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

## Standard X-ray Diffraction Powder Patterns

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No. 25-17  
1980  
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# Standard X-ray Diffraction Powder Patterns Section 17—Data for 54 Substances

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Marlene C. Morris, Howard F. McMurdie, Eloise H. Evans, and  
Boris Paretzkin

International Centre for  
Diffraction Data

Camden R. Hubbard and Simon J. Carmel

National Measurement Laboratory  
National Bureau of Standards  
Washington, DC 20234



International Centre for  
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## STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Previous work has been published as a book entitled Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976) (JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081). The volume is sold with an accompanying search manual, and contains 949 card images of patterns of experimental data, published originally as Circular 539 (vols. 1-10) and Monograph 25, Sections 1-12, and most of Section 13.

Individual copies of the Circular and Monograph are still available and may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161. If a publication listed below is identified with a number, it must be used in ordering. All are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

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### ERRATA

#### Monograph 25

- Section 16, pp. iii, 66, 176, 183: The corrected formula for sodium borate hydroxide hydrate (borax) is  $\text{Na}_2\text{B}_4\text{O}_5(\text{OH})_4 \cdot 8\text{H}_2\text{O}$ .
- p. 1: In the 2nd column, last paragraph, line 5 from the bottom, the symbols should be  $K\alpha_1$ .
- p. 129: In the paragraph "Structure", the space group should be  $P2_1/c$ .

# STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 17. --- Data for 54 Substances

by

Marlene C. Morris, Howard F. McMurdie,  
Eloise H. Evans and Boris Paretzkin  
JCPDS--International Centre for Diffraction Data

and

Camden R. Hubbard and Simon J. Carmel  
National Bureau of Standards

Standard x-ray diffraction patterns are presented for 54 substances. 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 in some cases.

Key words: Crystal structure; lattice constants; 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 JCPDS--International Centre for Diffraction Data,<sup>1</sup> the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the JCPDS, 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 54 experimental patterns, and is the twenty-seventh of the series of <sup>2</sup> Standard X-ray Diffraction Powder Patterns.

## EXPERIMENTAL POWDER PATTERNS

CAS registry number. The Chemical Abstracts Service Registry Number is included, when available, to help identify the sample. This number forms the basis for computer aided searching of Chemical Abstracts.

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory.

<sup>1</sup>JCPDS--International Centre for Diffraction Data, 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.

<sup>2</sup>See previous page for other published volumes.

Appropriate annealing or recrystallization of the samples improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

Optical data. When reported, optical measurements were made by grain immersion methods, in white light, using oils standardized in sodium light, in the refractive index range 1.49 to 2.1 [Hartshorne and Stuart, 1970].

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

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard. Choice of the standard was determined by the need for low angle and unobstructed reflections. The amount of standard was estimated so that the intensity of its strongest peak would be about equal to the intensity of the strongest peak of the sample.

To avoid errors associated with aberrations at the very top of the peaks, the readings of  $2\theta$  were taken at positions about 20% of the way down from the top, and in the center of the peak width. The  $K\alpha_2$  peaks were occasionally read to assist in establishing a  $K\alpha_1$  peak position, but  $K\alpha_2$  peaks were not reported.

At low angles,  $K\alpha_1$  and  $K\alpha_2$  peaks were unresolved for both the sample and the internal standard. The internal standard corrections were established from the theoretical values for  $K\alpha_1$  and were applied to the unresolved low angle peaks, as well as to the resolved  $K\alpha_1$  peaks in the higher angle regions. If the internal standard correction varied along the length of the pattern, linear interpolations were used.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in Table 1; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Table 1

hkl	Calculated 2θ Angles, CuKα <sub>1</sub> λ = 1.540598Å		
	W a=3.16524Å ±.00004	Ag a=4.08651Å ±.00002	Si a=5.43088Å ±.00004
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.303
310	100.632		
311		77.390	56.123
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.131
331		110.499	76.377
420		114.914	
422		134.871	88.032
511/333		156.737	94.954
440			106.710
531			114.094
620			127.547
533			136.897
444			158.638

The internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Single crystal cell parameter data were also collected. The lattice parameters from the two methods agreed within three parts in 10<sup>5</sup> [Hubbard et al., 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

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

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]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of Crystal Data [1973].

A computer program [Evans et al., 1963] assigned hkl's and refined the lattice constants.

Cell refinement was based only upon 2θ<sub>obs</sub> values which could be indexed without ambiguity. The program minimized the value Σ(θ<sub>obs</sub>-θ<sub>calc</sub>)<sup>2</sup>. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

In indexing cubic patterns, for a given reflection multiple hkl's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

The number of significant figures at any reported d-value was derived from the average error in |2θ<sub>obs</sub> - 2θ<sub>calc</sub>| and Δd/d = -cotθ Δθ. With these conditions, the rounding of any specific d at the given number of significant digits yielded an error in its corresponding 2θ which was less than the average error in 2θ.

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943 x 10<sup>23</sup> [Deslattes et al., 1974] and 1977 atomic weights published by the International Union of Pure and Applied Chemistry [1979].

Figure of merit. Several figures of merit ratings are available for assessing indexed powder data. M<sub>20</sub> [de Wolff, 1968] is a criterion for the reliability of the unit cell and indexing. A value of M<sub>20</sub> > 10 will guarantee the essential correctness of the indexing provided there are not more than 2 spurious lines (X<sub>20</sub> < 2) [de Wolff, 1968]. In general, patterns reported in this publication had M<sub>20</sub> > 20 and X = 0. M<sub>20</sub> was specified for any pattern indexed with a cell derived only through computer indexing from powder data, without further confirmation.

The accuracy and completeness of measured interplanar spacings was conveniently reported as F<sub>N</sub> [Smith and Snyder, 1979]. The format used in this publication was F<sub>N</sub> = overall value (|Δ2θ|, N<sub>poss</sub>), where N, the number of observed reflections was chosen as 30, or the maximum number of lines of the pattern if the entire pattern had fewer than 30 lines. The "overall value" was the figure of merit, F<sub>N</sub>, as defined by Smith and Snyder [1979], and |Δ2θ| was the average absolute magnitude of discrepancy between observed and calculated 2θ values for each reported hkl. N<sub>poss</sub> was the number of diffraction lines allowed in the space group, up to the N<sup>th</sup> observed and indexed line. Co-positional lines such as the cubic 221 and 300 are counted as one possible line.

Intensity measurements. It was found that samples which gave satisfactory intensity patterns



usually had an average particle size smaller than 10  $\mu\text{m}$ , as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (see Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. Occasionally, a rotating sample holder was used instead. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line.

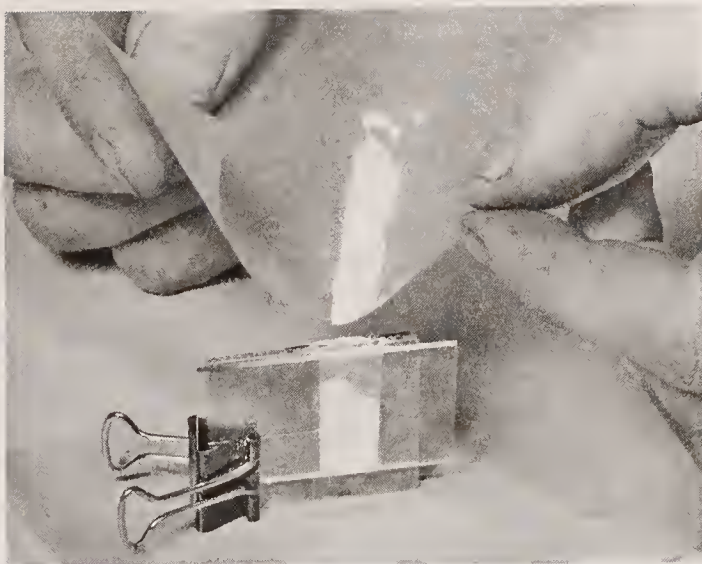


Figure 1.

As a check on reproducibility, each sample was mounted at least 3 times. The intensity values were determined for each of the mountings. Theta-compensating (variable divergence) slits were sometimes used to gather the intensity data. In that case, the average  $I(\text{comp})$  for each spacing was converted to an equivalent fixed slit value, using the approximate equation:

$$I(\text{fixed}) = \frac{I(\text{comp})}{\sin \theta}$$

The reported  $I^{\text{rel}}$  value for each observed spacing was the scaled average of the separate measurements, rounded to the nearest integer. The estimated standard deviation,  $\sigma$ , in the relative intensity values was calculated from the values of the five strongest lines, excluding the line with  $I = 100$ .

$$\sigma_i^2 = \frac{1}{n-1} \sum_{j=1}^n (I_j^{\text{rel}}(k) - \langle I \rangle_j)^2$$

and

$$\sigma = \left\{ \frac{1}{m} \sum_{i=1}^m \sigma_i^2 \right\}^{\frac{1}{2}}$$

where .

$m$  is the number of strong lines (usually 5), and

$n$  is the number of independent observations  $i$ , per line.

Where conversion of intensities for effects of theta-compensating slits was required, each  $\sigma_i$  was multiplied by the conversion factor

$$f = \frac{I(\text{comp})}{I(\text{fixed})}$$

#### Reference Intensity Ratio, $I/I_{\text{corundum}}$ .

The reference intensity ratio,  $I/I_c$ , has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the reflection 113 (hexagonal) of corundum ( $\alpha\text{-Al}_2\text{O}_3$ ) [Visser and de Wolff, 1964]. In this publication the ratios  $I/I_c$  were tabulated for copper  $K\alpha$  radiation, for a 1:1 mixture



Figure 2.

by weight of the sample and corundum. Occasionally  $I/I_c$  was not determined because it was not feasible.

