00
1.495	2	-2 6 2	62.01
1.474	2	-5 5 1	63.03
1.473	2	5 5 1	63.06
1.471	2	0 5 4	63.18
1.458	1	1 5 4	63.78
1.455	2	0 0 6	63.93
1.450	1	5 4 3	64.15
1.434	1	-3 6 2	64.97
1.428	2	6 3 3	65.30
1.426	4	6 0 4	65.39

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2) . The structure was determined by Zintl and Baumbach [1931].

Lattice parameters

a = 5.56Å [ibid.]

Density

(calculated) 2.39 g/cm^3 [ibid.]

Thermal parameters

Isotropic; overall B = 2.0

Scattering factors

Na^+ [3.3.1A]
O^{2-} [Suzuki, 1960]

Scale factors

(integrated intensities) 0.6209×10^4

Additional patterns

1. PDF card 3-1074 [Mathews, F.W., Canadian Industries Limited]
2. Zintl and Baumbach [1931]

Reference

Suzuki, T. (1960). Acta Cryst. 13, 279.
Zintl, E. and H.H.von Baumbach (1931). Z. anorg. u. allgem. Chem. 198, 88.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.21	33	1 1 1	27.76
2.78	41	2 0 0	32.18
1.966	100	2 2 0	46.14
1.677	5	3 1 1	54.70
1.605	7	2 2 2	57.36
1.390	8	4 0 0	67.30
1.275	1	3 3 1	74.30
1.243	5	4 2 0	76.56
1.135	9	4 2 2	85.48
.983	2	4 4 0	103.20
.927	1	4 4 2	112.46
.879	2	6 2 0	122.38

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.21	29	1 1 1	27.77
2.78	37	2 0 0	32.17
1.966	100	2 2 0	46.14
1.676	5	3 1 1	54.71
1.605	8	2 2 2	57.36
1.390	10	4 0 0	67.31
1.276	1	3 3 1	74.30
1.243	7	4 2 0	76.57
1.135	14	4 2 2	85.48
.983	4	4 4 0	103.20
.927	2	4 4 2	112.45
.879	5	6 2 0	122.37
.838	2	6 2 2	133.55
.803	2	4 4 4	147.41

Sodium selenide, Na_2Se

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a=6.823Å [ibid.]

Density

(calculated) 2.612 g/cm^3

Thermal parameters

Isotropic: Na 1.0
Se 0.6

Scattering factors

Na^+ [3.3.1A]
Se^0 [3.3.1B]

Scale factors

(integrated intensities) 5.559×10^4

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
3.938	100	1 1 1	22.56
3.411	7	2 0 0	26.10
2.412	86	2 2 0	37.24
2.057	37	3 1 1	43.96
1.970	2	2 2 2	46.04
1.705	11	4 0 0	53.70
1.565	12	3 3 1	58.96
1.526	2	4 2 0	60.64
1.393	18	4 2 2	67.16
1.313	7	5 1 1 +	71.84
1.206	4	4 4 0	79.38
1.153	6	5 3 1	83.80
1.137	1	4 4 2	85.28
1.079	5	6 2 0	91.12
1.040	2	5 3 3	95.52
.985	1	4 4 4	102.92
.955	3	7 1 1 +	107.46
.912	6	6 4 2	115.30
.888	4	7 3 1 +	120.26
.853	1	8 0 0	129.16
.834	1	7 3 3	135.06
.827	1	8 2 0 +	137.16
.804	4	8 2 2 +	146.64
.788	4	7 5 1 +	155.76

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
3.939	100	1 1 1	22.55
3.412	7	2 0 0	26.10
2.412	100	2 2 0	37.24
2.057	46	3 1 1	43.98
1.970	2	2 2 2	46.04
1.706	15	4 0 0	53.69
1.565	17	3 3 1	58.96
1.526	3	4 2 0	60.65
1.393	27	4 2 2	67.16
1.313	9	5 1 1	71.83
1.313	3	3 3 3	71.83
1.206	8	4 4 0	79.38
1.153	11	5 3 1	83.81
1.137	1	4 4 2	85.28
1.079	10	6 2 0	91.12
1.040	4	5 3 3	95.51
1.029	1	6 2 2	96.98
.985	3	4 4 4	102.92
.955	4	7 1 1	107.46
.955	4	5 5 1	107.46
.946	1	6 4 0	109.00
.912	15	6 4 2	115.31
.888	8	7 3 1	120.26
.888	4	5 5 3	120.26
.853	2	8 0 0	129.15
.834	4	7 3 3	135.06
.827	2	8 2 0	137.17
.827	2	6 4 4	137.17
.804	6	6 6 0	146.65
.804	11	8 2 2	146.65
.788	15	7 5 1	155.75
.788	3	5 5 5	155.75
.783	3	6 6 2	159.60

Additional patterns

1. Zintl et al. [1934]

Reference

Zintl,E., A.Harder, and B.Dauth (1934). Z. Electrochem. 40, 588.

Structure

Monoclinic, $P2_1/c$ (14), Z=4. The structure was determined by Grund [1954]. It was refined by Pant [1968] who published his data in terms of the $P2_1/a$ cell with a=12.329(4), b=4.848(4), c=8.133(3)Å, and β=104.24(4).

Lattice parameters

a=8.133(3), b=4.848(4), c=12.329(4)Å
β=104.24(4)°

Density

(calculated) 2.568 g/cm^3

Thermal parameters

Isotropic:sodium(1) B=1.014; sodium(2) B=1.045; silicon(1) B=0.438; silicon(2) B=0.428; oxygen(1) B=0.777; oxygen(2) B=0.756; oxygen(3) B=0.755; oxygen(4) B=0.837; oxygen(5) B=0.773

Polymorphism

At one bar pressure, sodium disilicate glass can be crystallized to yield six crystalline polymorphs. The beta phase described here occurs over the range 610 to 700°C. [Pant,1968]

Scattering factors

O^0, Na^0, Si^0 [3.3.1A]

Scale factors

(integrated intensities) 1.1764×10^4

Additional patterns

1. PDF card 18-1243 [K.J. Range and A.W. Willgallis, Mineralogisches Institut, Freie Universität, Berlin, Germany]
2. Donnay and Donnay [1953]

References

Donnay,G. and J.D.H. Donnay (1953). Am. Mineralogist 38, 163.
Grund,A.(1954). Bull. Soc. Franc. Mineral. Crist. 77, 775.
Pant, A.K. (1968). Acta Cryst. B24, 1077.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(^\circ)$ $\lambda = 1.54056$ Å
7.88	9	1	0	0		11.22
5.97	87	0	0	2		14.82
5.45	10	-1	0	2		16.26
4.494	2	0	1	1		19.74
4.279	31	1	0	2		20.74
4.130	71	1	1	0		21.50
3.941	87	2	0	0		22.54
3.764	26	0	1	2	+	23.62
3.622	96	-1	1	2		24.56
3.108	18	-2	1	1		28.70
3.079	19	0	1	3		28.98
3.054	43	-1	0	4	+	29.22
2.988	29	0	0	4		29.88
2.970	63	2	0	2		30.06
2.963	50	-2	1	2		30.14
2.836	2	2	1	1		31.52
2.725	1	-2	0	4		32.84
2.698	8	1	1	3		33.18
2.685	20	-2	1	3		33.34
2.659	45	-3	0	2		33.68
2.627	7	3	0	0		34.10
2.590	17	1	0	4		34.60
2.584	29	-1	1	4		34.68
2.534	19	2	1	2		35.40
2.424	100	0	2	0		37.06
2.376	2	0	2	1		37.84
2.331	9	-3	1	2		38.60
2.285	5	1	1	4		39.40
2.270	9	-3	0	4		39.68
2.214	3	-1	2	2	+	40.72
2.182	2	3	1	1		41.34
2.141	13	2	0	4	+	42.18
2.109	5	1	2	2		42.84
2.086	8	-2	1	5		43.34
2.081	6	-2	2	1		43.46
2.069	3	-1	2	3	+	43.72
2.064	4	2	2	0		43.82
2.055	3	-1	0	6	+	44.02
2.034	2	-2	2	2		44.50
2.026	7	-4	0	2		44.70
1.992	1	0	0	6		45.50
1.971	3	4	0	0		46.02
1.958	3	2	1	4		46.32
1.898	10	-1	2	4		47.88
1.893	7	-1	1	6		48.02
1.882	4	0	2	4		48.32
1.878	7	2	2	2		48.42
1.870	13	-4	0	4	+	48.66
1.837	7	-2	1	6		49.58
1.833	6	3	1	3		49.70

Sodium silicate, beta $Na_2Si_2O_5$ – continued

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.827	19	1 0 6 +	49.86
1.817	7	-3 0 6	50.16
1.812	5	-2 2 4	50.32
1.791	16	-3 2 2	50.94
1.782	2	3 2 0	51.22
1.770	8	1 2 4	51.60
1.748	12	4 0 2	52.30
1.744	11	-4 1 4	52.42
1.738	4	-3 2 3	52.60
1.727	2	-1 2 5	52.98
1.710	1	1 1 6	53.56
1.662	2	3 1 4	55.22
1.657	4	-3 2 4	55.42
1.643	1	-4 1 5 +	55.92
1.634	1	3 2 2	56.24
1.629	1	-2 1 7	56.44
1.624	2	2 0 6	56.62
1.613	8	-4 0 6	57.04
1.610	5	0 1 7	57.18
1.605	2	2 2 4	57.36
1.583	2	1 3 0	58.24
1.576	6	5 0 0	58.50
1.559	4	-3 2 5	59.24
1.555	5	-4 2 2	59.40
1.549	4	-1 3 2	59.62
1.540	4	2 1 6 +	60.02
1.529	6	4 2 0	60.50
1.527	6	-2 0 8	60.60
1.506	2	3 1 5	61.52
1.501	5	-2 3 1	61.76
1.497	7	0 3 3	61.92
1.494	5	0 0 8	62.08
1.487	2	-5 1 4	62.42
1.483	4	-2 3 2	62.58
1.481	4	-4 2 4 +	62.70
1.471	1	2 2 5	63.14
1.467	3	-1 1 8	63.36
1.459	8	1 2 6	63.74
1.456	7	-2 1 8	63.90
1.454	7	-3 2 6	63.98
1.447	4	1 3 3	64.34
1.445	6	-2 3 3	64.44
1.440	7	5 0 2	64.70
1.428	6	-1 3 4 +	65.30
1.424	5	-1 2 7	65.48
1.420	7	4 1 4 +	65.68
1.418	7	4 2 2	65.82
1.406	2	1 0 8	66.46
1.396	1	0 2 7	66.98
1.381	2	-3 3 2	67.82

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.371	1	1 3 4	68.36
1.369	1	3 1 6	68.48
1.363	1	-4 0 8	68.84
1.350	1	-3 2 7	69.58
1.348	1	3 3 1	69.72
1.343	5	-4 2 6 +	70.00
1.339	4	0 3 5 +	70.24
1.329	2	-6 0 4 +	70.84
1.325	4	-2 3 5	71.12
1.322	4	5 2 0	71.30
1.305	4	-6 1 2	72.34
1.295	1	2 0 8	72.98
1.292	3	-2 2 8	73.20
1.272	2	0 2 8 +	74.56
1.263	3	-4 3 1	75.14
1.252	2	3 3 3 +	75.92
1.249	3	-4 3 3 +	76.12
1.247	3	-6 0 6	76.32
1.238	3	5 2 2	76.98
1.230	1	3 2 6	77.56
1.215	1	4 1 6 +	78.70
1.212	2	0 4 0	78.92
1.209	8	-5 1 8 +	79.16
1.196	2	-1 4 1	80.16
1.193	1	3 3 4	80.42
1.190	3	-1 1 10	80.70
1.188	3	0 4 2 +	80.86
1.185	3	6 1 2	81.12
1.180	2	3 0 8	81.50
1.174	1	0 3 7	82.04
1.170	2	-3 1 10	82.38
1.166	1	-6 2 4	82.66
1.160	5	0 1 10	83.20
1.156	2	-4 0 10 +	83.60
1.153	2	-2 4 2	83.84
1.146	4	3 1 8 +	84.44
1.141	2	1 0 10	84.94
1.140	2	-5 3 3	85.04
1.136	1	1 4 3	85.42
1.132	2	3 3 5	85.80
1.128	2	-7 1 2	86.12