A procedure has been adopted, to achieve greater statistical accuracy [Hubbard and Smith, 1977]. For any weight fractions of sample and corundum,  $x_s$  and  $x_c$  ( $x_s = 1 - x_c$ ), the intensities for reflection  $\underline{h}$  of the sample and  $\underline{k}$  of corundum were measured for several combinations of  $\underline{h}$  and  $\underline{k}$  usually within the same region of  $2\theta$ , to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{I(h_o)}{I_c(113)} = \frac{x_c}{x_s} \cdot \frac{I_c^{\text{rel}}(\underline{k})}{I^{\text{rel}}(\underline{h})} \cdot \frac{I(\underline{h})}{I(\underline{k})}$$

and ( $h_0$ ) indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection ( $h_0$ ) will be the one with  $I = 100$  since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio,  $I/I_c$ . These values yield the tabulated average  $\langle I/I_c \rangle$ . From these data, the estimated deviation,  $\Delta$ , was obtained from

$$\Delta = \frac{\sum_{i=1}^n \left| (I/I_c)_i - \langle I/I_c \rangle \right|}{n}$$

where  $n$  is the number of measurements of the reference intensity ratio. The estimated deviation in the least significant figures is given in parentheses.

Format of tables. The printing of the data has been computerized. Superimposed reflections were treated in one of two ways. If a d-spacing had only two possible indices, an  $\underline{M}$  was added to the d-spacing which was repeated on the next line, but with the second index. However, if there were more than two possible indices, a plus sign was used in like manner. In both cases, the composite intensity was printed only once and aligned with the first reflection. The symbol "1L" in the intensity column was used to indicate "less than 1".

#### UNITS

In this publication the Ångström unit ( $1\text{Å} = 100\text{ pm}$ ) was selected for presentation of the d-spacings and lattice parameters to maintain consistency with (a) the earlier publications of Standard X-ray Diffraction Powder Patterns (Circular 539 volumes 1-10 and Monograph 25 sections 1-16), (b) the publications of the International Union of Crystallography: Acta Crystallographica and the Journal of Applied Crystallography, and (c) the continuing publication of cards and search manuals of the Powder Diffraction File (now consisting of over 33,000 entries). The PDF search manuals are based on the d-spacings in Å of the three strongest lines. Consistent with the choice of the Å unit for length, the volume of the unit cell is expressed in Å<sup>3</sup> ( $1\text{Å}^3 = 1 \times 10^{-30}\text{ m}^3$ ). Densities are reported in g/cm<sup>3</sup> ( $1\text{ gm/cm}^3 = 10^3\text{ kg/m}^3$ ).

#### ACKNOWLEDGMENTS

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Standard Reference Material 640 (1974), Silicon Powder X-ray Diffraction Standard, obtainable from the National Bureau of Standards, Office of Standard Reference Materials, Washington, DC 20234. Current price will be quoted on request.

Swanson, H. E., Morris, M. C., and Evans, E. H. (1966). *Nat'l. Bur. Std. U.S. Monogr.* 25, Sec. 4, 3.

Visser, J. W. and de Wolff, P. M. (1964). "Absolute Intensities," Report 641.109, Technisch Physische Dienst, Delft, Netherlands.

Wolff, P. M. de (1968). *J. Appl. Crystallogr.* 1, 108.

Aluminum Borate, Al<sub>18</sub>B<sub>4</sub>O<sub>33</sub>

CAS registry no.  
12005-61-7

Sample

The sample was prepared by heating a 1:1 mixture of Al<sub>2</sub>O<sub>3</sub> and H<sub>3</sub>BO<sub>3</sub> together at 1250 °C. The compound was later annealed at 1500 °C.

Color

Colorless

Structure

Orthorhombic, Amam (63), A2<sub>1</sub>am (36), or Ama2 (40), Z = 1 [Scholze, 1956]. Baumann and Moore [1942] reported data for this phase. Although the lattice constants were in good agreement with NBS constants, their pattern does not index on the given cell.

Lattice constants of this sample

a = 7.6874(8) Å  
b = 15.0127(15)  
c = 5.6643(6)

a/b = 0.5121  
c/b = 0.3773

Volume

653.70 Å<sup>3</sup>

Density

(calculated) 2.685 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 65.2(0.010,45)

Reference intensity

I/I<sub>corundum</sub> = 1.27(5)

Additional pattern

1. PDF card 9-248 [Scholze, 1956]

References

Baumann, H. N., Jr. and Moore, C. H., Jr. (1942). J. Amer. Chem. Soc. 25, No. 14, 391.  
Scholze, H. (1956). Z. Anorg. Allg. Chem. 284, 272.

CuKα <sub>1</sub> γ = 1.540598 Å; temp. 25±1 °C				
Internal standard Ag, a = 4.08651 Å				
d(Å)	I <sup>rel</sup>	hkl	2θ(°)	
σ = ±3				
7.52	1	0 2 0	11.76	
5.375	100	1 2 0	16.48	
5.301	18	0 1 1	16.71	
4.365	52	1 1 1	20.33	
3.846	8	2 0 0	23.11	
3.750M	16	0 4 0	23.71	
3.750M		0 3 1	23.71	
3.419	14	2 2 0	26.04	
3.373M	42	1 4 0	26.40	
3.373M		1 3 1	26.40	
3.111	2	2 1 1	28.67	
2.831	7	0 0 2	31.58	
2.685M	41	2 4 0	33.35	
2.685M		2 3 1	33.35	
2.649	4	0 2 2	33.81	
2.505	25	1 2 2	35.82	
2.424	4	3 2 0	37.05	
2.307	5	3 1 1	39.01	
2.281	3	2 0 2	39.48	
2.260	14	0 4 2	39.85	
2.181	27	2 2 2	41.36	
2.169	10	1 4 2	41.61	
2.116M	21	3 4 0	42.69	
2.116M		3 3 1	42.69	
2.097	3	2 6 0	43.11	
2.005	1L	0 7 1	45.18	
1.9474	4	2 4 2	46.60	
1.9415	2	1 7 1	46.75	
1.9218	2	4 0 0	47.26	
1.8733	5	0 1 3	48.56	
1.8618	4	4 2 0	48.88	
1.8424M	13	3 5 1	49.43	
1.8424M		3 2 2	49.43	
1.8196	12	1 1 3	50.09	
1.7896	3	3 6 0	50.99	
1.7776	5	2 7 1	51.36	
1.7215	2	1 3 3	53.16	
1.7105M	6	4 4 0	53.53	
1.7105M		4 3 1	53.53	
1.6852	14	2 6 2	54.40	
1.5904	7	4 0 2	57.94	
1.5650M	6	1 5 3	58.97	
1.5650M		0 8 2	58.97	
1.5564M	3	4 5 1	59.33	
1.5564M		4 2 2	59.33	

Aluminum Borate, Al<sub>18</sub>B<sub>4</sub>O<sub>33</sub> - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$	hkl	$2\theta(^{\circ})$
	$\sigma = \pm 3$		
1.5330	2	1 8 2	60.33
1.5130M	19	3 6 2	61.21
1.5130M		3 1 3	61.21
1.4764+	3	5 1 1	62.90
1.4764+		2 5 3	62.90
1.4643	2	4 4 2	63.48
1.4496	7	2 8 2	64.20
1.4159	9	0 0 4	65.92
1.3982	2	2 10 0	66.86
1.3876	1	4 7 1	67.44
1.3694	2	1 2 4	68.46
1.3560	3	3 5 3	69.23
1.3425M	3	4 8 0	70.03
1.3425M		4 6 2	70.03
1.3299+	10	5 2 2	70.79
1.3299+		2 7 3	70.79
1.3067	6	1 10 2	72.24
1.2953	2	3 10 0	72.98
1.2810	1	6 0 0	73.93
1.2716	1	5 4 2	74.57
1.2631	1	6 2 0	75.16
1.2533M	7	2 10 2	75.85
1.2533M		2 4 4	75.85
1.2513	6	0 12 0	75.99
1.2339	2	1 9 3	77.26
1.2296	1	4 9 1	77.58
1.2231	1	3 2 4	78.07
1.2129+	1	4 8 2	78.85
1.2129+		6 4 0	78.85
1.1890+	1	5 6 2	80.76
1.1890+		2 9 3	80.76
1.1770	2	3 4 4	81.76

Ammonium Borate Hydrate,  $\text{NH}_4\text{B}_5\text{O}_8 \cdot 4\text{H}_2\text{O}$

Synonyms

1. Ammonium pentaborate tetrahydrate
2. APT

CAS registry no.  
12229-12-8

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was recrystallized from an aqueous solution at room temperature.

Color

Colorless

Structure

Orthorhombic, Bba2 (41), Z = 4 [Cook and Jaffe, 1957; Clark and Christ, 1959].

Lattice constants of this sample

a = 11.033(3) Å

b = 11.332(3)

c = 9.238(3)

a/b = 0.9736

c/b = 0.8152

Volume

1155.0 Å<sup>3</sup>

Density

(calculated) 1.565 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 57.2 (0.014,38)

Reference intensity

I/I<sub>corundum</sub> = 1.08(6)

Additional pattern

1. PDF card 12-638 [Clark and Christ, 1959]

References

- Clark, J. R. and Christ, C. L. (1959).  
Amer. Mineral. 44, 1150.  
Cook, W. R., Jr. and Jaffe, H. (1957).  
Acta Crystallogr. 10, 705.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C				
Internal standard Si, a = 5.43088 Å				
d(Å)	I <sup>rel</sup> σ = ±2	hkl		2θ(°)
6.00	63	1 1 1		14.74
5.67	12	0 2 0		15.63
5.52	46	2 0 0		16.04
4.951	2	2 1 0		17.90
4.617	7	0 0 2		19.21
4.427	1	1 2 1		20.04
3.544	80	2 0 2		25.11
3.383	100	2 1 2		26.32
3.334	11	1 3 1		26.72
3.271	9	3 1 1		27.24
3.003	4	2 2 2		29.73
2.926	7	3 2 1		30.53
2.868	4	1 1 3		31.16
2.834	31	0 4 0		31.54
2.760	2	4 0 0		32.41
2.680	2	4 1 0		33.41
2.627	5	1 2 3		34.10
2.586	1	2 3 2		34.66
2.533	8	3 3 1		35.41
2.479	1L	4 2 0		36.20
2.414	1	0 4 2		37.21
2.367	4	4 0 2		37.98
2.332	4	1 3 3		38.58
2.317	9	4 1 2		38.83
2.312M	9	3 1 3		38.93
2.312M		0 0 4		38.93
2.212	8	2 4 2		40.75
2.182	16	3 4 1		41.35
2.178	16	3 2 3		41.43
2.158	4	1 5 1		41.83
2.138	3	0 2 4		42.24
2.107	7	5 1 1		42.88
2.095M	2	2 5 0		43.14
2.095M		2 1 4		43.14
2.048	2	1 4 3		44.18
2.007M	7	5 2 1		45.15
2.007M		4 3 2		45.15
1.909	6	2 5 2		47.59
1.888M	2	3 5 1		48.16
1.888M		0 6 0		48.16
1.856	4	2 3 4		49.03
1.817	4	4 4 2		50.16
1.7998M	2	1 5 3		50.68
1.7998M		1 1 5		50.68
1.7715M	3	5 1 3		51.55

Ammonium Borate Hydrate,  $\text{NH}_4\text{B}_5\text{O}_8 \cdot 4\text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 2$	hkl	$2\theta(^{\circ})$
1.7715M		4 0 4	51.55
1.7506M	3	4 5 0	52.21
1.7506M		4 1 4	52.21
1.7102M	2	5 4 1	53.54
1.7102M		5 2 3	53.54
1.7029	2	2 4 4	53.79
1.6533M	1	6 3 0	55.54
1.6533M		3 6 1	55.54
1.6206	1L	5 3 3	56.76
1.5780	1	1 7 1	58.44
1.5427	1	6 4 0	59.91

Ammonium Nickel Sulfate Hydrate,  $(\text{NH}_4)_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$

CAS registry no.  
51287-85-5

Sample  
The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color  
Strong bluish green

Structure  
Monoclinic,  $P2_1/a$  (14),  $Z = 2$ . The structure was determined by Grimes et al. [1963] and by Montgomery and Lingafelter [1964]. It is isostructural with other "Tutton" salts [Tutton, 1916].

Lattice constants of this sample

$a = 9.1862(15) \text{ \AA}$   
 $b = 12.468(2)$   
 $c = 6.2423(10)$   
 $\beta = 106.93(2)^\circ$

$a/b = 0.7368$   
 $c/b = 0.5007$

Volume  
 $684.0 \text{ \AA}^3$

Density  
(calculated)  $1.918 \text{ g/cm}^3$

Figure of merit  
 $F_{30} = 63.7(0.012, 38)$

Reference intensity  
 $I/I_{\text{corundum}} = 0.92(5)$

Additional pattern  
1. PDF card 12-454 [Institute of Physics, Cardiff, Wales]

References  
Grimes, N. W., Kay, H. F., and Webb, M. W. (1963). *Acta Crystallogr.* 16, 823.  
Montgomery, H. and Lingafelter, E. C. (1964). *Acta Crystallogr.* 17, 1478.  
Tutton, A. E. (1916). *Trans. Roy. Soc. London Ser. A* 216, 1.

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 5$	hkℓ	$2\theta(^\circ)$
5.090	20	1 2 0	17.41
4.397	19	2 0 0	20.18
4.316	21	0 2 1	20.56
4.243	36	-1 2 1	20.92
4.166	100	-2 0 1	21.31
4.147	66	2 1 0	21.41
3.952	6	-2 1 1	22.48
3.757	88	1 3 0	23.66
3.586	16	1 2 1	24.81
3.466	4	-2 2 1	25.68
3.410	14	0 3 1	26.11
3.376	18	-1 3 1	26.38
3.119	20	0 4 0	28.60
3.037	32	2 1 1	29.39
3.027	44	-1 1 2	29.49
2.943	4	-2 3 1	30.35
2.913	4	-3 1 1	30.67
2.903	5	0 1 2	30.77
2.892	6	-2 0 2	30.89
2.853	6	3 1 0	31.33
2.816	6	-2 1 2	31.75
2.796	28	2 2 1	31.98
2.790	26	-1 2 2	32.05
2.742	3	-1 4 1	32.63
2.703	8	-3 2 1	33.12
2.651	1	3 2 0	33.79
2.623	2	-2 2 2	34.16
2.550	6	1 1 2	35.17
2.541M	11	2 4 0	35.29
2.541M		1 4 1	35.29
2.501	7	2 3 1	35.88
2.430	25	-3 3 1	36.96
2.395	3	3 3 0	37.52
2.374	2	-2 3 2	37.86
2.302	2	0 5 1	39.10
2.208M	16	1 3 2	40.84
2.208M		2 4 1	40.84
2.166+	7	1 5 1	41.67
2.166+		4 1 0	41.67
2.156M	9	0 4 2	41.86
2.156M		2 1 2	41.86
2.134	9	3 4 0	42.31
2.120	6	-2 4 2	42.62
2.072	10	4 2 0	43.64
2.052	2	-2 0 3	44.09
2.049	2	-1 1 3	44.17
2.024	3	-2 1 3	44.74
2.005	1	-4 3 1	45.19
1.990	4	0 0 3	45.54
1.975	2	-4 2 2	45.92
1.963	4	0 6 1	46.22
1.956	3	-1 6 1	46.39
1.950M	2	2 5 1	46.53
1.950M		-2 2 3	46.53
1.942M	2	4 3 0	46.73

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard W, $a = 3.16524 \text{ \AA}$			
$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 5$	hkℓ	$2\theta(^\circ)$
7.19	4	1 1 0	12.30
6.24	30	0 2 0	14.19
5.98	14	0 0 1	14.80
5.388	36	0 1 1	16.44
5.248	7	-1 1 1	16.88

Ammonium Nickel Sulfate Hydrate,  $(\text{NH}_4)_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 5$	hkl	$2\theta(^{\circ})$
1.942M		-3 4 2	46.73
1.915	7	0 5 2	47.43
1.905	10	-3 1 3	47.71
1.899	10	3 5 0	47.87
1.878M	3	1 6 1	48.44
1.878M		2 6 0	48.44
1.8575	7	-1 3 3	49.00
1.8389	6	-2 3 3	49.53
1.8179	3	-5 1 1	50.14
1.8095M	5	4 2 1	50.39
1.8095M		1 1 3	50.39
1.7949M	10	0 3 3	50.83
1.7949M		4 4 0	50.83
1.7919	8	2 4 2	50.92
1.7632	2	-5 2 1	51.81
1.7588	4	-3 5 2	51.95
1.7401	4	5 1 0	52.55
1.7288M	2	-1 6 2	52.92
1.7288M		-1 4 3	52.92
1.7176	5	3 5 1	53.29
1.7132	6	-2 4 3	53.44
1.7052	2	0 6 2	53.71
1.6855M	5	-4 2 3	54.39
1.6855M		-4 5 1	54.39
1.6826	4	3 3 2	54.49
1.6750	3	1 3 3	54.76



Ammonium Sulfate, (NH<sub>4</sub>)<sub>2</sub>S<sub>2</sub>O<sub>3</sub>

Synonym  
1. Ammonium thiosulfate

CAS registry no.  
7783-18-8

Sample  
The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color  
Colorless

Structure  
Monoclinic, C2/m (12), Z = 4. The structure was determined by Brunt [1946]. A line at 2θ = 23.06 with I = 4, could not be indexed.

Lattice constants of this sample  
a = 10.2233(15) Å  
b = 6.4956(9)  
c = 8.8074(10)  
β = 94.66(1)°  
a/b = 1.5739  
c/b = 1.3559

Volume  
582.93 Å<sup>3</sup>

Density  
(calculated) 1.689 g/cm<sup>3</sup>

Figure of merit  
F<sub>30</sub> = 91.0(0.010,34)

Reference intensity  
I/I<sub>corundum</sub> = 0.94(3)

Additional pattern  
1. PDF card 1-844 [Hanawalt et al., 1938]

References  
Brunt, N. A. (1946). Diss. Leiden pp. 64.  
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

d(Å)	I <sup>rel</sup> σ = ±8	hkl	2θ(°)
4.257	18	2 0 1	20.85
3.501	16	-1 1 2	25.42
3.469	14	-2 0 2	25.66
3.353	32	1 1 2	26.56
3.248	18	0 2 0	27.44
3.199	28	2 0 2	27.87
3.046	22	0 2 1	29.30
3.010	74	3 1 0	29.66
2.925	8	0 0 3	30.54
2.915	9	-3 1 1	30.65
2.785	9	3 1 1	32.11
2.739	6	2 2 0	32.67
2.629M	62	-2 0 3	34.07
2.629M		-1 1 3	34.07
2.612	32	0 2 2	34.31
2.582	14	2 2 1	34.71
2.569	13	-3 1 2	34.90
2.547	8	4 0 0	35.21
2.536	8	1 1 3	35.36
2.500	2	-4 0 1	35.89
2.453	5	2 0 3	36.61
2.402	6	3 1 2	37.41
2.395	6	4 0 1	37.52
2.371	20	-2 2 2	37.92
2.286	6	-4 0 2	39.39
2.280	6	2 2 2	39.50
2.195	6	0 0 4	41.09
2.178	6	-3 1 3	41.42
2.129	3	4 0 2	42.42
2.118	2	1 3 0	42.65
2.078	4	-2 0 4	43.51
2.0688M	5	-1 1 4	43.72
2.0688M		-1 3 1	43.72
2.0510	4	1 3 1	44.12
2.0444	4	-2 2 3	44.27
2.0270	2	3 1 3	44.67
2.0065	6	1 1 4	45.15
1.9824	2	-4 2 1	45.73
1.9582M	7	2 0 4	46.33
1.9582M		2 2 3	46.33
1.9451	3	5 1 0	46.66
1.9271	3	4 2 1	47.12
1.8946	3	1 3 2	47.98
1.8686M	3	-4 2 2	48.69
1.8686M		5 1 1	48.69
1.8368	2	-3 1 4	49.59
1.8319	2	-5 1 2	49.73
1.8261	4	3 3 0	49.90
1.8186	12	0 2 4	50.12
1.8031	7	-3 3 1	50.58

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Si, a = 5.43088 Å			
d(Å)	I <sup>rel</sup> σ = ±8	hkl	2θ(°)
5.480	16	1 1 0	16.16
5.093	44	2 0 0	17.40
4.741	93	-1 1 1	18.70
4.553	100	1 1 1	19.48
4.386	76	0 0 2	20.23

Ammonium Sulfate,  $(\text{NH}_4)_2\text{S}_2\text{O}_3$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 8$	hkl	$2\theta(^{\circ})$
1.7814	2	4 2 2	51.24
1.7559	5	0 0 5	52.04
1.7294M	10	-1 3 3	52.90
1.7294M		5 1 2	52.90
1.7159	3	3 1 4	53.35
1.7117	4	-3 3 2	53.49
1.7052	6	-4 2 3	53.71
1.7023M	6	-2 0 5	53.81
1.7023M		1 3 3	53.81
1.6933M	6	-1 1 5	54.12
1.6933M		-6 0 1	54.12
1.6801	4	-5 1 3	54.58
1.6775	4	2 2 4	54.67
1.6599	2	3 3 2	55.30
1.6508	2	1 1 5	55.63
1.6196	1	2 0 5	56.80
1.6066	1	4 2 3	57.30
1.5967	1	0 4 1	57.69
1.5809	2	-3 3 3	58.32
1.5665	4	-3 1 5	58.91

Ammonium Sulfate,  $(\text{NH}_4)_2\text{S}_2\text{O}_8$

Synonym  
Ammonium persulfate

Sample  
The sample was from Fisher Scientific Co.  
Fair Lawn, NJ. The sample was hygroscopic.