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.88	6	1 0 0	11.21
5.98	66	0 0 2	14.81
5.45	8	-1 0 2	16.25
4.492	1	0 1 1	19.75
4.282	27	1 0 2	20.73
4.130	60	1 1 0	21.50
3.942	74	2 0 0	22.54
3.765	22	0 1 2	23.61
3.757	2	1 1 1	23.66
3.740	1	-2 0 2	23.77
3.623	85	-1 1 2	24.55
3.109	16	-2 1 1	28.69
3.078	17	0 1 3	28.99
3.058	1	2 1 0	29.18
3.054	38	-1 0 4	29.22
2.988	24	0 0 4	29.88
2.971	57	2 0 2	30.05
2.961	19	-2 1 2	30.15
2.836	2	2 1 1	31.52
2.725	1	-2 0 4	32.83
2.698	6	1 1 3	33.17
2.686	19	-2 1 3	33.33
2.658	45	-3 0 2	33.69
2.628	6	3 0 0	34.09
2.590	13	1 0 4	34.60
2.584	22	-1 1 4	34.69
2.533	18	2 1 2	35.40
2.424	100	0 2 0	37.06
2.376	1	0 2 1	37.84
2.331	9	-3 1 2	38.59
2.285	5	1 1 4	39.41
2.269	9	-3 0 4	39.69
2.215	2	-1 2 2	40.70
2.213	2	3 0 2	40.74
2.182	2	3 1 1	41.34
2.144	6	0 1 5	42.12
2.141	11	2 0 4	42.18
2.109	5	1 2 2	42.84
2.086	8	-2 1 5	43.33
2.080	2	-2 2 1	43.47
2.071	1	0 2 3	43.68
2.069	2	-1 2 3	43.72
2.065	3	2 2 0	43.81
2.055	1	-3 1 4	44.02
2.055	3	-1 0 6	44.03
2.034	2	-2 2 2	44.50
2.026	7	-4 0 2	44.70
1.992	1	0 0 6	45.50
1.971	4	4 0 0	46.01
1.958	3	2 1 4	46.32
1.899	11	-1 2 4	47.87
1.892	5	-1 1 6	48.05
1.862	3	0 2 4	48.31
1.878	6	2 2 2	48.42
1.870	5	-4 0 4	48.65
1.869	5	-4 1 1	48.67
1.869	5	-4 1 2	48.68
1.837	6	-2 1 6	49.58
1.834	2	3 1 3	49.68
1.827	19	1 0 6	49.87
1.826	2	4 1 0	49.91
1.825	4	-4 1 3	49.94
1.817	7	-3 0 6	50.17
1.811	1	-2 2 4	50.34
1.791	18	-3 2 2	50.94
1.782	1	3 2 0	51.23
1.770	9	1 2 4	51.60
1.748	14	4 0 2	52.29
1.745	5	-4 1 4	52.40
1.738	3	-3 2 3	52.61
1.727	1	-1 2 5	52.97
1.710	1	1 1 6	53.55
1.662	2	3 1 4	55.23
1.657	4	-3 2 4	55.42
1.644	1	4 1 2	55.86
1.643	1	-4 1 5	55.93
1.634	1	3 2 2	56.24
1.629	1	-2 1 7	56.45
1.624	2	2 0 6	56.63
1.613	9	-4 0 6	57.04
1.610	2	0 1 7	57.16
1.605	1	2 2 4	57.38
1.583	2	1 3 0	58.23
1.577	7	5 0 0	58.49
1.558	4	-3 2 5	59.24
1.554	3	-4 2 2	59.41
1.549	4	-1 3 2	59.63
1.542	1	-5 1 2	59.94
1.540	4	2 1 6	60.03
1.539	1	-1 0 8	60.09
1.529	6	4 2 0	60.49
1.527	5	-2 0 8	60.60
1.506	2	3 1 5	61.51
1.501	5	-2 3 1	61.75
1.497	6	0 3 3	61.91
1.494	3	0 0 8	62.08
1.487	1	-5 1 4	62.41
1.483	3	-2 3 2	62.56
1.482	1	4 2 1	62.65
1.481	3	-4 2 4	62.70

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.471	1	2 2 5	63.13
1.466	3	-1 1 8	63.37
1.459	9	1 2 6	63.73
1.456	3	-2 1 8	63.87
1.454	6	-3 2 6	63.99
1.447	3	1 3 3	64.33
1.445	7	-2 3 3	64.43
1.440	7	5 0 2	64.70
1.428	4	-1 3 4	65.27
1.428	2	0 1 8	65.31
1.427	2	3 0 6	65.33
1.424	2	-1 2 7	65.47
1.420	6	4 1 4	65.68
1.420	2	2 3 2	65.72
1.418	5	4 2 2	65.81
1.406	2	1 0 8	66.45
1.396	1	0 2 7	66.99
1.381	3	-3 3 2	67.81
1.371	1	1 3 4	68.36
1.369	1	3 1 6	68.47
1.363	1	-4 0 8	68.84
1.350	1	-3 2 7	69.56
1.348	1	3 3 1	69.71
1.344	1	4 2 3	69.92
1.344	1	-5 2 1	69.92
1.343	5	-4 2 6	70.00
1.340	1	-5 2 3	70.19
1.339	3	0 3 5	70.25
1.329	1	1 2 7	70.83
1.329	2	-6 0 4	70.83
1.324	4	-2 3 5	71.13
1.322	4	5 2 0	71.30
1.305	5	-6 1 2	72.35
1.295	1	2 0 8	72.98
1.292	3	-2 2 8	73.20
1.273	1	-5 2 5	74.46
1.272	3	0 2 8	74.56
1.263	4	-4 3 1	75.13
1.253	1	-2 3 6	75.85
1.252	2	3 3 3	75.93
1.250	1	4 3 0	76.11
1.249	2	-4 3 3	76.13
1.247	2	-6 0 6	76.32
1.238	5	5 2 2	76.97
1.230	1	3 2 6	77.56
1.216	1	1 2 8	78.61
1.215	1	4 1 6	78.69
1.212	1	0 4 0	78.92
1.209	1	-5 1 8	79.15
1.207	1	-3 3 6	79.27

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.196	2	-1 4 1	80.16
1.193	1	3 3 4	80.42
1.190	3	-1 1 10	80.71
1.188	2	0 4 2	80.86
1.188	1	1 4 1	80.88
1.185	3	6 1 2	81.11
1.180	2	3 0 8	81.51
1.174	1	0 3 7	82.04
1.170	3	-3 1 10	82.38
1.165	1	-6 2 4	82.74
1.160	7	0 1 10	83.19
1.156	1	-4 0 10	83.60
1.154	1	5 1 5	83.72
1.153	1	-2 4 2	83.84
1.146	4	3 1 8	84.43
1.146	1	-5 3 2	84.44
1.146	1	2 3 6	84.51
1.141	1	1 0 10	84.95
1.140	1	-5 3 3	85.04
1.136	1	1 4 3	85.43
1.131	2	3 3 5	85.81
1.128	2	-7 1 2	86.14

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a=6.539(2)Å [ibid.]

Density

(calculated) 1.854 g/cm^3

Thermal parameters

Isotropic: Na 1.0
S 0.6

Scattering factors

Na^+, S^{2-} [3.3.1A]

Scale factors

(integrated intensities) 1.930×10^4

Additional patterns

1. PDF card 3-933 [Zintl et al., 1934]

Reference

Zintl,E., A.Harder, and B.Dauth (1934). Z. Electrochem. 40, 588.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
3.776	62	1	1	1	23.54
3.269	5	2	0	0	27.26
2.312	100	2	2	0	38.92
1.971	16	3	1	1	46.00
1.888	1	2	2	2	48.16
1.635	12	4	0	0	56.22
1.500	5	3	3	1	61.80
1.462	1	4	2	0	63.58
1.335	18	4	2	2	70.50
1.258	3	5	1	1 +	75.48
1.156	5	4	4	0	83.58
1.105	3	5	3	1	88.36
1.034	6	6	2	0	96.32
.997	1	5	3	3	101.14
.944	1	4	4	4	109.40
.916	2	7	1	1 +	114.54
.874	7	6	4	2	123.66
.851	3	7	3	1 +	129.60
.817	1	8	0	0	140.92
.799	1	7	3	3	149.26

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
3.775	54	1	1	1	23.55
3.269	4	2	0	0	27.25
2.312	100	2	2	0	38.92
1.972	17	3	1	1	46.00
1.888	2	2	2	2	48.17
1.635	14	4	0	0	56.22
1.500	7	3	3	1	61.79
1.462	1	4	2	0	63.58
1.335	25	4	2	2	70.49
1.258	4	5	1	1	75.48
1.258	1	3	3	3	75.48
1.156	7	4	4	0	83.57
1.105	5	5	3	1	88.36
1.034	10	6	2	0	96.32
.997	2	5	3	3	101.15
.944	3	4	4	4	109.40
.916	2	5	5	1	114.54
.916	2	7	1	1	114.54
.874	16	6	4	2	123.65
.851	5	7	3	1	129.60
.851	2	5	5	3	129.60
.817	3	8	0	0	140.91
.799	3	7	3	3	149.25

Structure

Cubic, Fm3m (225), Z=4, isostructural with fluorite (CaF_2). The structure was determined by Zintl et al. [1934].

Lattice parameters

a=7.329(3)Å [ibid.]

Density

(calculated) 2.928 g/cm^3

Thermal parameters

Isotropic: Na 1.0
Te 0.6

Scattering factors

Na^+ [3.3.1A]
Te^0 [3.3.1B]

Scale factors

(integrated intensities) 12.74×10^4

Additional patterns

1. Zintl et al. [1934]

Reference

Zintl,E., A.Harder, and B.Dauth (1934). Z. Electrochem. 40, 588.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ*(°) λ = 1.54056 Å
4.231	100	1 1 1	20.96
3.663	17	2 0 0	24.28
2.592	65	2 2 0	34.58
2.210	41	3 1 1	40.80
2.116	4	2 2 2	42.70
1.832	10	4 0 0	49.72
1.681	14	3 3 1	54.54
1.639	5	4 2 0	56.08
1.496	16	4 2 2	61.96
1.411	9	5 1 1 +	66.20
1.296	4	4 4 0	72.96
1.239	8	5 3 1	76.90
1.222	2	4 4 2 +	76.18
1.159	5	6 2 0	83.32
1.118	2	5 3 3	87.14
1.105	1	6 2 2	88.40
1.058	1	4 4 4	93.46
1.026	4	7 1 1 +	97.28
1.016	1	6 4 0	98.56
.979	5	6 4 2	103.72
.954	4	7 3 1 +	107.66
.895	1	7 3 3	118.70
.889	1	8 2 0 +	120.16
.864	3	8 2 2 +	126.20
.846	3	7 5 1 +	131.06
.841	1	6 6 2	132.76
.819	2	8 4 0	140.12
.804	4	7 5 3 +	146.48
.800	2	8 4 2	148.84

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
4.231	100	1 1 1	20.98
3.664	19	2 0 0	24.27
2.591	79	2 2 0	34.59
2.210	50	3 1 1	40.80
2.116	6	2 2 2	42.70
1.832	13	4 0 0	49.72
1.681	20	3 3 1	54.53
1.639	8	4 2 0	56.07
1.496	25	4 2 2	61.98
1.410	11	5 1 1	66.20
1.410	4	3 3 3	66.20
1.296	7	4 4 0	72.96
1.239	14	5 3 1	76.89
1.221	1	6 0 0	78.19
1.221	3	4 4 2	78.19
1.159	9	6 2 0	83.32
1.118	5	5 3 3	87.13
1.105	2	6 2 2	88.40
1.058	2	4 4 4	93.46
1.026	4	5 5 1	97.28
1.026	4	7 1 1	97.28
1.016	2	6 4 0	98.56
.979	12	6 4 2	103.72
.954	7	7 3 1	107.66
.954	4	5 5 3	107.66
.916	1	8 0 0	114.45
.895	4	7 3 3	118.70
.889	2	8 2 0	120.15
.889	2	6 4 4	120.15
.864	3	6 6 0	126.20
.864	6	8 2 2	126.20
.846	8	7 5 1	131.06
.846	1	5 5 5	131.06
.841	2	6 6 2	132.77
.819	7	8 4 0	140.12
.804	11	7 5 3	146.48
.804	6	9 1 1	146.48
.800	7	8 4 2	148.84