Color  
Colorless

Structure  
Monoclinic,  $P2_1/n(14)$ ,  $Z = 2$ . The structure of  $(\text{NH}_4)_2\text{S}_2\text{O}_8$  has been determined by Zachariassen and Mooney [1934] and refined by Sivertsen and Sorum [1969].

Lattice constants of this sample

$a = 7.829(2)$   
 $b = 8.0075(14)$   
 $c = 6.1483(12)$   
 $\beta = 95.12(2)^\circ$

$a/b = 0.9777$   
 $c/b = 0.7678$

Volume  
 $383.90 \text{ \AA}^3$

Density  
(calculated)  $1.974 \text{ g/cm}^3$

Figure of merit  
 $F_{30} = 41.9(0.015, 48)$

Additional pattern  
1. PDF card 11-551 [University College, Cardiff, Wales]

References  
Sivertsen, B. K. and Sorum, H. (1969) Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 130, 449.  
Zachariassen, W. H. and Mooney, R. C. L. (1934) Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 88, 63.

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 6$	hkl	$2\theta(^\circ)$
3.996M	50	0 2 0	22.23
3.996M		1 1 1	22.23
3.560	62	1 2 0	24.99
3.501	69	2 1 0	25.42
3.347	100	0 2 1	26.61
3.154	50	-2 1 1	28.27
3.063	16	0 0 2	29.13
3.027	2	1 2 1	29.49
2.945	19	2 1 1	30.33
2.860	18	0 1 2	31.25
2.761	2	-1 1 2	32.40
2.606	6	-2 2 1	34.39
2.526	3	1 3 0	35.51
2.483	28	2 2 1	36.15
2.475M	25	-3 0 1	36.27
2.475M		3 1 0	36.27
2.433	6	0 2 2	36.92
2.403	13	-2 1 2	37.39
2.370	4	-1 2 2	37.93
2.309M	8	1 3 1	38.97
2.309M		2 0 2	38.97
2.220	10	2 1 2	40.61
2.204	8	2 3 0	40.92
2.181	2	3 2 0	41.36
2.041	16	2 3 1	44.35
2.019	2	-1 0 3	44.85
2.012	4	0 3 2	45.01
2.007	6	3 2 1	45.14
1.978M	5	0 1 3	45.84
1.978M		-1 3 2	45.84
1.940	3	1 4 0	46.80
1.933	8	1 0 3	46.97
1.921	4	1 3 2	47.27
1.8791	4	1 1 3	48.40
1.8625	6	3 3 0	48.86
1.8424	2	-3 2 2	49.43
1.8368	6	1 4 1	49.59
1.8145	2	-3 3 1	50.24
1.7805	8	2 4 0	51.27
1.7660	2	4 1 1	51.72
1.7509	3	3 3 1	52.20
1.7459	3	2 3 2	52.36
1.7285	2	-2 4 1	52.93
1.7221	11	-4 2 1	53.14
1.6750	2	0 4 2	54.76
1.6549	2	-1 4 2	55.48
1.6505	4	4 2 1	55.64
1.6000	3	2 2 3	57.56

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard W, $a = 3.16524 \text{ \AA}$			
$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 6$	hkl	$2\theta(^\circ)$
5.583	42	1 1 0	15.86
5.038	62	-1 0 1	17.59
4.862	14	0 1 1	18.23
4.621	10	1 0 1	19.19
4.261	12	-1 1 1	20.83

Cadmium Bromate Hydrate,  $\text{Cd}(\text{BrO}_3)_2 \cdot 2\text{H}_2\text{O}$

Synonym

1. Cadmium bromate dihydrate

CAS registry no.

19320-65-1

Sample

The sample was prepared by dissolving anhydrous  $\text{Cd}(\text{BrO}_3)_2$  in water and letting it dry. The sample was then washed.

Color

Light orange yellow.

Structure

Orthorhombic,  $P2_12_12_1$  (19),  $Z = 4$ . The structure was studied by Garcia-Blanco and Perales [1963].

Lattice constants of this sample

$a = 9.2417(10) \text{ \AA}$

$b = 12.5015(13)$

$c = 6.1762(6)$

$a/b = 0.7392$

$c/b = 0.4940$

Volume

$713.57 \text{ \AA}^3$

Density

(calculated)  $3.763 \text{ g/cm}^3$

Figure of merit

$F_{30} = 62.5(0.012, 39)$

Reference intensity

$I/I_{\text{corundum}} = 2.9(2)$

Additional pattern

1. PDF card 1-0353 (labelled monohydrate) [Hanawalt et al. 1938]

References

Garcia-Blanco, S. and Perales, A. (1963).

Acta Crystallogr. 16, A34.

Hanawalt, J. D., Rinn, H. W., and

Frevel, L. K. (1938). Ind. Eng. Chem.

Anal. Ed. 10, 457.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$				
Internal standard W, $a = 3.16524 \text{ \AA}$				
$d(\text{Å})$	$I^{\text{rel}}$	hkl	$2\theta(^\circ)$	
$\sigma = \pm 1$				
6.24	22	0 2 0	14.18	
5.538	28	0 1 1	15.99	
5.172	1	1 2 0	17.13	
5.131	1	1 0 1	17.27	
4.746	4	1 1 1	18.68	
4.621	1	2 0 0	19.19	
4.397	100	0 2 1	20.18	
3.969	4	1 2 1	22.38	
3.799	2	1 3 0	23.40	
3.714	15	2 2 0	23.94	
3.700	15	2 0 1	24.03	
3.546	21	2 1 1	25.09	
3.453	22	0 3 1	25.78	
3.236	11	1 3 1	27.54	
3.184	26	2 2 1	28.00	
3.123	12	0 4 0	28.56	
3.091M	24	2 3 0	28.86	
3.091M		0 0 2	28.86	
2.996	5	0 1 2	29.80	
2.990	5	3 1 0	29.86	
2.959	3	1 4 0	30.18	
2.929	1L	1 0 2	30.50	
2.851	14	1 1 2	31.35	
2.769M	16	0 2 2	32.31	
2.769M		2 3 1	32.31	
2.692	5	3 1 1	33.25	
2.669	3	1 4 1	33.55	
2.651	3	1 2 2	33.79	
2.590	3	2 4 0	34.61	
2.568	2	2 0 2	34.91	
2.514	10	2 1 2	35.68	
2.480	4	0 3 2	36.19	
2.477	3	3 3 0	36.24	
2.396	5	1 3 2	37.51	
2.389	6	2 4 1	37.62	
2.375	7	2 2 2	37.85	
2.318	5	0 5 1	38.81	
2.273	8	4 1 0	39.62	
2.248	5	1 5 1	40.07	
2.196M	22	0 4 2	41.07	
2.196M		3 4 0	41.07	
2.181	5	3 0 2	41.36	
2.164	2	4 0 1	41.70	
2.148	3	3 1 2	42.02	
2.137	6	1 4 2	42.25	

Cadmium Bromate Hydrate,  $\text{Cd}(\text{BrO}_3)_2 \cdot 2\text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 1$	hkl	$2\theta(^{\circ})$
2.133	5	4 1 1	42.35
2.083	4	0 6 0	43.41
2.071	11	2 5 1	43.68
2.067	10	3 4 1	43.77
2.044	5	4 2 1	44.27
2.033M	9	1 6 0	44.54
2.033M		0 1 3	44.54
2.011	3	1 0 3	45.05
1.9845M	4	1 1 3	45.68
1.9845M		2 4 2	45.68
1.9747	2	0 6 1	45.92
1.9443	10	0 5 2	46.68
1.9322M	3	3 3 2	46.99
1.9322M		1 6 1	46.99
1.9195	4	4 3 1	47.32
1.9122	5	1 2 3	47.51
1.9013	1	1 5 2	47.80
1.8810	1	2 0 3	48.35
1.8597	1	2 1 3	48.94
1.8501	2	4 0 2	49.21
1.8462	1	0 3 3	49.32
1.8285	1	5 1 0	49.83
1.8159	5	2 6 1	50.20
1.8008	3	2 2 3	50.65
1.7886	4	3 4 2	51.02
1.7789	3	4 4 1	51.32
1.7547M	1	1 7 0	52.08
1.7547M		5 1 1	52.08
1.7194	2	0 4 3	53.23
1.7147M	4	0 7 1	53.39
1.7147M		2 3 3	53.39
1.7040	2	5 2 1	53.75
1.6967+	3	4 5 0	54.00
1.6967+		3 1 3	54.00
1.6904+	6	1 4 3	54.22
1.6904+		5 3 0	54.22
1.6872	5	1 7 1	54.33
1.6665	2	2 7 0	55.06
1.6621	3	3 6 1	55.22
1.6511	1	3 2 3	55.62
1.6432	3	3 5 2	55.91
1.6362	2	4 5 1	56.17
1.6298	3	5 3 1	56.41
1.6177	1	2 6 2	56.87
1.6110	3	2 4 3	57.13

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 1$	hkl	$2\theta(^{\circ})$
1.6084	3	2 7 1	57.23
1.5921	2	4 4 2	57.87
1.5901M	2	5 4 0	57.95
1.5901M		0 5 3	57.95
1.5831	4	3 3 3	58.23
1.5735	1	5 1 2	58.62
1.5633	2	0 8 0	59.04
1.5457M	2	0 7 2	59.78
1.5457M		3 7 0	59.78
1.5413M	3	1 8 0	59.97
1.5413M		5 4 1	59.97
1.5373M	2	5 2 2	60.14
1.5373M		4 0 3	60.14
1.5327	3	0 1 4	60.34
1.5243	1	1 7 2	60.71
1.5146	2	0 8 1	61.14
1.5117	3	1 1 4	61.27
1.5030	1	2 5 3	61.66
1.5006M	1	3 4 3	61.77
1.5006M		4 6 1	61.77
1.4989M	1	0 2 4	61.85
1.4989M		3 7 1	61.85
1.4945M	1	1 8 1	62.05
1.4945M		6 0 1	62.05
1.4866M	2	4 5 2	62.42
1.4866M		5 5 0	62.42
1.4838	3	6 1 1	62.55
1.4657	3	2 7 2	63.41
1.4641M	3	2 0 4	63.49
1.4641M		0 6 3	63.49
1.4482	3	0 3 4	64.27
1.4445M	2	5 5 1	64.45
1.4445M		6 3 0	64.45
1.4303	2	1 3 4	65.17
1.4255	1	2 2 4	65.42
1.4130M	1	4 7 0	66.07
1.4130M		3 5 3	66.07
1.4070	1	6 3 1	66.39
1.3942M	2	0 8 2	67.08
1.3942M		3 8 0	67.08

Calcium Sulfate Hydrate (Gypsum),  $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$

Synonym

1. Calcium sulfate dihydrate

CAS registry no.