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

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4—Acetyl—2′—fluorobiphenyl, $C_{14}H_{11}OF$	8m	91
L-Alanine, $C_3H_7O_2N$	8m	93
Aluminum, Al	1	11
Aluminum antimony, AlSb	4	72
Aluminum calcium sulfate hydrate (ettringite), $Al_2O_3 \cdot 6CaO \cdot 3SO_3 \cdot 31H_2O$	8	3
Aluminum chloride, $AlCl_3$	9m	61
Aluminum chloride hexahydrate (chloraluminite), $AlCl_3 \cdot 6H_2O$	7	3
Aluminum fluosilicate, topaz, $Al_2SiO_4(F,OH)_2$	1m	4
Aluminum metaphosphate, $Al(PO_3)_3$	2m	3
Aluminum nickel, AlNi	6m	82
Aluminum orthophosphate (berlinite), $AlPO_4$ (trigonal)	10	3
Aluminum orthophosphate, $AlPO_4$ (orthorhombic)	10	4
Aluminum oxide, (corundum), alpha Al_2O_3	9	3
Aluminum oxide monohydrate (böhmite), alpha $Al_2O_3 \cdot H_2O$	3	38
Aluminum oxide monohydrate, diaspore, beta $Al_2O_3 \cdot H_2O$	3	41
Aluminum silicate (mullite) $3Al_2O_3 \cdot 2SiO_2$	3m	3
Ammonium acetate, $NH_4 \cdot CH_3CO_2$	8m	95
Ammonium aluminum fluoride, $(NH_4)_3AlF_6$	9m	5
Ammonium aluminum selenate hydrate, $NH_4Al(SeO_4)_2 \cdot 12H_2O$	9m	6
Ammonium aluminum sulfate, $NH_4Al(SO_4)_2$	10m	5
Ammonium aluminum sulfate dodecahydrate (tschermigite), $NH_4Al(SO_4)_2 \cdot 12H_2O$	6	3
Ammonium azide, NH_4N_3	9	4
Ammonium bicarbonate (teschemacherite), $(NH_4)HCO_3$	9	5
Ammonium bromide, NH_4Br	2	49
Ammonium bromoosmate, $(NH_4)_2OsBr_6$	3	71
Ammonium bromoplatinate, $(NH_4)_2PtBr_6$	9	6
Ammonium bromoselenate, $(NH_4)_2SeBr_6$	8	4
Ammonium bromotellurate, $(NH_4)_2TeBr_6$	8	5
Ammonium cadmium sulfate, $(NH_4)_2Cd_2(SO_4)_3$	7m	5
Ammonium cadmium sulfate hydrate, $(NH_4)_2Cd(SO_4)_2 \cdot 6H_2O$	8m	5
Ammonium cadmium trichloride, NH_4CdCl_3	5m	6
Ammonium calcium sulfate, $(NH_4)_2Ca_2(SO_4)_3$	8m	7
Ammonium chloride (sal-ammoniac), NH_4Cl	1	59
Ammonium chloroiridate, $(NH_4)_2IrCl_6$	8	6
Ammonium chloroosmate, $(NH_4)_2OsCl_6$	1m	6
Ammonium chloropalladate, $(NH_4)_2PdCl_6$	8	7
Ammonium chloropalladite, $(NH_4)_2PdCl_4$	6	6
Ammonium chloroplatinate, $(NH_4)_2PtCl_6$	5	3
Ammonium chlorostannate $(NH_4)_2SnCl_6$	5	4
Ammonium chlorotellurate, $(NH_4)_2TeCl_6$	8	8
Ammonium chromium sulfate dodecahydrate, $NH_4Cr(SO_4)_2 \cdot 12H_2O$	6	7
Ammonium cobalt fluoride, NH_4CoF_3	8m	9
Ammonium cobalt (II) trichloride, NH_4CoCl_3	6m	5
Ammonium copper bromide hydrate, $(NH_4)_2CuBr_4 \cdot 2H_2O$	10m	6
Ammonium copper chloride, NH_4CuCl_3	7m	7
Ammonium copper chloride hydrate, $(NH_4)_2CuCl_4 \cdot 2H_2O$	9m	8
Ammonium dihydrogen phosphate, $NH_4H_2PO_4$	4	64
Ammonium fluoberyllate, $(NH_4)_2BeF_4$	3m	5
Ammonium fluoborate, NH_4BF_4	3m	6
Ammonium fluogermanate, $(NH_4)_2GeF_6$	6	8
Ammonium fluosilicate (cryptohalite), $(NH_4)_2SiF_6$	5	5
Ammonium gallium sulfate dodecahydrate, $NH_4Ga(SO_4)_2 \cdot 12H_2O$	6	9
Ammonium iodate, NH_4IO_3	10m	7
Ammonium iodide, NH_4I	4	56
Ammonium iron fluoride, $(NH_4)_3FeF_6$	9m	9
Ammonium iron sulfate, $NH_4Fe(SO_4)_2$	10m	8
Ammonium iron sulfate dodecahydrate, $NH_4Fe(SO_4)_2 \cdot 12H_2O$	6	10
Ammonium magnesium aluminum fluoride, NH_4MgAlF_6	10m	9
Ammonium magnesium chromium oxide hydrate, $(NH_4)_2Mg(CrO_4)_2 \cdot 6H_2O$	8m	10
Ammonium manganese sulfate, $(NH_4)_2Mn_2(SO_4)_3$	7m	8
Ammonium manganese sulfate hydrate, $(NH_4)_2Mn(SO_4)_2 \cdot 6H_2O$	8m	12
Ammonium manganese(II) trifluoride, NH_4MnF_3	5m	8
Ammonium mercury chloride, NH_4HgCl_3 (revised)	8m	14
Ammonium metavanadate, NH_4VO_3	8	9
Ammonium nickel chromium oxide hydrate, $(NH_4)_2Ni(CrO_4)_2 \cdot 6H_2O$	8m	16
Ammonium nickel (II) trichloride, NH_4NiCl_3	6m	6
Ammonium nitrate (ammonia-niter), NH_4NO_3	7	4
Ammonium oxalate monohydrate (oxammite), $(NH_4)_2C_2O_4 \cdot H_2O$	7	5
Ammonium perchlorate, NH_4ClO_4 (orthorhombic)	7	6
Ammonium perrhenate, NH_4ReO_4	9	7
Ammonium phosphomolybdate tetrahydrate, $(NH_4)_3PO_4(MoO_3)_{12} \cdot 4H_2O$	8	10
Ammonium sulfate (mascagnite), $(NH_4)_2SO_4$ (revised)	9	8
Ammonium yttrium oxalate hydrate, $NH_4Y(C_2O_4)_2 \cdot H_2O$	8m	97
Ammonium zinc fluoride, NH_4ZnF_3	8m	18
Ammonium zirconium fluoride, $(NH_4)_3ZrF_7$	6	14
Antimony(III) fluoride, SbF_3	2m	4
Antimony(III) iodide, SbI_3	6	16
Antimony(III) oxide (senarmontite), Sb_2O_3 (cubic)	3	31
Antimony(III) oxide, valentinite, Sb_2O_3 (orthorhombic)	10	6
Antimony(IV) oxide (cervantite), Sb_2O_4	10	8
Antimony(V) oxide, Sb_2O_5	10	10
Antimony, Sb	3	14
Antimony scandium, SbSc	4m	44
Antimony selenide, Sb_2Se_3	3m	7
Antimony (III) sulfide (stibnite), Sb_2S_3	5	6
Antimony telluride, Sb_2Te_3	3m	8
Antimony terbium, SbTb	5m	61

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

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

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Antimony thorium, SbTh	4m	44
Antimony thulium, SbTm	4m	45
Antimony ytterbium, SbYb	4m	45
Antimony yttrium, SbY	4m	46
Arsenic acid, $H_5As_3O_{10}$	7m	84
Arsenic, As	3	6
Arsenic(III) iodide, AsI_3	6	17
Arsenic trioxide (arsenolite), As_2O_3 (cubic)	1	51
Arsenic trioxide, claudetite, As_2O_3 (monoclinic)	3m	9
L-Ascorbic acid, $C_6H_8O_6$	8m	99
Azobenzene, $C_{12}H_{10}N_2$	7m	86
Barium aluminum oxide, $BaAl_2O_4$	5m	11
Barium arsenate, $Ba_3(AsO_4)_2$	2m	6
Barium, Ba	4	7
Barium borate, BaB_8O_{13}	7m	10
Barium boron oxide, high form, BaB_2O_4	4m	4
Barium boron oxide, BaB_4O_7	4m	6
Barium bromate hydrate, $Ba(BrO_3)_2 \cdot H_2O$	8m	19
Barium bromide, $BaBr_2$	10m	63
Barium bromide fluoride, BaBrF	10m	10
Barium bromide monohydrate, $BaBr_2 \cdot H_2O$	3m	10
Barium calcium tungsten oxide, Ba_2CaWO_6	9m	10
Barium carbonate (witherite), $BaCO_3$ (orthorhombic)	2	54
Barium carbonate, $BaCO_3$(cubic) at 1075 °C	10	11
Barium chlorate hydrate, $Ba(ClO_3)_2 \cdot H_2O$	8m	21
Barium chloride, $BaCl_2$, (orthorhombic)	9m	11
Barium chloride, $BaCl_2$, (cubic)	9m	13
Barium chloride fluoride, BaClF	10m	11
Barium fluoride, BaF_2	1	70
Barium fluosilicate, $BaSiF_6$	4m	7
Barium iodide, BaI_2	10m	66
Barium molybdate, $BaMoO_4$	7	7
Barium nitrate (nitrobarite), $Ba(NO_3)_2$	1	81
Barium oxide, BaO	9m	63
Barium perchlorate trihydrate, $Ba(ClO_4)_2 \cdot 3H_2O$	2m	7
Barium peroxide, BaO_2	6	18
Barium selenide, BaSe	5m	61
Barium stannate, $BaSnO_3$	3m	11
Barium sulfate (barite), $BaSO_4$ (revised)	10m	12
Barium sulfide, BaS	7	8
Barium titanate, $BaTiO_3$	3	45
Barium titanium silicate (fresnoite), $Ba_2TiSi_2O_8$	9m	14
Barium tungstate, $BaWO_4$	7	9
Barium zirconate, $BaZrO_3$	5	8
Beryllium, alpha, Be	9m	64
Beryllium aluminum oxide (chrysoberyl), $BeAl_2O_4$	9	10
Beryllium aluminum silicate, beryl, $Be_3Al_2(SiO_3)_6$	9	13
Beryllium calcium oxide, $Be_{17}Ca_{12}O_{29}$	7m	89
Beryllium chromium oxide, $BeCr_2O_4$	10	12
Beryllium cobalt, BeCo	5m	62
Beryllium germanate, Be_2GeO_4	10	13
Beryllium lanthanum oxide, $Be_2La_2O_5$	9m	65
Beryllium niobium, Be_2Nb	7m	92
Beryllium orthosilicate, phenacite, $BeSi_2O_4$	8	11
Beryllium oxide (bromellite), BeO	1	36
Beryllium palladium, BePd	5m	62
Bis (o-dodecacarborane), $C_4B_{20}H_{22}$	6m	7
Bismuth, Bi	3	20
Bismuth cerium, BiCe	4m	46
Bismuth dysprosium, BiDy	4m	47
Bismuth erbium, BiEr	4m	47
Bismuth fluoride, BiF_3	1m	7
Bismuth holmium, BiHo	4m	48
Bismuth(III) iodide, BiI_3	6	20
Bismuth lanthanum, BiLa	4m	48
Bismuth neodymium, BiNd	4m	49
Bismuth orthophosphate, $BiPO_4$ (monoclinic)	3m	11
Bismuth orthophosphate, $BiPO_4$ (trigonal)	3m	13
Bismuth orthovanadate, low form, $BiVO_4$ (tetragonal)	3m	14
Bismuth orthovanadate, high form, $BiVO_4$ (monoclinic)	3m	14
Bismuth oxybromide, BiOBr	8	14
Bismuth oxychloride (bismoclite), BiOCl	4	54
Bismuth oxyiodide, BiOI	9	16
Bismuth praseodymium, BiPr	4m	49
Bismuth sulfide (bismuthinite), Bi_2S_3 (revised)	5m	13
Bismuth telluride, BiTe	4m	50
Bismuth telluride (tellurobismuthite), Bi_2Te_3	3m	16
Bismuth trioxide (bismite), alpha Bi_2O_3	3m	16
Boron oxide, B_2O_3, phase I	10m	70
Cadmium, Cd	3	10
Cadmium ammine chloride, $Cd(NH_3)_2Cl_2$	10m	14
Cadmium bromide, $CdBr_2$	9	17
Cadmium carbonate (otavite), $CdCO_3$	7	11
Cadmium cerium, CdCe	5m	63
Cadmium chloride, $CdCl_2$	9	18
Cadmium chromite, $CdCr_2O_4$	5m	16
Cadmium cyanide, $Cd(CN)_2$	2m	8
Cadmium fluoride, CdF_2	10m	15
Cadmium imidazole nitrate, $Cd(C_3H_4N_2)_6(NO_3)_2$	8m	23
Cadmium iron oxide, $CdFe_2O_4$	9m	16
Cadmium lanthanum, CdLa	5m	63
Cadmium manganese oxide, $CdMn_2O_4$	10m	16
Cadmium molybdate, $CdMoO_4$	6	21
Cadmium nitrate tetrahydrate, $Cd(NO_3)_2 \cdot 4H_2O$	7m	93
Cadmium oxide, CdO	2	27
Cadmium oxide, CdO (ref. standard)	8m	2
Cadmium perchlorate hexahydrate, $Cd(ClO_4)_2 \cdot 6H_2O$	3m	19
Cadmium praseodymium, CdPr	5m	64
Cadmium selenide, CdSe (hexagonal)	7	12
Cadmium sulfate, $CdSO_4$	3m	20
Cadmium sulfate hydrate, $3CdSO_4 \cdot 8H_2O$	6m	8
Cadmium sulfate monohydrate, $CdSO_4 \cdot H_2O$	6m	10
Cadmium sulfide (greenockite), CdS	4	15
Cadmium telluride, CdTe	3m	21
Cadmium tungstate, $CdWO_4$	2m	8
Calcium, Ca	9m	68
Calcium aluminate, $12CaO \cdot 7Al_2O_3$	9	20
Calcium aluminum germanate, $Ca_3Al_2(GeO_4)_3$	10	15
Calcium aluminum oxide, $Ca_3Al_2O_6$	5	10

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

	Vol. or sec.	Page
Calcium bromide hexahydrate, $CaBr_2 \cdot 6H_2O$	8	15
Calcium carbonate (aragonite), $CaCO_3$ (orthorhombic)	3	53
Calcium carbonate (calcite) $CaCO_3$ (hexagonal)	2	51
Calcium chloride fluoride, CaClF	10m	17
Calcium chromate, $CaCrO_4$	7	13
Calcium chromium germanate, $Ca_3Cr_2(GeO_4)_3$	10	16
Calcium chromium silicate (uvarovite), $Ca_3Cr_2(SiO_4)_3$	10	17
Calcium fluoride (fluorite), CaF_2	1	69
Calcium fluoride phosphate (fluorapatite), $Ca_5F(PO_4)_3$	3m	22
Calcium formate, $Ca(HCO_2)_2$	8	16
Calcium gallium germanate, $Ca_3Ga_2(GeO_4)_3$	10	18
Calcium hydroxide (portlandite), $Ca(OH)_2$	1	58
Calcium iron germanate, $Ca_3Fe_2(GeO_4)_3$	10	19
Calcium iron silicate (andradite), $Ca_3Fe_2Si_3O_{12}$	9	22
Calcium iron silicate hydroxide, julgoldite, $Ca_2Fe_3Si_3O_{10}(OH,O)_2(OH)_2$	10m	72
Calcium magnesium silicate (diopside), $CaMg(SiO_3)_2$	5m	17
Calcium malate hydrate, $C_4H_4Ca\ O_5 \cdot 2H_2O$	10m	76
Calcium molybdate (powellite), $CaMoO_4$	6	22
Calcium nitrate, $Ca(NO_3)_2$	7	14
Calcium oxide, CaO	1	43
Calcium phosphate, beta-pyro-, $Ca_2P_2O_7$	7m	95
Calcium platinum oxide, Ca_4PtO_6	10m	18
Calcium selenide, CaSe	5m	64
Calcium sulfate (anhydrite), $CaSO_4$	4	65
Calcium sulfide (oldhamite), CaS	7	15
Calcium telluride, CaTe	4m	50
Calcium titanium oxide (perovskite), $CaTiO_3$	9m	17
Calcium tungstate, scheelite, $CaWO_4$	6	23
Calcium tungsten oxide, Ca_3WO_6	9m	19
Carbon, diamond, C	2	5
Cerium, antimony CeSb	4m	40
Cerium arsenate, $CeAsO_4$	4m	8
Cerium arsenide, CeAs	4m	51
Cerium(III) chloride, $CeCl_3$	1m	8
Cerium copper, $CeCu_6$	7m	99
Cerium(III) fluoride, CeF_3	8	17
Cerium magnesium, CeMg	5m	65
Cerium magnesium nitrate 24-hydrate, $Ce_2Mg_3(NO_3)_{12} \cdot 24H_2O$	10	20
Cerium niobium titanium oxide (eschynite), $CeNbTiO_6$	3m	24
Cerium nitride, CeN	4m	51
Cerium(IV) oxide (cerianite), CeO_2	1	56
Cerium phosphide, CeP	4m	52
Cerium(III) vanadate, $CeVO_4$	1m	9
Cerium zinc, CeZn	5m	65
Cesium aluminum sulfate dodecahydrate, $CsAl(SO_4)_2 \cdot 12H_2O$	6	25
Cesium beryllium fluoride, $CsBeF_3$	9m	69
Cesium bromate, $CsBrO_3$	8	18
Cesium bromide, CsBr	3	49
Cesium bromoosmate(IV), Cs_2OsBr_6	2m	10
Cesium bromoplatinate, Cs_2PtBr_6	8	19
Cesium bromoselenate, Cs_2SeBr_6	8	20
Cesium bromotellurate, Cs_2TeBr_6	9	24
Cesium cadmium bromide, $CsCdBr_3$ (hexagonal)	10m	20
Cesium cadmium trichloride, $CsCdCl_3$ (hexagonal)	5m	19
Cesium calcium fluoride, $CsCaF_3$	8m	25
Cesium calcium sulfate, $Cs_2Ca_2(SO_4)_3$	7m	12
Cesium calcium trichloride, $CsCaCl_3$	5m	21
Cesium cerium chloride, Cs_2CeCl_6	7m	101
Cesium chlorate, $CsClO_3$	8	20
Cesium chloride, CsCl	2	44
Cesium chloroosmate(IV), Cs_2OsCl_6	2m	11
Cesium chloroplatinate, Cs_2PtCl_6	5	14
Cesium chlorostannate, Cs_2SnCl_6	5	16
Cesium chromate, Cs_2CrO_4	3m	25
Cesium chromium sulfate dodecahydrate, $CsCr(SO_4)_2 \cdot 12H_2O$	8	21
Cesium cobalt (II) trichloride, $CsCoCl_3$	6m	11
Cesium copper sulfate hexahydrate, $Cs_2Cu(SO_4)_2 \cdot 6H_2O$	7m	14
Cesium copper(II) trichloride, $CsCuCl_3$	5m	22
Cesium dichloroiodide, $CsICl_2$	3	50
Cesium fluoantimonate, $CsSbF_6$	4m	9
Cesium fluoborate, $CsBF_4$	8	22
Cesium fluogermanate, Cs_2GeF_6	5	17
Cesium fluoplatinate, Cs_2PtF_6	6	27
Cesium fluoride, CsF	3m	26
Cesium fluosilicate, Cs_2SiF_6	5	19
Cesium gallium sulfate dodecahydrate, $CsGa(SO_4)_2 \cdot 12H_2O$	8	23
Cesium iodine bromide, CsI_2Br	7m	103
Cesium iodide, CsI	4	47
Cesium iron sulfate dodecahydrate, $CsFe(SO_4)_2 \cdot 12H_2O$	6	28
Cesium iron sulfate hexahydrate, $Cs_2Fe(SO_4)_2 \cdot 6H_2O$	7m	16
Cesium lead fluoride, $CsPbF_3$	8m	26
Cesium lead(II) trichloride, $CsPbCl_3$ (tetragonal)	5m	24
Cesium lithium cobalt cyanide, $CsLiCo(CN)_6$	10m	79
Cesium lithium fluoride, $CsLiF_2$	7m	105
Cesium magnesium chromium oxide, $Cs_2Mg_2(CrO_4)_3$	8m	27
Cesium magnesium chromium oxide hydrate, $Cs_2Mg(CrO_4)_2 \cdot 6H_2O$	8m	29
Cesium magnesium sulfate hexahydrate, $Cs_2Mg(SO_4)_2 \cdot 6H_2O$	7m	18
Cesium manganese fluoride, $CsMnF_3$	10m	21
Cesium manganese sulfate hexahydrate, $Cs_2Mn(SO_4)_2 \cdot 6H_2O$	7m	20
Cesium mercury chloride, $CsHgCl_3$	7m	22
Cesium nickel sulfate hexahydrate, $Cs_2Ni(SO_4)_2 \cdot 6H_2O$	7m	23
Cesium nickel (II) trichloride, $CsNiCl_3$	6m	12
Cesium nitrate, $CsNO_3$	9	25
Cesium perchlorate, $CsClO_4$, (orthorhombic)	1m	10
Cesium strontium trichloride, $CsSrCl_3$	6m	13

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Cesium sulfate Cs_2SO_4	7	17
Cesium vanadium sulfate dodecahydrate, $CsV(SO_4)_2 \cdot 12H_2O$	1m	11
Cesium zinc sulfate hexahydrate, $Cs_2Zn(SO_4)_2 \cdot 6H_2O$	7m	25
Chromium, Cr	5	20
Chromium fluoride, Cr_2F_5	7m	108
Chromium fluoride, CrF_2	10m	81
Chromium(III) fluoride trihydrate, $CrF_3 \cdot 3H_2O$	5m	25
Chromium iridium 3:1, Cr_3Ir	6m	14
Chromium orthophosphate, alpha, $CrPO_4$	2m	12
Chromium orthophosphate, beta, $CrPO_4$	9	26
Chromium(III) oxide, Cr_2O_3	5	22
Chromium rhodium 3:1, Cr_3Rh	6m	15
Chromium silicide, Cr_3Si	6	29
Cobalt, Co (cubic)	4m	10
Cobalt aluminum oxide, $CoAl_2O_4$	9	27
Cobalt ammine iodide, $Co(NH_3)_6I_3$	10m	83
Cobalt antimony oxide, $CoSb_2O_6$	5m	26
Cobalt arsenide (skutterudite), $CoAs_3$	10	21
Cobalt(II) carbonate (spherocobaltite), $CoCO_3$	10	24
Cobalt chromium oxide, $CoCr_2O_4$	9m	21
Cobalt diarsenide, $CoAs_2$ (revised)	4m	10
Cobalt fluoride, CoF_2	10m	85
Cobalt fluosilicate hexahydrate, $CoSiF_6 \cdot 6H_2O$	3m	27
Cobalt gallate, $CoGa_2O_4$	10	27
Cobalt germanate, Co_2GeO_4	10	27
Cobalt iodide, CoI_2	4m	52
Cobalt iron arsenide (safflorite), $CoFeAs_4$	10	28
Cobalt iron oxide, $CoFe_2O_4$	9m	22
Cobalt mercury thiocyanate, $Co[Hg(CNS)_4]$	2m	13
Cobalt(II) oxide, CoO	9	28
Cobalt(II, III) oxide, Co_3O_4	9	29
Cobalt perchlorate hexahydrate, $Co(ClO_4)_2 \cdot 6H_2O$	3m	28
Cobalt silicate, Co_2SiO_4 (orthorhombic)	4m	11
Cobalt sulfate, beta, $CoSO_4$	2m	14
Cobalt titanate, $CoTiO_3$	4m	13
Cobalt tungstate, $CoWO_4$	4m	13
Copper, Cu	1	15
Copper ammine selenate, $Cu(NH_3)_4SeO_4$	10m	87
Copper ammine sulfate hydrate, $Cu(NH_3)_4SO_4 \cdot H_2O$	10m	90
Copper antimony oxide, $CuSb_2O_6$	5m	27
Copper(I) bromide, CuBr	4	36
Copper carbonate, basic, azurite, $CU_3(OH)_2(CO_3)_2$	10	30
Copper carbonate, basic, (malachite), $CU_2(OH)_2CO_3$	10	31
Copper (I) chloride (nantokite), CuCl	4	35
Copper glutamate dihydrate, $CuC_5H_7NO_4 \cdot 2H_2O$	7m	110
Copper(I) iodide (marchite), CuI	4	38
Copper (I) oxide (cuprite), Cu_2O	2	23
Copper(II) oxide (tenorite), CuO	1	49
Copper phosphate, alpha-pyro-, $Cu_2P_2O_7$	7m	113
Copper pyrazole chloride, $Cu(C_3H_4N_2)_4Cl_2$	8m	31
Copper sulfate (chalcocyanite), $CuSO_4$	3m	29
Copper(II) sulfide (covellite), CuS	4	13
Copper uranium oxide, $CuUO_4$	10m	93
Dibenzoylmethane, $C_{15}H_{12}O_2$	7m	115
Dysprosium antimony, DySb	4m	41
Dysprosium arsenate, $DyAsO_4$	3m	30
Dysprosium arsenide, DyAs	4m	53
Dysprosium gallium oxide, $Dy_3Ga_2(GaO_4)_3$	2m	15
Dysprosium nitride, DyN	4m	53
Dysprosium sesquioxide, Dy_2O_3	9	30
Dysprosium telluride, DyTe	4m	54
Dysprosium vanadate, $DyVO_4$	4m	15
Erbium antimony, ErSb	4m	41
Erbium arsenate, $ErAsO_4$	3m	31
Erbium arsenide, ErAs	4m	54
Erbium gallium oxide, $Er_3Ga_2(GaO_4)_3$	1m	12
Erbium manganite, $ErMnO_3$	2m	16
Erbium nitride, ErN	4m	55
Erbium phosphate, $ErPO_4$	9	31
Erbium sesquioxide, Er_2O_3	8	25
Erbium telluride, ErTe	4m	55
Erbium vanadate, $ErVO_4$	5m	29
Europium arsenate, $EuAsO_4$	3m	32
Europium(III) chloride, $EuCl_3$	1m	13
Europium gallium oxide, $Eu_3Ga_2(GaO_4)_3$	2m	17
Europium nitride, EuN	4m	56
Europium oxide, EuO	4m	56
Europium oxychloride, EuOCl	1m	13
Europium(III) vanadate, $EuVO_4$	4m	16
Gadolinium antimony, GdSb	4m	42
Gadolinium arsenate, $GdAsO_4$	4m	17
Gadolinium arsenide, GdAs	4m	57
Gadolinium chloride hexahydrate, $GdCl_3 \cdot 6H_2O$	7m	118
Gadolinium fluoride, GdF_3	1m	14
Gadolinium gallium oxide, $Gd_3Ga_2(GaO_4)_3$	2m	18
Gadolinium indium, GdIn	5m	67
Gadolinium nitride, GdN	4m	57
Gadolinium oxide, Gd_2O_3	1m	16
Gadolinium oxychloride, GdOCl	1m	17
Gadolinium titanium oxide, Gd_2TiO_5	8m	32
Gadolinium vanadate, $GdVO_4$	5m	30
Gallium, Ga	2	9
Gallium antimonide, GaSb	6	30
Gallium arsenide, GaAs	3m	33
Gallium oxide, alpha, Ga_2O_3	4	25
Gallium phosphate hydrate, $GaPO_4 \cdot 2H_2O$	8m	34
Gallium phosphate (α-quartz type), $GaPO_4$	8	27
Germanium, Ge	1	18
Germanium dioxide, GeO_2 (hexagonal) (low form)	1	51
Germanium dioxide, GeO_2 (tetragonal) (high form)	8	28
Germanium iodide, GeI_2	4m	58
Germanium(IV) iodide, GeI_4	5	25
Glyoxime, $H_2C_2(NOH)_2$	8m	102
Gold, Au	1	33
Gold antimony 1:2 (aurostibite), $AuSb_2$	7	18
Gold(I) cyanide, AuCN	10	33
Gold dysprosium, AuDy	5m	66