10101-41-4

Sample

The sample was prepared by adding  $\text{H}_2\text{SO}_4$  to a water solution of  $\text{Ca}(\text{NO}_3)_2$ . The precipitate was filtered out, washed in water, and bottled while moist. The crystals were dried immediately before use, and care was taken to prevent dehydration.

Color

Colorless

Structure

Monoclinic,  $\text{C}2/c$  (15),  $Z = 4$ . The structure was determined by Wooster [1936] and refined by Atoji and Rundle [1958].

Lattice constants of this sample

$a = 6.2845(11) \text{ \AA}$   
 $b = 15.2079(15)$   
 $c = 5.6776(7)$   
 $\beta = 114.09(1)^\circ$

$a/b = 0.4132$   
 $c/b = 0.3733$

Volume

$495.37 \text{ \AA}^3$

Density

(calculated)  $2.308 \text{ g/cm}^3$

Figure of merit

$F_{30} = 47.4(0.013,49)$

Reference intensity

$I/I_{\text{corundum}} = 1.83(4)$

Additional patterns

- PDF card 6-0046 [F. H. Gillery, Pennsylvania State University, University Park, PA]
- PDF card 21-816 [Technisch Physische Dienst, Delft, Holland]

References

- Atoji, M. and Rundle, R. E. (1958). *J. Chem. Phys.* **29**, 1306.  
 Wooster, W. A. (1936). *Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem.* **94**, 375.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$				
$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 4$	hkl	$2\theta(^\circ)$	
7.63	100	0 2 0	11.59	
4.283	98	0 2 1	20.72	
3.799M	17	0 4 0	23.40	
3.799M		1 3 0	23.40	
3.172	4	1 1 1	28.11	
3.065	74	0 4 1	29.11	
2.873	47	-2 2 1	31.10	
2.789	10	-1 1 2	32.07	
2.732	2	1 3 1	32.75	
2.685M	34	1 5 0	33.35	
2.685M		2 2 0	33.35	
2.597	6	-1 5 1	34.51	
2.534	2	0 6 0	35.39	
2.495	11	-2 0 2	35.97	
2.476	1	-1 3 2	36.25	
2.452	6	0 2 2	36.62	
2.406	4	-2 4 1	37.35	
2.291	1L	2 4 0	39.29	
2.219	15	1 5 1	40.63	
2.142	2	0 4 2	42.15	
2.086	24	-2 4 2	43.34	
2.074M	15	-1 5 2	43.60	
2.074M		-3 1 1	43.60	
2.048	6	1 1 2	44.18	
2.032	1L	1 7 0	44.56	
1.992	4	-1 7 1	45.51	
1.963	3	-2 6 1	46.22	
1.8998M	16	0 8 0	47.84	
1.8998M		2 6 0	47.84	
1.8795	12	2 4 1	48.39	
1.8650	3	-1 1 3	48.79	
1.8118	13	0 6 2	50.32	
1.7995	6	-2 2 3	50.69	
1.7844	9	0 8 1	51.15	
1.7785	12	-2 6 2	51.33	
1.7093	1	1 5 2	53.57	
1.6846	3	0 2 3	54.42	
1.6640	6	-2 4 3	55.15	
1.6456	4	2 6 1	55.82	
1.6209+	9	-2 8 1	56.75	
1.6209+		1 9 0	56.75	
1.6005	1	-1 9 1	57.54	
1.5846	4	2 8 0	58.17	
1.5327	2	0 8 2	60.34	
1.5209+	1	0 10 0	60.86	

Calcium Sulfate Hydrate (Gypsum),  $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 4$	hkl	$2\theta(^{\circ})$
1.5209+		-4 2 2	60.86
1.5119	1	-2 8 2	61.26
1.4982	1L	1 9 1	61.88
1.4947	1L	-2 6 3	62.04
1.4591+	3	-3 7 2	63.73
1.4591+		0 10 1	63.73
1.4392	5	-4 4 1	64.72
1.4354	3	3 7 0	64.91
1.4278M	2	2 8 1	65.30
1.4278M		0 6 3	65.30
1.4178	3	-2 0 4	65.82
1.4015	2	-4 2 3	66.68
1.3657M	5	2 6 2	68.67
1.3657M		-2 10 1	68.67
1.3440M	1	1 11 0	69.94
1.3440M		2 10 0	69.94
1.3324	2	-1 11 1	70.64
1.3262	4	-2 8 3	71.02
1.3234	4	-4 6 2	71.19
1.2785	1	0 8 3	74.10
1.2722	1L	1 11 1	74.53
1.2674	1L	0 12 0	74.86
1.2481M	3	4 6 0	76.22
1.2481M		-4 0 4	76.22
1.2441	2	2 10 1	76.51
1.2336	3	2 8 2	77.28
1.2309+	2	-4 2 4	77.48
1.2309+		0 12 1	77.48

Calcium Tin Oxide, CaSnO<sub>3</sub>

Synonym

1. Calcium stannate

CAS registry no.

12013-46-6

Sample

The sample was obtained from CERAC, Inc. Milwaukee, WI. The material was heated to 800 °C for one hour. A small amount of SnO<sub>2</sub> was present in the sample.

Color

White

Structure

Orthorhombic, P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> (19), Z = 4. The structure of CaSnO<sub>3</sub> was studied by Smith and Welch [1960].

Lattice constants of this sample

a = 5.6615(5) Å  
b = 7.8825(7)  
c = 5.5162(5)

a/b = 0.7182  
c/b = 0.6998

Volume

246.17 Å<sup>3</sup>

Density

(calculated) 5.579 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 55.5(0.011,51)

Reference intensity

I/I<sub>corundum</sub> = 6.5(4)

Additional patterns

- PDF card 3-755 [H. D. Megaw, Philips Lamps Ltd.]
- Coughanour et al. [1955]

References

Coughanour, L. W., Roth, R. S., Marzullo, S., and Sennett, F. E. (1955). J. Res. Nat. Bur. Stand. 54, No. 3, 149.  
Smith, A. J. and Welch, A. J. E. (1960). Acta. Crystallogr. 13, 653.

d(Å)	I <sup>rel</sup> σ = ±1	hkl	2θ(°)
2.518	1L	2 0 1	35.62
2.480	1	1 0 2	36.19
2.398	1	2 1 1	37.47
2.371	3	0 3 1	37.91
2.366	3	1 1 2	38.00
2.298	3	2 2 0	39.17
2.259	3	0 2 2	39.87
2.188	2	1 3 1	41.22
2.122	1	2 2 1	42.56
2.099	1L	1 2 2	43.06
1.9751	32	2 0 2	45.91
1.9714	29	0 4 0	46.00
1.9256	1	2 3 0	47.16
1.9168	1	2 1 2	47.39
1.8183	1L	2 3 1	50.13
1.8038	1L	1 3 2	50.56
1.7853	7	3 0 1	51.12
1.7638	19	1 4 1	51.79
1.7484	4	1 0 3	52.28
1.7076	1	1 1 3	53.63
1.6266	15	3 2 1	56.53
1.6177	12	2 4 0	56.87
1.6030	15	0 4 2	57.44
1.5984	23	1 2 3	57.62
1.5420M	1L	1 4 2	59.94
1.5420M		2 0 3	59.94
1.4766	1	3 3 1	62.89
1.4155	2	4 0 0	65.94
1.3951	2	2 4 2	67.03
1.3788	10	0 0 4	67.93
1.3393M	1L	1 0 4	70.22
1.3393M		3 3 2	70.22
1.3362	1	2 5 1	70.41
1.3320	2	4 2 0	70.66
1.3301M	2	1 5 2	70.78
1.3301M		2 3 3	70.78
1.3231	4	3 4 1	71.21
1.3173	2	3 0 3	71.57
1.3082	2	1 4 3	72.15
1.3021	1	0 2 4	72.54
1.2592	2	4 0 2	75.43
1.2489	7	3 2 3	76.16
1.2466M	9	1 6 1	76.33
1.2466M		4 3 0	76.33
1.2398	3	2 0 4	76.82
1.2324	1L	2 5 2	77.37
1.2247	1L	2 1 4	77.95
1.2144	1L	2 4 3	78.74
1.1994	2	4 2 2	79.92
1.1966	2	0 5 3	80.14

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup> σ = ±1	hkl	2θ(°)
3.943	60	0 2 0	22.53
3.531	2	1 1 1	25.20
2.830	26	2 0 0	31.59
2.789	100	1 2 1	32.07
2.758	23	0 0 2	32.44



Calcium Tin Oxide,  $\text{CaSnO}_3$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 1$	hkl	$2\theta(^{\circ})$
1.1916	1	2 6 0	80.55
1.1861	1	0 6 2	81.00
1.1825	3	2 2 4	81.30
1.1708	1L	1 5 3	82.28
1.1499	2	4 4 0	84.12
1.1358	1L	4 3 2	85.41
1.1300	2	0 4 4	85.95
1.1092	1	5 0 1	87.97
1.0948	2	3 4 3	89.43
1.0939	2	2 6 2	89.53

Cerium Nitrate Hydrate,  $\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$

Synonym

1. Cerous nitrate hexahydrate

CAS registry no.