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Gold holmium, AuHo	5m	68
Gold magnesium, AuMg	6m	83
Gold niobium 1:3, $AuNb_3$	6m	16
Gold potassium cyanide, $AuK(CN)_2$	8m	36
Gold tin, 1:1 AuSn	7	19
Gold titanium 1:3, $AuTi_3$	6m	17
Gold vanadium 1:3, AuV_3	6m	18
Hafnium, Hf	3	18
Hexamethylenediammonium adipate, $C_{12}H_{26}N_2O_4$	7m	121
Holmium arsenate, $HoAsO_4$	3m	34
Holmium ethylsulfate nonahydrate, $Ho[(C_2H_5)SO_4]_3 \cdot 9H_2O$	1m	18
Holmium fluoride, HOF_3	10m	23
Holmium nitride, HoN	4m	58
Holmium selenide, HoSe	4m	59
Holmium sesquioxide, Ho_2O_3	9	32
Holmium vanadate, $HoVO_4$	4m	18
Hydrogen borate, beta, HBO_2	9m	71
Hydrogen iodate, HI_3O_8	8m	104
Hydroquinone, gamma, $C_6H_6O_2$	8m	107
Imidazole nickel nitrate, $(C_3H_4N_2)_6Ni(NO_3)_2$	7m	27
Imidazole zinc chloride, $(C_3H_4N_2)_2ZnCl_2$	7m	123
Indium, In	3	12
Indium antimony, InSb	4	73
Indium arsenide, InAs	3m	35
Indium oxide, In_2O_3	5	26
Indium phosphate, $InPO_4$	8	29
Iodic acid, HIO_3	5	28
Iodine, I_2	3	16
Iridium, Ir	4	9
Iridium dioxide, IrO_2	4m	19
Iridium niobium 1:3, $IrNb_3$	6m	19
Iridium titanium 1:3, $IrTi_3$	6m	20
Iridium vanadium 1:3, IrV_3	6m	21
Iron, alpha Fe	4	3
Iron arsenide, FeAs	1m	19
Iron arsenide (loellingite), $FeAs_2$	10	34
Iron bromide, $FeBr_2$	4m	59
Iron iodide, FeI_2	4m	60
Iron oxalate hydrate (humboldtine) $FeC_2O_4 \cdot 2H_2O$	10m	24
Iron(II,III) oxide (magnetite), Fe_3O_4	5m	31
Iron sulfate hydrate (melanterite), $FeSO_4 \cdot 7H_2O$	8m	38
Iron sulfate hydroxide, butlerite, $FeSO_4(OH) \cdot 2H_2O$	10m	95
Iron sulfide (pyrite), FeS_2	5	29
bis-(N-Isopropyl-3-ethylsalicylaldiminato) palladium, $(C_{12}H_{16}NO)_2Pd$	7m	144
Lanthanum antimony, LaSb	4m	42
Lanthanum arsenate, $LaAsO_4$	3m	36
Lanthanum arsenide, LaAs	4m	60
Lanthanum borate, $LaBO_3$	1m	20
Lanthanum chloride, $LaCl_3$	1m	20
Lanthanum fluoride, LaF_3	7	21
Lanthanum magnesium, LaMg	5m	69
Lanthanum magnesium nitrate 24-hydrate, $La_2Mg_3(NO_3)_{12} \cdot 24H_2O$	1m	22
Lanthanum niobium titanium oxide, $LaNbTiO_6$	3m	37
Lanthanum nitrate hydrate, $La(NO_3)_3 \cdot 6H_2O$	8m	40
Lanthanum nitride, LaN	4m	61
Lanthanum oxide, La_2O_3	3	33
Lanthanum oxychloride, LaOCl	7	22
Lanthanum phosphide, LaP	5m	69
Lanthanum selenide, LaSe	4m	61
Lanthanum zinc, LaZn	5m	70
Lead, Pb	1	34
Lead boron oxide, PbB_4O_7	4m	19
Lead bromide, $PbBr_2$	2	47
Lead bromide fluoride, PbBrF	10m	25
Lead carbonate (cerrussite), $PbCO_3$	2	56
Lead chloride (cotunnite), $PbCl_2$	2	45
Lead fluochloride (matlockite), PbFCl	1	76
Lead fluoride, alpha PbF_2 (orthorhombic)	5	31
Lead fluoride, beta PbF_2 (cubic)	5	33
Lead fluoride iodide, PbFI	10m	26
Lead formate, $Pb(HCO_2)_2$	8	30
Lead(II) iodide, PbI_2	5	34
Lead molybdate (wulfenite), $PbMoO_4$	7	23
Lead monoxide (litharge), PbO (red) tetragonal	2	30
Lead monoxide (massicot), PbO (yellow) (orthorhombic)	2	32
Lead nitrate, $Pb(NO_3)_2$	5	36
Lead(II, III) oxide (minium), Pb_3O_4	8	32
Lead oxide sulfate, $Pb_5O_4SO_4$	10m	27
Lead oxybromide, $Pb_3O_2Br_2$	5m	32
Lead phosphate hydrate, $Pb_5(PO_4)_3OH$	8	33
Lead selenide (clausthalite), PbSe	5	38
Lead sulfate (anglesite), $PbSO_4$	3	67
Lead sulfide (galena), PbS	2	18
Lead tin oxide, Pb_2SnO_4	10m	29
Lead titanate, $PbTiO_3$	5	39
Lead tungstate (stolzite), $PbWO_4$ (tetragonal) (revised)	5m	34
Lead uranium oxide, Pb_3UO_6	8m	109
Lithium aluminum, Li_9Al_4	10m	98
Lithium aluminum fluoride, alpha, Li_3AlF_6	8m	111
Lithium arsenate, Li_3AsO_4	2m	19
Lithium azide, LiN_3	8m	113
Lithium barium trifluoride, $LiBaF_3$	5m	35
Lithium beryllium fluoride, Li_2BeF_4	7m	126
Lithium borate, $Li_2B_4O_7$	8m	114
Lithium bromide, LiBr	4	30
Lithium carbonate, Li_2CO_3	8m	42
Lithium chloride, LiCl	1	62
Lithium fluoride, LiF	1	61
Lithium gallium oxide, $LiGaO_2$	10m	31
Lithium iodate, $LiIO_3$	7	26
Lithium iodate, $LiIO_3$(tetragonal)	10m	33
Lithium molybdate, Li_2MoO_4 (trigonal)	1m	23
Lithium niobate, $LiNbO_3$	6m	22
Lithium nitrate, $LiNO_3$	7	27
Lithium oxalate, $Li_2C_2O_4$	10m	34
Lithium oxide, Li_2O	1m	25
Lithium perchlorate trihydrate, $LiClO_4 \cdot 3H_2O$	8	34
Lithium phosphate, low form (lithiophosphate), Li_3PO_4 (orthorhombic) revised	4m	21
Lithium phosphate, high form, Li_3PO_4	3m	39

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Lithium rubidium fluoride, $LiRbF_2$	7m	128
Lithium selenide, Li_2Se	10m	100
Lithium sodium aluminum fluoride, cryolithionite, $Li_3Na_3Al_2F_{12}$	9m	23
Lithium sodium sulfate, $LiNaSO_4$	6m	24
Lithium sulfate, Li_2SO_4	6m	26
Lithium sulfate monohydrate, $Li_2SO_4 \cdot H_2O$	4m	22
Lithium sulfide, Li_2S	10m	101
Lithium telluride, Li_2Te	10m	102
Lithium trimetaphosphate trihydrate, $Li_3P_3O_9 \cdot 3H_2O$	2m	20
Lithium tungstate, Li_2WO_4 (trigonal)	1m	25
Lithium tungstate hemihydrate, $Li_2WO_4 \cdot \frac{1}{2}H_2O$	2m	20
Lithium uranium fluoride, $LiUF_5$	7m	131
Lutetium arsenate, $LuAsO_4$	5m	36
Lutetium gallium oxide, $Lu_3Ga_2(GaO_4)_3$	2m	22
Lutetium manganite, $LuMnO_3$	2m	23
Lutetium nitride, LuN	4m	62
Lutetium oxide, Lu_2O_3	1m	27
Lutetium vanadate, $LuVO_4$	5m	37
Magnesium, Mg	1	10
Magnesiun aluminum oxide (spinel), $MgAl_2O_4$ (revised)	9m	25
Magnesium aluminum silicate (pyrope), $Mg_3Al_2(SiO_4)_3$	4m	24
Magnesium aluminum silicate (low cordierite), $Mg_2Al_4Si_5O_{18}$ (orthorhombic)	1m	28
Magnesium aluminum silicate (high cordierite), $Mg_2Al_4Si_5O_{18}$ (hexagonal)	1m	29
Magnesium ammonium phosphate hexahydrate (struvite), $MgNH_4PO_4 \cdot 6H_2O$	3m	41
Magnesium boron oxide, $Mg_2B_2O_5$ (triclinic)	4m	25
Magnesium bromide, $MgBr_2$	4m	62
Magnesium carbonate (magnesite), $MgCO_3$	7	28
Magnesium chloride dodecahydrate, $MgCl_2 \cdot 12H_2O$	7m	135
Magnesium chromite (picrochromite), $MgCr_2O_4$	9	34
Magnesium fluoride (sellaite), MgF_2	4	33
Magnesium gallate, $MgGa_2O_4$	10	36
Magnesium germanate, Mg_2GeO_4 (cubic)	10	37
Magnesium germanate, Mg_2GeO_4 (orthorhombic)	10	38
Magnesium hydrogen phosphate trihydrate, newberyite, $MgHPO_4 \cdot 3H_2O$	7m	139
Magnesium hydroxide (brucite), $Mg(OH)_2$	6	30
Magnesium iron carbonate hydroxide hydrate, pyroaurite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$, phase II	10m	104
Magnesium iron carbonate hydroxide hydrate, sjögrenite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$, phase I	10m	103
Magnesium manganese oxide, $MgMn_2O_4$	10m	35
Magnesium molybdate, $MgMoO_4$	7m	28
Magnesium nickel oxide, $MgNiO_2$	10m	36
Magnesium oxide (periclase), MgO	1	37
Magnesium perchlorate hexahydrate, $Mg(ClO_4)_2 \cdot 6H_2O$	7m	30
Magnesium phosphate, alpha, $Mg_2P_2O_7$	9m	73
Magnesium selenide, MgSe	5m	70
Magnesium selenite hydrate, $MgSeO_3 \cdot 6H_2O$	3m	116
Magnesium silicate, enstatite, $MgSiO_3$	6	32
Magnesium silicate (forsterite), Mg_2SiO_4	1	83
Magnesium silicate fluoride (norbergite), $Mg_2SiO_4 \cdot MgF_2$	10	39
Magnesium silicate fluoride (humite), $3Mg_2SiO_4 \cdot MgF_2$	1m	30
Magnesium sulfate heptahydrate (epsomite), $MgSO_4 \cdot 7H_2O$	7	30
Magnesium sulfide, MgS	7	31
Magnesium sulfite hydrate, $MgSO_3 \cdot 6H_2O$	9m	26
Magnesium tin, Mg_2Sn	5	41
Magnesium tin oxide, Mg_2SnO_4	10m	37
Magnesium titanate (geikielite), $MgTiO_3$	5	43
Magnesium tungstate, $MgWO_4$	1	84
Manganese, alpha, Mn	7m	142
Manganese aluminate (galaxite), $MnAl_2O_4$	9	35
Manganese bromide, $MnBr_2$	4m	63
Manganese(II) carbonate (rhodochrosite), $MnCO_3$	7	32
Manganese chloride (scacchite), $MnCl_2$	8m	43
Manganese chloride hydrate, $MnCl_2 \cdot 4H_2O$	9m	28
Manganese cobalt oxide, $MnCo_2O_4$	9m	30
Manganese ferrite (jacobsite), $MnFe_2O_4$	9	36
Manganese fluoride, MnF_2	10m	105
Manganese iodide, MnI_2	4m	63
Manganese oxide (hausmannite), Mn_3O_4	10m	38
Manganese oxide (pyrolusite), beta, MnO_2	10m	39
Manganese(II) oxide (manganosite), MnO	5	45
Manganese(III) oxide (partridgeite), Mn_2O_3	9	37
Manganese selenide, MnSe	10	41
Manganese sulfide (alabandite), alpha MnS	4	11
Manganese(II) tungstate (huebnerite), $MnWO_4$	2m	24
Manganese vanadiun oxide, $Mn_2V_2O_7$	9m	75
Mercury amide chloride, $HgNH_2Cl$	10m	40
Mercury bromate, $Hg(BrO_3)_2$	10m	107
Mercury bromide, $HgBr_2$	10m	110
Mercury(I) bromide, Hg_2Br_2	7	33
Mercury(I) chloride (calomel), Hg_2Cl_2	1	72
Mercury(II) chloride, $HgCl_2$	1	73
Mercury(II) cyanide, $Hg(CN)_2$	6	35
Mercury(II) fluoride, HgF_2	2m	25
Mercury(I) iodide, HgI	4	49
Mercury iodide, HgI_2 (tetragonal) (revised)	7m	32
Mercury magnesium, HgMg	6m	84
Mercury(II) oxide (montroydite) HgO (revised)	9	39
Mercury phthalate, $C_6H_4(COOHg)_2$	10m	113
Mercury(II) selenide (tiemannite), HgSe	7	35
Mercury(II) sulfide (cinnabar), HgS (hexagonal)	4	17
Mercury(II) sulfide (metacinnabar), HgS (cubic)	4	21
Mercury sulfide chloride, alpha, $Hg_3S_2Cl_2$	8m	118
Metaboric acid, HBO_2 (cubic)	4m	27
Methanesulfonanilide, $C_6H_5\text{-}NH\text{-}SO_2CH_3$	9m	78
N-methylphenazinium tetracyanoquinodimethanide, $C_{25}H_{15}N_6$	7m	146
Molybdenum, Mo	1	20
Molybdenum arsenide, Mo_2As_3	10m	115
Molybdenum disulfide (molybdenite), MoS_2	5	47
Molybdenum osmium 3:1, Mo_3Os	6m	28

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Molybdenum trioxide (molybdite), MoO_3	3	30
2-Naphthylamine, n-phenyl—, $C_{16}H_{13}N$	6m	29
Neodymium antimony, NdSb	4m	43
Neodynium arsenate, $NdAsO_4$	4m	28
Neodymium arsenide, NdAs	4m	64
Neodymium borate, $NdBO_3$	1m	32
Neodymium chloride, $NdCl_3$	1m	33
Neodymium ethylsulfate nonahydrate, $Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$	9	41
Neodymium fluoride, NdF_3	8	36
Neodymium gallium oxide, $Nd_3Ga_2(GaO_4)_3$	1m	34
Neodymium oxide, Nd_2O_3	4	26
Neodymium oxychloride, NdOCl	8	37
Neodymium selenide, NdSe	5m	71
Neodymium vanadate, $NdVO_4$	4m	30
Neptunium nitride, NpN	4m	64
Nickel, Ni	1	13
Nickel aluminate, $NiAl_2O_4$	9	42
Nickel arsenic 1:2 (rammelsbergite), $NiAs_2$	10	42
Nickel arsenic sulfide (gersdorffite), NiAsS	1m	35
Nickel bromide, $NiBr_2$	10m	119
Nickel(II) carbonate, $NiCO_3$ (trigonal)	1m	36
Nickel chloride, $NiCl_2$	9m	81
Nickel ferrite (trevorite), $NiFe_2O_4$	10	44
Nickel fluoride, NiF_2	10m	121
Nickel fluosilicate hexahydrate, $NiSiF_6 \cdot 6H_2O$	8	38
Nickel gallate, $NiGa_2O_4$	10	45
Nickel germanate, Ni_2GeO_4	9	43
Nickel(II) oxide (bunsenite), NiO	1	47
Nickel phosphide, $Ni_{12}P_5$	9m	83
Nickel pyrazole chloride, $Ni(C_3H_4N_2)_4Cl_2$	8m	44
Nickel sulfate, $NiSO_4$	2m	26
Nickel sulfate hexahydrate (retgersite), $NiSO_4 \cdot 6H_2O$	7	36
Nickel sulfide, millerite, NiS	1m	37
Nickel tungstate, $NiWO_4$	2m	27
Nickel yttrium, Ni_3Y	10m	123
Niobium osmium 3:1, Nb_3Os	6m	30
Niobium oxychloride, $NbOCl_3$	7m	148
Niobium platinum 3:1, Nb_3Pt	6m	31
Niobium silicide, $NbSi_2$	8	39
Osmium, Os	4	8
Osmium titanium, OsTi	6m	85
Palladium, Pd	1	21
Palladium hydride, $PdH_{0.706}$	5m	72
Palladium oxide, PdO	4	27
Palladium vanadium 1:3, PdV_3	6m	32
Phosphorus bromide, PBr_7	7m	150
Phosphorus oxide (stable form I), P_2O_5, (orthorhombic)	9m	86
Phosphorus oxide (stable form II), P_2O_5, (orthorhombic)	9m	88
Phosphorus oxide (metastable form), P_4O_{10}, (rhombohedral)	9m	91
Pimelic acid, $C_7H_{12}O_4$	7m	153
Platinum, Pt	1	31
Platinum titanium 1:3, $PtTi_3$	6m	33
Platinum vanadium 1:3, PtV_3	6m	34
Plutonium arsenide, PuAs	4m	65
Plutonium phosphide, PuP	4m	65
Plutonium telluride, PuTe	4m	66
Potassium acid phthalate, $C_6H_4(COOH)(COOK)$	4m	30
Potassium aluminum sulfate, $KAl(SO_4)_2$	9m	31
Potassium aluminum sulfate dodecahydrate, (alum), $KAl(SO_4)_2 \cdot 12H_2O$	6	36
Potassium barium nickel nitrite, $K_2BaNi(NO_2)_6$	9m	32
Potassium borohydride, KBH_4	9	44
Potassium bromate, $KBrO_3$	7	38
Potassium bromide, KBr	1	66
Potassium bromide chloride, $KBr_{0.5}Cl_{0.5}$	8m	46
Potassium bromoplatinate, K_2PtBr_6	8	40
Potassium bromoselenate, K_2SeBr_6	8	41
Potassium cadmium fluoride, $KCdF_3$	8m	47
Potassium cadmium sulfate, $K_2Cd_2(SO_4)_3$	7m	34
Potassium cadmium trichloride, $KCdCl_3$	5m	38
Potassium calcium carbonate (fairchildite), $K_2Ca(CO_3)_2$	8m	48
Potassium calcium chloride (chlorocalcite), $KCaCl_3$	7m	36
Potassium calcium fluoride, $KCaF_3$	8m	49
Potassium calcium magnesium sulfate, $K_2CaMg(SO_4)_3$	7m	37
Potassium calcium nickel nitrite, $K_2CaNi(NO_2)_6$	9m	33
Potassium calcium sulfate, $K_2Ca_2(SO_4)_3$	7m	39
Potassium chlorate, $KClO_3$	3m	42
Potassium chloride (sylvite), KCl	1	35
Potassium chloroplatinate, K_2PtCl_6	5	49
Potassium chlororhenate, K_2ReCl_6	2m	28
Potassium chlororuthenate(IV), K_2RuCl_6	10	46
Potassium chlorostannate, K_2SnCl_6	6	38
Potassium chromium sulfate dodecahydrate, $KCr(SO_4)_2 \cdot 12H_2O$	6	39
Potassium cobalt (II) sulfate, $K_2Co_2(SO_4)_3$	6m	35
Potassium cobalt (II) trifluoride, $KCoF_3$	6m	37
Potassium cobaltinitrite, $K_3Co(NO_2)_6$	9	45
Potassium copper chloride, $KCuCl_3$	7m	41
Potassium copper chloride hydrate (mitscherlichite), $K_2CuCl_4.2H_2O$	9m	34
Potassium copper (II) trifluoride, $KCuF_3$	6m	38
Potassium cyanate, KCNO	7	39
Potassium cyanide, KCN	1	77
Potassium hydrogen diformate $KH(HCOO)_2$	9m	93
Potassium dihydrogen arsenate, KH_2AsO_4	1m	38
Potassium dihydrogen phosphate, KH_2PO_4	3	69
Potassium fluogermanate, K_2GeF_6	6	41
Potassium fluoplatinate, K_2PtF_6	6	42
Potassium fluoride, KF	1	64
Potassium fluosilicate (hieratite), K_2SiF_6	5	50
Potassium fluotitanate, K_2TiF_6	7	40
Potassium heptafluozirconate, K_3ZrF_7	9	46
Potassium hydroxide, KOH at 300 °C	4m	66
Potassium hydroxy-chlororuthenate, $K_4Ru_2Cl_{10}O \cdot H_2O$	10	47
Potassium iodide, KI	1	68
Potassium iron cyanide, $K_3Fe(CN)_6$	9m	35
Potassium iron fluoride, K_3FeF_6	9m	37
Potassium iron (II) trifluoride, $KFeF_3$	6m	39

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Potassium lithium sulfate, $KLiSO_4$	3m	43
Potassium magnesium chloride hydrate (carnallite), $KMgCl_3 \cdot 6H_2O$	8m	50
Potassium magnesium chromium oxide, $K_2Mg_2(CrO_4)_3$	8m	52
Potassium magnesium fluoride, K_2MgF_4	10m	42
Potassium magnesium selenate hydrate, $K_2Mg(SeO_4)_2 \cdot 6H_2O$	10m	43
Potassium magnesium sulfate (langbeinite), $K_2Mg_2(SO_4)_3$	6m	40
Potassium magnesium sulfate hydrate (picromerite), $K_2Mg(SO_4)_2 \cdot 6H_2O$	8m	54
Potassium magnesium trifluoride, $KMgF_3$	6m	42
Potassium manganese (II) sulfate (manganolangbeinite), $K_2Mn_2(SO_4)_3$	6m	43
Potassium manganese (II) trifluoride, $KMnF_3$	6m	45
Potassium nickel fluoride, $KNiF_3$	7m	42
Potassium nickel fluoride, K_2NiF_4	10m	45
Potassium nickel (II) sulfate, $K_2Ni_2(SO_4)_3$	6m	46
Potassium niobium fluoride, K_2NbF_7	8m	120
Potassium nitrate (niter), KNO_3	3	58
Potassium nitrite, KNO_2	9m	38
Potassium nitroso chlororuthenate, K_2RuCl_5NO	2m	29
Potassium oxalate hydrate, $K_2C_2O_4 \cdot H_2O$	9m	39
Potassium oxalate perhydrate, $K_2C_2O_4 \cdot H_2O_2$	9m	96
Potassium oxide, K_2O	10m	125
Potassium perchlorate, $KClO_4$	6	43
Potassium perchromate, K_3CrO_8	3m	44
Potassium periodate, KIO_4	7	41
Potassium permanganate, $KMnO_4$	7	42
Potassium perrhenate, $KReO_4$	8	41
Potassium phosphomolybdate tetrahydrate, $K_2PO_4(MoO_3)_{12} \cdot 4H_2O$	8	43
Potassium selenate, K_2SeO_4	9m	41
Potassium selenide, K_2Se	10m	126
Potassium sodium aluminum fluoride (elpasolite), K_2NaAlF_6	9m	43
Potassium sodium sulfate, $KNaSO_4$	6m	50
Potassium sodium sulfate, $K_{.67}Na_{1.33}SO_4$	6m	48
Potassium sodium sulfate (aphthitalite), $K_3Na(SO_4)_2$	6m	52
Potassium sulfate, $K_2S_2O_7$	9m	99
Potassium sulfate (arcanite), K_2SO_4	3	62
Potassium sulfide, K_2S	10m	127
Potassium telluride, K_2Te	10m	128
Potassium thiocyanate, KCNS	8	44
Potassium vanadium oxide, KV_3O_8	8m	56
Potassium zinc decavanadate 16 hydrate, $K_2Zn_2V_{10}O_{28} \cdot 16H_2O$	3m	45
Potassium zinc fluoride, $KZnF_3$	5	51
Potassium zinc fluoride, K_2ZnF_4	10m	46
Potassium zinc sulfate hexahydrate, $K_2Zn(SO_4)_2 \cdot 6H_2O$	7m	43
Potassium zinc sulfate, $K_2Zn_2(SO_4)_3$	6m	54
Praseodymium antimony, PrSb	4m	43
Praseodymium arsenate, $PrAsO_4$	4m	32
Praseodymium arsenide, PrAs	4m	67
Praseodymium chloride, $PrCl_3$	1m	39
Praseodymium fluoride, PrF_3	5	52
Praseodymium oxychloride, PrOCl	9	47
Praseodymium sulfide, PrS	4m	67
Praseodymium vanadate, $PrVO_4$	5m	40
Praseodymium zinc, PrZn	5m	72
Reserpine, $C_{33}H_{40}N_2O_9$	8m	123
Rhenium, Re	2	13
Rhodium, Rh	3	9
Rhodium vanadium 1:3, RhV_3	6m	56
Rubidium aluminum sulfate dodecahydrate, $RbAl(SO_4)_2 \cdot 12H_2O$	6	44
Rubidium amide, $RbNH_2$	5m	73
Rubidium bromate, $RbBrO_3$	8	45
Rubidium bromide, RbBr	7	43
Rubidium bromotellurate, Rb_2TeBr_6	8	46
Rubidium cadmium sulfate, $Rb_2Cd_2(SO_4)_3$	7m	45
Rubidium cadmium trichloride, high form, $RbCdCl_3$ (tetragonal)	5m	43
Rubidium cadmium trichloride, low form, $RbCdCl_3$ (orthorhombic)	5m	41
Rubidium calcium chloride, $RbCaCl_3$	7m	47
Rubidium calcium fluoride, $RbCaF_3$	8m	57
Rubidium calcium sulfate, $Rb_2Ca_2(SO_4)_3$	7m	48
Rubidium chlorate, $RbClO_3$	8	47
Rubidium chloride, RbCl	4	41
Rubidium chloroplatinate, Rb_2PtCl_6	5	53
Rubidium chlorostannate, Rb_2SnCl_6	6	46
Rubidium chlorotellurate, Rb_2TeCl_6	8	48
Rubidium chromate, Rb_2CrO_4	3m	46
Rubidium chromium sulfate dodecahydrate, $RbCr(SO_4)_2 \cdot 12H_2O$	6	47
Rubidium cobalt fluoride, $RbCoF_3$	8m	58
Rubidium cobalt sulfate, $Rb_2Co_2(SO_4)_3$	8m	59
Rubidium cobalt (II) trichloride, $RbCoCl_3$	6m	57
Rubidium copper chloride hydrate, $Rb_2CuCl_4 \cdot 2H_2O$	10m	47
Rubidium copper sulfate hydrate, $Rb_2Cu(SO_4)_2 \cdot 6H_2O$	8m	61
Rubidium fluoplatinate, Rb_2PtF_6	6	48
Rubidium fluoride, RbF	8m	63
Rubidum fluosilicate, Rb_2SiF_6	6	49
Rubidium iodide, RbI	4	43
Rubidium iron sulfate hydrate, $Rb_2Fe(SO_4)_2 \cdot 6H_2O$	8m	64
Rubidium magnesium chromium oxide, $Rb_2Mg_2(CrO_4)_3$	8m	66
Rubidium magnesium chromium oxide hydrate, $Rb_2Mg(CrO_4)_2 \cdot 6H_2O$	8m	68
Rubidium magnesium sulfate, $Rb_2Mg_2(SO_4)_3$	7m	50
Rubidium magnesium sulfate hydrate, $Rb_2Mg(SO_4)_2 \cdot 6H_2O$	8m	70
Rubidium manganese sulfate, $Rb_2Mn_2(SO_4)_3$	7m	52
Rubidium manganese(II) trifluoride, $RbMnF_3$	5m	44
Rubidium nickel sulfate, $Rb_2Ni_2(SO_4)_3$	8m	72
Rubidium nickel sulfate hydrate, $Rb_2Ni(SO_4)_2 \cdot 6H_2O$	8m	74
Rubidium nickel (II) trichloride, $RbNiCl_3$	6m	58
Rubidium nitrate, $RbNO_3$ (trigonal)	5m	45
Rubidium oxalate perhydrate, $Rb_2C_2O_4 \cdot H_2O_2$	9m	102
Rubidium perchlorate, $RbClO_4$	2m	30