10294-41-4

Sample

The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color

Colorless

Structure

Triclinic,  $\bar{P}1(2)$ ,  $Z = 2$ . The structure of  $\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$  was studied by Iveronova et al. [1955].

Lattice constants of this sample

$a = 8.905(2) \text{ \AA}$   
 $b = 10.683(3)$   
 $c = 6.6182(14)$   
 $\alpha = 101.18(2)^\circ$   
 $\beta = 102.19(2)$   
 $\gamma = 87.89(2)$

$a/b = 0.8336$   
 $c/b = 0.6195$

Volume

$603.7 \text{ \AA}^3$

Density

(calculated  $2.389 \text{ g/cm}^3$ )

Figure of merit

$F_{30} = 45.8(0.013,51)$

Reference intensity

$I/I_{\text{corundum}} = 0.44(3)$

Additional pattern

1. PDF card 14-3 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). *Ind. Eng. Chem. Anal. Ed.* **10**, 457.  
 Iveronova, V. I., Tarasova, V. P., Zolina, Z. K., Markhasin, G. V., and Sukhodereva, I. M. (1955). *Zh. Fiz. Khim.* **29**, 314.

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 5$	hkl	$2\theta(^\circ)$
5.437	42	-1 -1 1	16.29
5.245	42	0 2 0	16.89
5.024	44	0 1 1	17.64
4.701	100	-1 1 1	18.86
4.487M	39	0 -2 1	19.77
4.487M		1 2 0	19.77
4.358	46	2 0 0	20.36
4.017	22	2 1 0	22.11
4.001	27	-2 0 1	22.20
3.890	14	-2 -1 1	22.84
3.770	19	1 -2 1	23.58
3.711	6	0 2 1	23.96
3.576	4	-1 2 1	24.88
3.493	2	0 3 0	25.48
3.375	28	-2 -2 1	26.39
3.341M	21	0 -3 1	26.66
3.341M		2 2 0	26.66
3.247M	50	-1 3 0	27.45
3.247M		-1 -1 2	27.45
3.237M	33	1 3 0	27.53
3.237M		-1 -3 1	27.53
3.213	37	0 -1 2	27.74
3.175	15	0 0 2	28.08
3.048	14	2 1 1	29.28
3.013M	25	1 -3 1	29.63
3.013M		-2 2 1	29.63
3.002	28	-1 -2 2	29.74
2.979	29	0 -2 2	29.97
2.913	45	-1 1 2	30.67
2.892M	47	-2 -1 2	30.89
2.892M		0 1 2	30.89
2.875	11	-3 0 1	31.08
2.864	11	-2 0 2	31.20
2.839	31	0 3 1	31.49
2.832M	28	-3 -1 1	31.57
2.832M		1 -1 2	31.57
2.802M	11	1 0 2	31.91
2.802M		-3 1 0	31.91
2.794M	15	-2 -3 1	32.01
2.794M		3 1 0	32.01
2.715+	21	-3 1 1	32.96
2.715+		-2 -2 2	32.96
2.663M	19	1 -2 2	33.63
2.663M		2 2 1	33.63
2.651	35	-2 1 2	33.78
2.620	28	0 4 0	34.19
2.611M	30	-3 -2 1	34.32
2.611M		0 -3 2	34.32
2.550	19	-1 -4 1	35.16
2.542	14	-3 2 0	35.28

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard Si, $a = 5.43088 \text{ \AA}$			
$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 5$	hkl	$2\theta(^\circ)$
8.70	21	1 0 0	10.16
6.71	85	-1 1 0	13.19
6.37	60	0 0 1	13.90
5.96	76	0 -1 1	14.85
5.73	54	-1 0 1	15.44

Cerium Nitrate Hydrate,  $\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 5$	hkl	$2\theta(^{\circ})$
2.533	18	3 2 0	35.41
2.527M	24	-1 2 2	35.49
2.527M		2 -3 1	35.49
2.490	18	-2 3 1	36.04
2.452	20	3 0 1	36.62
2.440	15	1 -4 1	36.80
2.424	13	-2 -3 2	37.05
2.405	13	-3 0 2	37.36
2.393	5	1 -3 2	37.56
2.359	6	2 -1 2	38.12
2.352	12	-2 2 2	38.24
2.316M	23	-2 -4 1	38.85
2.316M		-3 -3 1	38.85
2.313M	26	-3 -2 2	38.91
2.313M		1 2 2	38.91
2.291	32	3 -2 1	39.30
2.280	31	2 3 1	39.49
2.265	14	2 -2 2	39.77
2.249M	28	-1 -4 2	40.06
2.249M		-2 4 0	40.06
2.243M	24	-1 4 1	40.17
2.243M		0 -4 2	40.17
2.227	5	3 3 0	40.47
2.204M	19	-1 -1 3	40.91
2.204M		-4 0 1	40.91
2.184	13	-4 -1 1	41.31
2.159+	27	1 4 1	41.80
2.159+		3 2 1	41.80
2.153M	27	0 3 2	41.92
2.153M		-1 -2 3	41.92
2.137	22	-3 3 1	42.26
2.129M	26	-4 1 1	42.43
2.129M		4 1 0	42.43
2.116M	35	0 0 3	42.70
2.116M		0 -5 1	42.70
2.107	28	0 -2 3	42.89
2.088	20	2 -3 2	43.29
2.081	20	-2 0 3	43.44
2.077M	21	-3 2 2	43.53
2.077M		-4 -2 1	43.53
2.053	11	-2 3 2	44.08
2.039	22	-1 5 0	44.39
2.035M	17	1 5 0	44.49
2.035M		2 2 2	44.49
2.024+	6	1 -5 1	44.74
2.024+		1 3 2	44.74
2.012	3	-4 2 0	45.01
1.999	19	-4 0 2	45.33
1.987M	8	-4 2 1	45.63
1.987M		0 -3 3	45.63
1.973	10	-2 1 3	45.97

Chromium Boride,  $\zeta$ -CrB

CAS registry no.  
12006-79-0

## Sample

The sample was obtained from Cerac, Menomonee Falls, WI.

## Color

Metallic gray

## Structure

Orthorhombic, Cmc $\bar{m}$  (63), Z = 4. The structure was determined by Kiessling [1949].

## Lattice constants of this sample

a = 2.9663(4) Å  
b = 7.8666(10)  
c = 2.9322(5)

a/b = 0.3771  
c/b = 0.3727

## Volume

68.422 Å<sup>3</sup>

## Density

(calculated) 6.097 g/cm<sup>3</sup>

## Figure of merit

F<sub>19</sub> = 62.9(0.013,24)

## Reference intensity

I/I<sub>corundum</sub> = 1.22(8)

## Polymorphism

Papesch et al., [1973] also observed a tetragonal low temperature form of CrB with 52-56 atom % B.

## Additional pattern

1. PDF card 9-361 [Plessey Co. Ltd., Caswell, Towcester, Northants, England].

## References

Kiessling, R. (1949). Acta Chem. Scand. 3, 595.  
Papesch, G., Nowotny, H., and Benesovsky, F. (1973). Monatsh. Chem. 104, 933.

CuK $\alpha_1$ $\lambda = 1.540598$ Å; temp. 25 $\pm$ 1 °C Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup> $\sigma = \pm 6$	hkl	2 $\theta$ (°)
3.936	5	0 2 0	22.57
2.776	38	1 1 0	32.22
2.351	74	0 2 1	38.25
2.016	100	1 1 1	44.92
1.965M	79	0 4 0	46.15
1.965M		1 3 0	46.15
1.6322	32	1 3 1	56.32
1.4829	14	2 0 0	62.59
1.4663	17	0 0 2	63.38
1.3881	1L	2 2 0	67.41
1.3111	6	0 6 0	71.96
1.2961	12	1 1 2	72.93
1.2555	34	1 5 1	75.69
1.2543	30	2 2 1	75.78
1.1970	9	0 6 1	80.11
1.1840	12	2 4 0	81.17
1.1752M	30	0 4 2	81.91
1.1752M		1 3 2	81.91
1.0980	13	2 4 1	89.10
1.0509	13	1 7 0	94.27
1.0427	14	2 0 2	95.25

Chromium Chloride CrCl<sub>3</sub>

Synonyms

1. Chromic chloride
2. Chromium trichloride

CAS registry no.  
10025-73-7

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, N.J.

Color

Deep purple red.

Structure

Monoclinic, A2/m (12), Z = 4, pseudo-hexagonal. The structure was determined by Morosin and Narath [1964]. This form exists at room temperature.

Lattice constants of this sample

a = 6.123(2) Å  
b = 10.311(3)  
c = 5.956(5)  
β = 108.64(5)°

a/b = 0.5938  
c/b = 0.5776

Volume  
356.3 Å<sup>3</sup>

Density

(calculated) 2.952 g/cm<sup>3</sup>

Figures of merit

F<sub>19</sub> = 13.2 (0.018,80)  
M<sub>19</sub> = 16.0

Reference intensity

I/I<sub>corundum</sub> = 4.5(2)

Polymorphism

There is a hexagonal form found by Wooster [1930] and a low temperature form also found by Morosin and Narath [1964].

Additional pattern

1. PDF card 6-535 [Handy and Gregory, 1952]

References

- Handy, L. L. and Gregory, N. W. (1952). J. Am. Chem. Soc. 74, 891.  
Morosin, B. and Narath, A. (1964). J. Chem. Phys. 40, 1958.  
Wooster, N. (1930). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 74, 363.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup>	hkl	2θ(°)
σ = ±3			
5.80	100	1 0 0	15.27
5.154	1	0 2 0	17.19
3.849	1L	1 2 0	23.09
2.936M	2	0 3 1	30.42
2.936M		-1 0 2	30.42
2.901	14	2 0 0	30.80
2.816	1	0 0 2	31.75
2.577	1	0 4 0	34.78
2.475	2	0 2 2	36.27
2.460	6	1 3 1	36.49
1.934	1	3 0 0	46.94
1.911	1	2 3 1	47.54
1.754	3	-3 3 1	52.09
1.720	3	-1 3 3	53.21
1.6511M	1	3 1 1	55.62
1.6511M		0 3 3	55.62
1.6478M	1	1 6 0	55.74
1.5039	1L	3 3 1	61.62
1.4498M	6	-3 5 1	64.19
1.4498M		4 0 0	64.19
1.4115M	1	0 0 4	66.15
1.4115M		-2 2 4	66.15
1.3954M	1	4 2 0	67.01
1.3954M		-4 3 1	67.01

Chromium Iron Oxide,  $\text{Cr}_{1.3}\text{Fe}_{0.7}\text{O}_3$

Sample

The sample was obtained from the City Chemical Corp., New York, N. Y. It was labelled iron chromite ( $\text{FeCr}_2\text{O}_4$ ). The approximate composition was determined by the relation of the cell parameters to those of  $\text{Fe}_2\text{O}_3$  and  $\text{Cr}_2\text{O}_3$ . This is a solid solution between hematite ( $\text{Fe}_2\text{O}_3$ ) and chromic oxide ( $\text{Cr}_2\text{O}_3$ ).

Color

Dark brown

Structure

Hexagonal,  $R\bar{3}c$  (167),  $Z = 6$ . The structure of  $\text{Cr}_2\text{O}_3$  was determined by Wretblad [1930]. The structure of hematite ( $\text{Fe}_2\text{O}_3$ ) was determined by Davey [1923].

Lattice constants of this sample

$a = 4.9965(6) \text{ \AA}$   
 $c = 13.621(3)$

$c/a = 2.7261$

Volume

$294.49 \text{ \AA}^3$

Density

(calculated)  $5.233 \text{ g/cm}^3$

Figure of merit

$F_{20} = 51.0(0.014, 29)$

Reference intensity

$I/I_{\text{corundum}} = 2.11(8)$

References

Davey, W. P. (1923). Phys. Rev. 21, 716.  
 Wretblad, P. E. (1930). Z. Anorg. Chem. 189, 329.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$			
$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 3$	hk $\ell$	$2\theta(^\circ)$
3.654	43	0 1 2	24.34
2.676	100	1 0 4	33.46
2.499	73	1 1 0	35.90
2.270	4	0 0 6	39.67
2.189	27	1 1 3	41.21
2.063	4	2 0 2	43.85
1.8268	33	0 2 4	49.88
1.6801	66	1 1 6	54.58
1.5896	5	1 2 2	57.97
1.5849	6	0 1 8	58.16
1.4738	23	2 1 4	63.02
1.4421	25	3 0 0	64.57
1.3380	1	2 0 8	70.30
1.2988	12	1 0 10	72.75
1.2488	6	2 2 0	76.17
1.2179	3	3 0 6	78.47
1.1794	2	1 2 8	81.56
1.1528	4	0 2 10	83.86
1.1319	7	1 3 4	85.77
1.0945	7	2 2 6	89.46

Chromium Oxide, CrO<sub>3</sub>

## Synonyms

1. Chromic acid anhydride
2. Chromium trioxide

## CAS registry no.

1333-82-0

## Sample

The sample was from J. T. Baker Chemical Co.,  
Phillipsburg, NJ.

## Color

Dark reddish brown.

## Structure

Orthorhombic, Ama2 (40), Z = 4. The structure  
of CrO<sub>3</sub> was studied by Bräkken [1931] and  
refined by Byström and Wilhelmi [1950].

## Lattice constants of this sample

a = 5.7494(15) Å

b = 8.556(2)

c = 4.7961(11)

a/b = 0.6720

c/b = 0.5606

## Volume

235.93 Å<sup>3</sup>

## Density

(calculated) 2.815 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 56.8(0.016,32)

## Reference intensity

I/I<sub>corundum</sub> = 1.41(13)

## Additional pattern

1. PDF card 9-47 [Byström and Wilhelmi, 1950]

## References

Bräkken, H. (1931). Z. Kristallogr. Kristall-  
geometrie Kristallphys. Kristallchem. 78,  
484.

Byström, A. and Wilhelmi, K.-A. (1950). Acta  
Chem. Scand., 4, 1131.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Si, a = 5.43088 Å			
d(Å)	I <sup>rel</sup>	hkl	2θ(°)
σ = ±3			
4.279	19	0 2 0	20.74
4.186	90	0 1 1	21.21
3.435	100	1 2 0	25.92
3.383	64	1 1 1	26.32
2.874	44	2 0 0	31.09
2.454	4	0 3 1	36.59
2.398	17	0 0 2	37.48
2.370	18	2 1 1	37.94
2.255	18	1 3 1	39.94
2.139	2	0 4 0	42.21
2.091	2	0 2 2	43.23
2.006	8	1 4 0	45.17
1.966	10	1 2 2	46.14
1.866	2	2 3 1	48.77
1.842	5	2 0 2	49.43
1.749	10	3 2 0	52.26
1.743	11	3 1 1	52.44
1.7168	5	2 4 0	53.32
1.6921	3	2 2 2	54.16
1.6112	3	0 5 1	57.12
1.5954	2	0 4 2	57.74
1.5706	3	0 1 3	58.74
1.5512	1	1 5 1	59.55
1.5380	2	1 4 2	60.11
1.5159	4	1 1 3	61.08
1.5097	4	3 3 1	61.36
1.4366	6	4 0 0	64.85
1.4262	3	0 6 0	65.38
1.4124	4	3 2 2	66.10
1.4062	6	2 5 1	66.43
1.3956	3	2 4 2	67.00
1.3795	5	2 1 3	67.89
1.3555	6	1 3 3	69.26
1.2773	2	2 6 0	74.18

Cinchonine, C<sub>19</sub>H<sub>22</sub>N<sub>2</sub>O

Synonym

1. (9S)-Cinchonan-9-ol

CAS registry no.

118-10-5

Sample

The sample was obtained from the Eastman Kodak Co., Rochester, N. Y. It was recrystallized from ethanol.

Color

Colorless

Structure

Monoclinic, P2<sub>1</sub>/\*, Z = 2. The unit cell and space group were determined by Paretzkin [1956].

Lattice constants of this sample

a = 11.091(2) Å  
 b = 7.200(3)  
 c = 10.774(2)  
 β = 107.95(2)°

a/b = 1.5404  
 c/b = 1.4964

Volume

818.48 Å<sup>3</sup>

Density

(calculated) 1.195 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 46.6(0.012,52)

Additional pattern

1. PDF card 7-526 [Paretzkin, Polytechnic Institute of Brooklyn].

References

Paretzkin, B. (1956). Acta Crystallogr. 9, 290.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å				
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)	
10.53	100	1 0 0	8.39	
8.84	1L	-1 0 1	10.00	
6.43	2	1 0 1	13.76	
5.898	10	0 1 1	15.01	
5.583	1	-1 1 1	15.86	
5.417	4	-2 0 1	16.35	
5.301	20	-1 0 2	16.71	
5.282	24	2 0 0	16.77	
5.119	19	0 0 2	17.31	
4.795	4	1 1 1	18.49	
4.423	3	-2 0 2	20.06	
4.327	5	-2 1 1	20.51	
4.251	7	2 1 0	20.88	
4.197	21	2 0 1	21.15	
4.135	10	1 0 2	21.47	
3.770	2	-2 1 2	23.58	
3.623	10	2 1 1	24.55	
3.586M	3	-1 0 3	24.81	
3.586M		1 1 2	24.81	
3.437	1L	-3 0 2	25.90	
3.409	1L	1 2 0	26.12	
3.288	1L	-3 1 1	27.10	
3.213M	1	2 0 2	27.74	
3.213M		-1 1 3	27.74	
3.161	1	3 1 0	28.21	
3.102	1	-3 1 2	28.76	
3.089	1	0 1 3	28.88	
3.049	1L	3 0 1	29.27	
2.936	2	2 1 2	30.42	
2.809	2	3 1 1	31.83	
2.770	1L	-4 0 1	32.29	
2.761	1L	1 1 3	32.40	
2.726	1L	-3 1 3	32.83	
2.708	1L	-4 0 2	33.05	
2.687	1	-1 0 4	33.32	
2.638	1L	4 0 0	33.96	
2.556	1	3 0 2	35.08	
2.541	1	-1 2 3	35.29	
2.534M	1	-4 1 2	35.39	
2.534M		2 0 3	35.39	
2.480	1L	0 2 3	36.19	
2.464M	1L	-2 2 3	36.43	
2.464M		-3 0 4	36.43	
2.408	1	3 1 2	37.31	
2.388	1L	2 1 3	37.63	



Cinchonine, C<sub>19</sub>H<sub>22</sub>N<sub>2</sub>O - (continued)

d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)
2.328	1L	3 2 1	38.64
2.279	1L	-3 2 3	39.51
2.263	1L	4 1 1	39.81
2.218	1L	1 1 4	40.65
2.208	1L	-4 0 4	40.83
2.165	1L	-4 2 2	41.69
2.140	1L	-1 0 5	42.19
2.111+	1	5 0 0	42.80
2.111+		-5 0 3	42.80
2.082	1L	2 3 1	43.43
2.069M	1L	-3 0 5	43.72
2.069M		2 0 4	43.72
2.051+	1L	-1 1 5	44.12
2.051+		0 0 5	44.12
2.024M	1L	5 1 0	44.74
2.024M		-5 1 3	44.74
2.012M	1L	4 1 2	45.02
2.012M		-3 3 1	45.02
1.9898	1L	-3 1 5	45.55
1.9570M	1L	-2 3 3	46.36
1.9570M		1 2 4	46.36
1.9514M	1L	5 0 1	46.50
1.9514M		-5 0 4	46.50
1.8846M	1L	5 1 1	48.25
1.8846M		-4 2 4	48.25
1.8795M	1L	-5 2 1	48.39
1.8795M		-5 2 2	48.39
1.8389	1L	-1 2 5	49.53
1.8115	1L	4 2 2	50.33
1.8065	1L	-6 0 3	50.48
1.7932	1L	2 2 4	50.88

Clopendixol Hydrate,  $C_{22}H_{25}ClN_2OS \cdot 2H_2O$

Synonym

1. 4-[3-(2-Chlorothioxanthen-9-ylidene)propyl]-1-piperazineethanol dihydrate

Sample

The sample was supplied by J. Rodgers, University of Adelaide, Adelaide, South Australia. Chemical analysis gave weight percents indicating that the dihydrate is the most probable formula.