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Rubidium periodate, $RbIO_4$	2m	31
Rubidium potassium chloride, $Rb_{0.5}K_{0.5}Cl$	8m	76
Rubidium selenate, Rb_2SeO_4	9m	44
Rubidium strontium chloride, $RbSrCl_3$	7m	54
Rubidium sulfate, Rb_2SO_4	8	48
Rubidium zinc fluoride, $RbZnF_3$	7m	57
Rubidium zinc sulfate hexahydrate, $Rb_2Zn(SO_4)_2 \cdot 6H_2O$	7m	55
Ruthenium, Ru	4	5
Ruthenium titanium, RuTi	6m	86
Samarium arsenate, $SmAsO_4$	4m	33
Samarium arsenide, SmAs	4m	68
Samarium chloride, $SmCl_3$	1m	40
Samarium fluoride, SmF_3	1m	41
Samarium gallium oxide, $Sm_3Ga_2(GaO_4)_3$	1m	42
Samarium oxide, Sm_2O_3 (cubic)	4m	34
Samarium oxychloride, SmOCl	1m	43
Samarium tin oxide, $Sm_2Sn_2O_7$	8m	77
Samarium vanadate, $SmVO_4$	5m	47
Scandium arsenate, $ScAsO_4$	4m	35
Scandium arsenide, ScAs	4m	68
Scandium oxide, Sc_2O_3	3	27
Scandium phosphate, $ScPO_4$	8	50
Scandium silicate (thortveitite), $Sc_2Si_2O_7$	7m	58
Selenium, Se	5	54
Selenium oxide (selenolite), SeO_2 (revised)	7m	60
Silicon, Si	2	6
Silicon dioxide, alpha or low quartz, SiO_2 (hexagonal)	3	24
Silicon dioxide (alpha or low cristobalite), SiO_2 (tetragonal) (revised)	10	48
Silicon dioxide (beta or high cristobalite), SiO_2 (cubic)	1	42
Silver, Ag	1	23
Silver, Ag (reference standard)	8m	2
Silver antimony sulfide, $AgSbS_2$ (cubic)	5m	48
Silver antimony sulfide (miargyrite), $AgSbS_2$ (monoclinic)	5m	49
Silver antimony sulfide (pyrargyrite), Ag_3SbS_3 (trigonal)	5m	51
Silver antimony telluride, $AgSbTe_2$	3m	47
Silver arsenate, Ag_3AsO_4	5	56
Silver arsenic sulfide, xanthoconite, Ag_3AsS_3	8m	126
Silver bromate, $AgBrO_3$	5	57
Silver bromide (bromyrite), AgBr	4	46
Silver carbonate, Ag_2CO_3	1m	44
Silver chlorate, $AgClO_3$	7	44
Silver chloride, (cerargyrite), AgCl	4	44
Silver cyanide, AgCN	9m	48
Silver dysprosium, AgDy	5m	66
Silver erbium, AgEr	5m	67
Silver gadolinium, AgGd	6m	87
Silver holmium, AgHo	5m	68
Silver iodide (iodyrite), AgI (hexagonal)	8	51
Silver iodide, gamma, AgI (cubic)	9	48
Silver molybdate, Ag_2MoO_4	7	45
Silver neodymium, AgNd	5m	71
Silver nitrate, $AgNO_3$	5	59
Silver nitrite, $AgNO_2$	5	60
Silver oxalate, $Ag_2C_2O_4$	9m	47
Silver oxide, Ag_2O	1m	45
Silver(II) oxynitrate, $Ag_7O_8NO_3$	4	61
Silver periodate, $AgIO_4$	9	49
Silver permanganate, $AgMnO_4$	7m	155
Silver perrhenate, $AgReO_4$	8	53
Silver phosphate, Ag_3PO_4	5	62
Silver potassium cyanide, $AgK(CN)_2$	8m	78
Silver samarium, AgSm	5m	73
Silver selenate, Ag_2SeO_4	2m	32
Silver sodium chloride, $Ag_{0.5}Na_{0.5}Cl$	8m	79
Silver subfluoride, Ag_2F	5m	53
Silver sulfate, Ag_2SO_4	7	46
Silver sulfide (argentite), Ag_2S	10	51
Silver terbium, AgTb	5m	74
Silver thulium, AgTm	5m	74
Silver yttrium, AgY	5m	75
Sodium, Na	9m	105
Sodium acid fluoride, $NaHF_2$	5	63
Sodium aluminum chloride silicate, sodalite, $Na_8Si_6Al_6O_{24}Cl_2$	7m	158
Sodium azide, alpha, NaN_3, at −90 to −100° C	8m	129
Sodium azide, beta, NaN_3	8m	130
Sodium borate, $Na_2B_8O_{13}$	7m	160
Sodium borohydride, $NaBH_4$	9	51
Sodium bromate, $NaBrO_3$	5	65
Sodium bromide, NaBr	3	47
Sodium calcium aluminum fluoride hydrate, thomsenolite, $NaCaAlF_6 \cdot H_2O$	8m	132
Sodium calcium beryllium aluminum fluorosilicate, meliphanite, $(Na_{0.63}Ca_{1.37})Be(Al_{0.13}Si_{1.87})(O_{6.25}F_{0.75})$	8m	135
Sodium calcium beryllium fluorosilicate, leucophanite, $NaCaBeFSi_2O_6$	8m	138
Sodium calcium carbonate hydrate, pirssonite, $Na_2Ca(CO_3)_2.2H_2O$	9m	106
Sodium calcium silicate, Na_2CaSiO_4	10m	48
Sodium calcium sulfate (glauberite), $Na_2Ca(SO_4)_2$	6m	59
Sodium carbonate monohydrate (thermonatrite), $Na_2CO_3 \cdot H_2O$	8	54
Sodium chlorate, $NaClO_3$	3	51
Sodium chloride (halite), NaCl	2	41
Sodium chromium oxide, Na_2CrO_4	9m	48
Sodium chromium oxide hydrate, $Na_2CrO_4.4H_2O$	9m	50
Sodium cobalt (II) sulfate tetrahydrate, $Na_2Co(SO_4)_2 \cdot 4H_2O$	6m	61
Sodium cyanate, NaCNO	2m	33
Sodium cyanide, NaCN (cubic)	1	78
Sodium cyanide, NaCN (orthorhombic) at 6 ° C	1	79
Sodium dichromate dihydrate, $Na_2Cr_2O_7 \cdot 2H_2O$	7m	62
Sodium fluoride (villiaumite), NaF	1	63
Sodium hexametaphosphate hexahydrate, $Na_6P_6O_{18} \cdot 6H_2O$	5m	54
Sodium hydrogen phosphate, $Na_3H(PO_3)_4$	10m	130
Sodium hydrogen silicate tetrahydrate, $Na_2H_2SiO_4 \cdot 4H_2O$	7m	163

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Sodium hydrogen sulfate hydrate, $NaHSO_4 \cdot H_2O$	9m	52
Sodium hydroxide, NaOH at 300 ° C	4m	69
Sodium iodate, $NaIO_3$	7	47
Sodium iodide, NaI	4	31
Sodium iron fluoride, Na_3FeF_6	9m	54
Sodium lanthanum fluosilicate, $(Na_2La_8)(SiO_4)_6F_2$	7m	64
Sodium lanthanum molybdenum oxide, $NaLa(MoO_4)_2$	10m	49
Sodium magnesium aluminum boron hydroxy silicate, dravite, $NaMg_3Al_6B_3Si_6O_{27}(OH)_4$	3m	47
Sodium magnesium sulfate tetrahydrate, bloedite, $Na_2Mg(SO_4)_2 \cdot 4H_2O$	6m	63
Sodium manganese (II) trifluoride, $NaMnF_3$	6m	65
Sodium mercury (II) trichloride dihydrate, $NaHgCl_3 \cdot 2H_2O$	6m	66
Sodium molybdate, Na_2MoO_4	1m	46
Sodium molybdenum oxide, $Na_2Mo_2O_7$	9m	110
Sodium neodymium fluosilicate, $(Na_2Nd_8)(SiO_4)_6F_2$	7m	66
Sodium nickel (II) sulfate tetrahydrate, $Na_2Ni(SO_4)_2 \cdot 4H_2O$	6m	68
Sodium nitrate (soda-niter), $NaNO_3$	6	50
Sodium nitrite, $NaNO_2$	4	62
Sodium orthotungstate(IV) dihydrate, $Na_2WO_4 \cdot 2H_2O$	2m	33
Sodium oxalate, $Na_2C_2O_4$	6m	70
Sodium oxide, Na_2O	10m	134
Sodium perchlorate, $NaClO_4$ (orthorhombic)	7	49
Sodium periodate, $NaIO_4$	7	48
Sodium praseodymium fluosilicate, $(Na_2Pr_8)(SiO_4)_6F_2$	7m	68
Sodium selenate, Na_2SeO_4	9m	55
Sodium selenide, Na_2Se	10m	135
Sodium silicate, alpha (III), $Na_2Si_2O_5$	8m	141
Sodium silicate, beta, $Na_2Si_2O_5$	10m	136
Sodium sulfate (thenardite), Na_2SO_4	2	59
Sodium sulfide, Na_2S	10m	140
Sodium sulfite, Na_2SO_3	3	60
Sodium telluride, Na_2Te	10m	141
Sodium tetrametaphosphate tetrahydrate, alpha, $Na_4P_4O_{12} \cdot 4H_2O$ (monoclinic)	10	52
Sodium tetrametaphosphate tetrahydrate, beta, $Na_4P_4O_{12} \cdot 4H_2O$ (triclinic)	2m	35
Sodium tin fluoride, $NaSn_2F_5$	7m	166
Sodium trimetaphosphate, $Na_3P_3O_9$	3m	49
Sodium trimetaphosphate monohydrate, $Na_3P_3O_9 \cdot H_2O$	3m	50
Sodium tungstate, Na_2WO_4	1m	47
Sodium zinc sulfate tetrahydrate, $Na_2Zn(SO_4)_2 \cdot 4H_2O$	6m	72
Sodium zinc trifluoride, $NaZnF_3$	6m	74
Sodium zirconium fluoride, $Na_7Zr_6F_{31}$	8m	144
Strontium aluminum hydroxide, $Sr_3Al_2(OH)_{12}$	10m	50
Strontium aluminum oxide, $Sr_3Al_2O_6$	10m	52
Strontium arsenate, $Sr_3(AsO_4)_2$	2m	36
Strontium azide, $Sr(N_3)_2$	8m	146
Strontium boron oxide, SrB_2O_4	3m	53
Strontium boron oxide, SrB_4O_7	4m	36
Strontium bromide fluoride, SrBrF	10m	54
Strontium bromide hexahydrate, $SrBr_2 \cdot 6H_2O$	4	60
Strontium carbonate (strontianite), $SrCO_3$	3	56
Strontium chloride, $SrCl_2$	4	40
Strontium chloride fluoride, SrClF	10m	55
Strontium chloride hexahydrate, $SrCl_2 \cdot 6H_2O$	4	58
Strontium fluoride, SrF_2	5	67
Strontium formate, $Sr(CHO_2)_2$	8	55
Strontium formate dihydrate, $Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic)	8	56
Strontium indium hydroxide, $Sr_3In_2(OH)_{12}$	6m	76
Strontium iodide hexahydrate, $SrI_2 \cdot 6H_2O$	8	58
Strontium manganese oxide, $SrMnO_3$ (cubic)	10m	56
Strontium manganese oxide, $SrMnO_3$ (hexagonal)	10m	58
Strontium molybdate, $SrMoO_4$	7	50
Strontium nitrate, $Sr(NO_3)_2$	1	80
Strontium oxide, SrO	5	68
Strontium peroxide, SrO_2	6	52
Strontium scandium oxide hexahydrate, $Sr_3Sc_2O_6 \cdot 6H_2O$	6m	78
Strontium sulfate (celestite), $SrSO_4$	2	61
Strontium sulfide, SrS	7	52
Strontium telluride, SrTe	4m	69
Strontium tin oxide, $SrSnO_3$	8m	80
Strontium titanate, $SrTiO_3$	3	44
Strontium tungstate, $SrWO_4$	7	53
Strontium zirconate, $SrZrO_3$	9	51
Sulfamic acid, NH_3SO_3	7	54
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d-Tartaric acid, $C_4H_6O_6$	7m	168
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Tellurium, Te	1	26
Tellurium(IV) oxide (paratellurite), TeO_2 (tetragonal)	7	56
Tellurium(IV) oxide, paratellurite, TeO_2 (tetragonal)	10	55
Tellurium(IV) oxide, tellurite, TeO_2 (orthorhombic)	9	57
Terbium arsenate, $TbAsO_4$	3m	54
Terbium arsenide, TbAs	5m	75
Terbium nitride, TbN	4m	70
Terbium phosphide, TbP	5m	76
Terbium selenide, TbSe	5m	76
Terbium sulfide, TbS	5m	77
Terbium telluride, TbTe	5m	77
Terbium vanadate, $TbVO_4$	5m	56
Thallium aluminum sulfate dodecahydrate, $TlAl(SO_4)_2 \cdot 12H_2O$	6	53
Thallium(I) arsenate, Tl_3AsO_4	2m	37
Thallium azide, TlN_3	8m	82
Thallium(I) bromate, $TlBrO_3$	8	60
Thallium bromide, TlBr	7	57
Thallium cadmium sulfate, $Tl_2Cd_2(SO_4)_3$	8m	83
Thallium(I) chlorate, $TlClO_3$	8	61
Thallium(I) chloride, TlCl	4	51
Thallium chloroplatinate, Tl_2PtCl_6	5	70
Thallium chlorostannate, Tl_2SnCl_6	6	54

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A mineral name in ( ) indicates a synthetic sample.

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Thallium chromate, Tl_2CrO_4	3m	54
Thallium chromium sulfate dodecahydrate, $TlCr(SO_4)_2 \cdot 12H_2O$	6	55
Thallium cobalt sulfate, $Tl_2Co_2(SO_4)_3$	8m	85
Thallium cobalt sulfate hexahydrate, $Tl_2Co(SO_4)_2 \cdot 6H_2O$	7m	70
Thallium copper sulfate hexahydrate, $Tl_2Cu(SO_4)_2 \cdot 6H_2O$	7m	72
Thallium fluosilicate, Tl_2SiF_6	6	56
Thallium gallium sulfate dodecahydrate, $TlGa(SO_4)_2 \cdot 12H_2O$	6	57
Thallium(I) iodate, $TlIO_3$	8	62
Thallium(I) iodide, TlI (orthorhombic)	4	53
Thallium iron sulfate hydrate, $Tl_2Fe(SO_4)_2 \cdot 6H_2O$	8m	87
Thallium magnesium chromium oxide, $Tl_2Mg_2(CrO_4)_3$	8m	89
Thallium magnesium sulfate hexahydrate, $Tl_2Mg(SO_4)_2 \cdot 6H_2O$	7m	74
Thallium manganese sulfate, $Tl_2Mn_2(SO_4)_3$	7m	76
Thallium nickel sulfate hexahydrate, $Tl_2Ni(SO_4)_2 \cdot 6H_2O$	7m	78
Thallium(I) nitrate, $TlNO_3$	6	58
Thallium(III) oxide, Tl_2O_3	2	28
Thallium(I) perchlorate, $TlClO_4$	2m	38
Thallium(I) phosphate, Tl_3PO_4	7	58
Thallium(III) phosphate, $TlPO_4$	7	59
Thallium(I) sulfate, Tl_2SO_4	6	59
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Thallium(I) tungstate, Tl_2WO_4	1m	48
Thallium zinc sulfate hexahydrate, $Tl_2Zn(SO_4)_2 \cdot 6H_2O$	7m	80
Thorium arsenide, ThAs	4m	70
Thorium oxide (thorianite), ThO_2	1	57
Thulium arsenate, $TmAsO_4$	3m	56
Thulium arsenide, TmAs	4m	71
Thulium nitride, TmN	4m	71
Thulium sesquioxide, Tm_2O_3	9	58
Thulium telluride, TmTe	4m	72
Thulium vanadate, $TmVO_4$	5m	57
Tin, alpha, Sn (cubic)	2	12
Tin, beta, Sn (tetragonal)	1	24
Tin arsenide, SnAs	4m	37
Tin(II) fluoride, SnF_2	3m	51
Tin(IV) iodide, SnI_4	5	71
Tin(II) oxide, SnO	4	28
Tin(IV) oxide (cassiterite), SnO_2	1	54
Tin sulfide (berndtite), beta, SnS_2	9m	57
Tin(II) telluride, SnTe	7	61
Titanium, Ti	3	1
Titanium dioxide, brookite, TiO_2 (orthorhombic)	3m	57
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Titanium oxide (rutile), TiO_2 (revised)	7m	83
Titanium(III) oxide, $TiO_{1.515}$	9	59
Titanium silicide, Ti_5Si_3	8	64
Titanium sulfide, TiS_2	4m	72
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Yttrium oxide, Y_2O_3	3	28
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Zinc cobalt oxide, $ZnCo_2O_4$	10m	60
Zinc cyanide, $Zn(CN)_2$	5	73
Zinc fluoride, ZnF_2	6	60
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Zinc germanate, Zn_2GeO_4	10	56
Zinc glutamate dihydrate, $ZnC_5H_7NO_4 \cdot 2H_2O$	7m	170
Zinc iodide, ZnI_2	9	60
Zinc iron oxide (franklinite), $ZnFe_2O_4$	9m	60
Zinc manganese oxide (hetaerolite), $ZnMn_2O_4$	10m	61
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Zinc selenide, ZnSe	3	23
Zinc sulfate (zinkosite), $ZnSO_4$	7	64
Zinc sulfate heptahydrate (goslarite), $ZnSO_4 \cdot 7H_2O$	8	71
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A mineral name in ( ) indicates a synthetic sample.

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Zirconium oxide, ZrO	5m	81
Zirconium phosphide, ZrP	4m	75
Zirconium silicate, zircon, $ZrSiO_4$	4	68
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A mineral name in ( ) indicates a synthetic sample.

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*Natural mineral.

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Paratellurite, TeO_2	7	56
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*Thomsenolite, $NaCaAlF_6 \cdot H_2O$	8m	132
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* 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 84 substances. Forty-seven of these patterns represent experimental data and 37 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.

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Aluminum nitrate hydrate, $Al(NO_3)_3 \cdot 9H_2O$

Sample

The sample was prepared by slow evaporation of an aqueous solution of $Al(NO_3)_3$. The crystals were filtered out and washed with ethyl alcohol.

Color

Colorless

Optical data

Biaxial (-), $N_\alpha = 1.401$, $N_\beta = 1.514$, $N_\gamma = 1.525$; $2V \simeq 25°$.

Structure

Monoclinic, $P2_1/c$ (14), Z=4, isostructural with $Cr(NO_3)_3 \cdot 9H_2O$ [Kannan and Viswamitra, 1965].

NBS lattice constants:

a = 13.847(8)Å
b = 9.617(2)
c = 10.908(5)
β = 95.68(2)°

Density

(calculated) 1.724 g/cm³

Reference intensity

$I/I_{corundum}$ 0.5

Additional patterns

1. PDF card 1-435 [Hanawalt et al., 1938]
2. PDF card 12-472 [Aluminium Lab. Ltd.,Kingston Canada].

References

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Kannan, K. K. and Viswamitra, M. A. (1965). Acta Cryst. 19, 151.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.87	1	110	11.24
7.20	12	011	12.29
6.55	70	$\bar{1}11$	13.51
6.21	60	111	14.26
5.60	14	210	15.81
5.22	6	$\bar{1}02$	16.97
4.89	18	102	18.13
4.82	25	211,020	18.41
4.729	4	012	18.75
4.595	4	$\bar{1}12$,300	19.30
4.539	15	120	19.54
4.487	45	$\bar{2}02$	19.77
4.362	3	112	20.34
4.231	2	$\bar{1}21$	20.98
4.143	10	310,121	21.43
4.074	60	202	21.80
3.994	45	$\bar{3}11$	22.24
3.943	50	220	22.53
3.762	30	311	23.63
3.639	12	221	24.44
3.599	65	022	24.72
3.541	6	$\bar{1}22$	25.13
3.449	9	$\bar{3}12$,400	25.81
3.426	12	122	25.99
3.387	6	013	26.29
3.278	16	$\bar{2}22$	27.18
3.244	35	410,$\bar{3}21$	27.47
3.219	19	113	27.69
3.123	20	130	28.56
3.112	20	321	28.66
3.074	12	031	29.02
3.049	20	$\bar{4}02$	29.27
3.017	100	$\bar{1}31$	29.58
2.982	45	131	29.93
2.907	35	230,$\bar{4}12$	30.73
2.878	7	$\bar{1}23$	31.05
2.854	5	$\bar{3}13$	31.32
2.835	4	$\bar{2}31$	31.53
2.788	3	402,123	32.08
2.779	7	231	32.18
2.761	18	032	32.40
2.680	6	132	33.41
2.615	20	$\bar{2}04$,104,+	34.26
2.609	30	014,$\bar{2}32$,+	34.34
2.590	50	$\bar{3}31$	34.60
2.538	16	$\bar{3}23$	35.33
2.522	35	331,114,+	35.57
2.446	3	$\bar{3}04$,204	36.71
2.422	2	$\bar{3}32$	37.09
2.399	6	033	37.45
2.393	4	520,$\bar{1}33$	37.56
2.369	40	$\bar{3}14$,140,+	37.95
2.363	25	$\bar{1}24$,024,+	38.05
2.348	30	041,430	38.31
2.326	4	$\bar{4}31$	38.68
2.307	12	$\bar{4}23$,141	39.01
2.301	14	$\bar{2}24$,600,+	39.16
2.271	16	240	39.65
2.263	8	431,$\bar{5}22$	39.80
2.242	10	$\bar{4}04$,$\bar{5}13$,+	40.19
2.210	2	$\bar{4}32$,241	40.79
2.184	16	$\bar{1}42$,$\bar{4}14$,+	41.30

Aluminum tungsten oxide, $Al_2(WO_4)_3$

Sample

The sample was prepared by adding $NaWO_4$ solution to one of $AlCl_3$ and heating the precipitate two hours at 800 °C and 15 minutes at 900 °C.

Color

Colorless

Structure

Orthorhombic, Pnca (60), Z=2, isostructural with other tungstates and molybdates of the smaller trivalent rare-earth elements such as $Gd_2(WO_4)_3$ [Craig and Stephenson, 1968].

NBS lattice constants:

a = 9.139(2) Å
b = 12.596(2)
c = 9.060(2)

Density

(calculated) 2.539 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.3

Additional patterns

1. PDF card 18-72 [Waring, 1965] (incorrectly called $2Al_2O_3 \cdot 5WO_3$)

References

Craig, D. C. and Stephenson, N. C. (1968). Acta Cryst. B24, 1250.

Waring, J. (1965). J. Am. Ceram. Soc. 48, 493.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.30	11	020	14.04
5.73	13	111	15.46
4.53	11	002	19.59
4.50	6	121	19.73
4.296	35	210	20.66
4.059	40	102	21.88
3.877	50	211	22.92
3.867	45	112	22.98
3.810	100	031	23.33
3.697	16	220	24.05
3.676	7	022	24.19
3.519	25	131	25.29
3.422	50	221	26.02
3.219	15	202	27.69
3.147	12	040	28.34
3.115	4	212	28.63
3.090	6	230	28.87
2.933	19	013	30.45
2.926	10	231	30.53
2.865	13	222	31.19
2.828	6	141	31.61
2.816	9	311	31.75
2.624	7	321	34.14
2.610	16	123	34.33
2.593	7	240	34.56
2.555	2	232	35.10
2.528	7	302	35.48
2.493	8	241	36.00
2.488	9	142	36.07
2.480	7	312	36.19
2.471	6	213	36.32
2.429	5	051	36.98
2.380	5	331	37.76
2.368	19	133	37.97
2.346	3	322,151	38.34
2.340	4	223	38.45
2.285	2	400	39.40
2.265	3	004	39.77
2.252	7	242	40.01
2.206	11	250	40.87
2.182	17	411	41.35
2.166	6	114,332	41.67
2.161	5	233	41.77
2.142	10	251,152	42.15
2.132	5	024	42.35
2.114	5	313	42.73
2.100	13	060	43.03
2.076	1	124	43.56
2.030	3	323,204	44.61
2.004	9	214	45.21
1.984	3	252	45.70
1.972	9	342	45.99
1.959	2	431	46.30
1.941	6	422	46.77
1.935	5	053	46.92
1.907	6	260	47.66
1.8926	3	153	48.03
1.8650	13	162	48.79
1.8490	13	440	49.24
1.8385	9	044	49.54
1.8271	3	234	49.87
1.7987	2	314	50.73
1.7931	5	015	50.88
1.7833	5	352	51.18