Color

Colorless

Structure

Triclinic,  $P\bar{3}$ ,  $Z = 2$ . The unit cell was measured on a single crystal diffractometer by V. Himes at NBS (priv. comm.). The value of  $Z$  was assumed from the measured density.

Lattice constants of this sample

$a = 7.773(3) \text{ \AA}$   
 $b = 21.939(11)$   
 $c = 6.518(4)$   
 $\alpha = 91.60(5)^\circ$   
 $\beta = 93.06(4)$   
 $\gamma = 90.06(4)$

$a/b = 0.3543$   
 $c/b = 0.2971$

Volume  $\text{\AA}^3$   
 1110.  $\text{\AA}^3$

Density

(calculated)  $1.308 \text{ g/cm}^3$   
 (measured)  $1.34 \text{ g/cm}^3$

Figure of merit

$F_{30} = 23.0(0.016, 80)$

Reference intensity

$I/I_{\text{corundum}} = 1.01(5)$

Polymorphism

The form described here is the inactive isomer having no neuroleptic activity. An active isomer also exists.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 6$	hkl	$2\theta(^\circ)$
22.02	100	0 1 0	4.01
11.00	15	0 2 0	8.03
7.32+	38	-1 1 0	12.08
7.32+		1 1 0	12.08
6.29	39	0 -1 1	14.07
5.65	11	0 -2 1	15.66
5.48	4	0 4 0	16.15
5.34	16	-1 3 0	16.59
5.122	7	-1 0 1	17.30
5.012	13	-1 -1 1	17.68
4.792	43	0 3 1	18.50
4.721	33	1 1 1	18.78
4.609	55	-1 2 1	19.24
4.405	3	1 2 1	20.14
4.243	12	-1 -3 1	20.92
4.135	4	0 4 1	21.47
3.882	20	2 0 0	22.89
3.824+	18	-2 1 0	23.24
3.824+		-1 5 0	23.24
3.703	12	-1 4 1	24.01
3.658+	45	-2 2 0	24.31
3.658+		2 2 0	24.31
3.597	7	1 4 1	24.73
3.431	32	-2 3 0	25.95
3.371M	44	-2 1 1	26.42
3.371M		-1 -5 1	26.42
3.294	17	1 -5 1	27.05
3.269	21	-2 -2 1	27.26
3.248M	19	0 0 2	27.44
3.248M		-2 2 1	27.44
3.221M	15	0 -6 1	27.67
3.221M		1 5 1	27.67
3.167M	11	-2 4 0	28.15
3.167M		2 4 0	28.15
3.136M	10	2 -2 1	28.44
3.136M		0 7 0	28.44
3.094	4	0 2 2	28.83
2.993	8	2 -3 1	29.83
2.960	6	2 3 1	30.17
2.941M	5	1 0 2	30.37
2.941M		0 3 2	30.37
2.795M	4	-1 3 2	32.00
2.795M		0 7 1	32.00
2.780	3	2 4 1	32.17
2.740	1	0 8 0	32.66

Clopendixol Hydrate,  $C_{22}H_{25}ClN_2OS \cdot 2H_2O$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 6$	hkl	$2\theta(^{\circ})$
2.678	6	-2 5 1	33.43
2.643	3	-1 4 2	33.89
2.516	1	3 2 0	35.66
2.449M	1	2 -6 1	36.66
2.449M		-3 0 1	36.66
2.440+	1	-3 3 0	36.81
2.440+		-2 7 0	36.81
2.317M	5	-1 6 2	38.84
2.317M		-3 3 1	38.84
2.299M	5	-2 4 2	39.15
2.299M		3 2 1	39.15
2.237	4	2 8 0	40.29

Copper Hydroxide Phosphate (Libethenite),  $\text{Cu}_2(\text{OH})\text{PO}_4$

Synonym

1. Copper phosphate hydrate

CAS registry no.

1318-84-9

Sample

The sample was prepared at NBS by D. Misra by reaction of hydroxyapatite with  $\text{Cu}(\text{NO}_3)_2$  solution. The material was dried at 55 °C.

Color

Light yellow green

Structure

Orthorhombic, Pnmm (58), Z = 4. The lattice constants of libethenite were determined by Strunz [1936]. The structure was determined by Heritsch [1940].

Lattice constants of this sample

a = 8.0678(10) Å

b = 8.4100(15)

c = 5.8896(7)

a/b = 0.9593

c/b = 0.7003

Volume

399.61 Å<sup>3</sup>

Density

(calculated) 3.974 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 53.6(0.012,45)

Reference intensity

I/I<sub>corundum</sub> = 1.13(4)

Additional patterns

1. PDF card 8-107 [Strunz, 1936]
2. PPF card 1-274 [Hanawalt et al., 1938]

References

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

Heritsch, H. (1940). Z. Kristallogr. Kristallogeometrie Kristallphys. Kristallchem. 102, 1.

Strunz, H. (1936). Z. Kristallogr. Kristallogeometrie Kristallphys. Kristallchem. 94, 63.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C				
Internal standard Ag, a = 4.08651 Å				
d(Å)	I <sup>rel</sup>	hkl	2θ(°)	
σ = ±3				
5.813	93	1 1 0	15.23	
4.818	100	0 1 1	18.40	
4.751	68	1 0 1	18.66	
4.137	6	1 1 1	21.46	
3.729	42	1 2 0	23.84	
3.638	15	2 1 0	24.45	
2.946	18	0 0 2	30.32	
2.912	72	2 2 0	30.68	
2.647	43	1 3 0	33.84	
2.627	61	1 1 2	34.10	
2.610	19	2 2 1	34.33	
2.561	25	3 1 0	35.01	
2.532	10	0 3 1	35.43	
2.446	11	3 0 1	36.71	
2.414M	26	1 3 1	37.21	
2.414M		0 2 2	37.21	
2.377	21	2 0 2	37.81	
2.348	10	3 1 1	38.30	
2.312	21	1 2 2	38.93	
2.288	4	2 1 2	39.34	
2.265	3	3 2 0	39.77	
2.071	6	2 2 2	43.67	
2.017	1	4 0 0	44.91	
1.9682	3	1 3 2	46.08	
1.9411	3	3 3 0	46.76	
1.9326	6	3 1 2	46.98	
1.9237	6	1 4 1	47.21	
1.9077	5	1 0 3	47.63	
1.8607M	5	4 1 1	48.91	
1.8607M		1 1 3	48.91	
1.8196	2	4 2 0	50.09	
1.8139	2	2 3 2	50.26	
1.7955	2	3 2 2	50.81	
1.7370M	2	4 2 1	52.65	
1.7370M		1 2 3	52.65	
1.7111	11	0 4 2	53.51	
1.6643	7	4 0 2	55.14	
1.6462	3	1 5 0	55.80	
1.6330	2	4 1 2	56.29	
1.6277	3	2 2 3	56.49	
1.6201	10	3 3 2	56.78	
1.5951	4	3 4 1	57.75	
1.5849+	9	3 0 3	58.16	
1.5849+		5 1 0	58.16	
1.5767M	7	4 3 1	58.49	

Copper Hydroxide Phosphate (Libethenite),  $\text{Cu}_2(\text{OH})\text{PO}_4$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$	hkl	$2\theta(^{\circ})$
	$\sigma = \pm 3$		
1.5767M		1 3 3	58.49
1.5590	4	3 1 3	59.22
1.5472	9	4 2 2	59.72
1.5302	3	5 1 1	60.45
1.5063	3	5 2 0	61.51
1.4724	7	0 0 4	63.09
1.4554	6	4 4 0	63.91
1.4276	3	1 1 4	65.31

β-L-Glutamic Acid, C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>

Synonyms

1. β-L-glutaminic acid
2. β-L-2-aminopentanedioic acid

CAS registry no.

56-86-0

Sample

The sample was obtained from Sigma Chemical Co., St. Louis, MO.

Color

Colorless

Structure

Orthorhombic, P<sub>2</sub><sub>1</sub>2<sub>1</sub>2<sub>1</sub> (19), Z = 8. The structure was determined by Hirokawa [1955].

Lattice constants of this sample

a = 6.9651(15) Å

b = 17.308(3)

c = 5.1690(14)

a/b = 0.4024

c/b = 0.2986

Volume

623.12 Å<sup>3</sup>

Density

(calculated) 1.568 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 48.3(0.016,39)

Reference intensity

I/I<sub>corundum</sub> = 0.65(3)

Polymorphism

There is also an orthorhombic α-form found by Bernal [1931].

References

Bernal, J. D. (1931). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 78, 363.

Hirokawa, S. (1955). Acta Crystallogr. 8, 637.

CuKα<sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I <sup>rel</sup> σ = ±3	hkl	2θ(°)
8.65	34	0 2 0	10.22
6.46	10	1 1 0	13.69
4.960	9	0 1 1	17.87
4.445M	28	1 3 0	19.96
4.445M		0 2 1	19.96
4.323	40	0 4 0	20.53
4.155	100	1 0 1	21.37
4.042	75	1 1 1	21.97
3.854	13	0 3 1	23.06
3.746	24	1 2 1	23.73
3.678	10	1 4 0	24.18
3.482	64	2 0 0	25.56
3.415	43	2 1 0	26.07
3.372	6	1 3 1	26.41
3.320	3	0 4 1	26.83
3.232	18	2 2 0	27.58
3.101	10	1 5 0	28.77
2.983	26	2 3 0	29.93
2.887M	70	2 0 1	30.95
2.887M		0 6 0	30.95
2.849	12	2 1 1	31.37
2.741	6	2 2 1	32.64
2.712	12	2 4 0	33.00
2.664	31	1 6 0	33.62
2.583M	12	0 0 2	34.70
2.583M		2 3 1	34.70
2.520	29	0 6 1	35.60
2.475	8	0 2 2	36.27
2.455	4	2 5 0	36.57
2.402	3	2 4 1	37.41
2.398	3	1 1 2	37.47
2.367	12	1 6 1	37.99
2.358	5	0 3 2	38.13
2.330	8	1 7 0	38.61
2.303	2	3 1 0	39.09
2.231	14	0 7 1	40.39
2.154	5	3 3 0	41.91
2.125	6	1 7 1	42.50
2.102	8	3 1 1	42.99
2.057	6	3 2 1	43.98

$\beta$  -L-Glutamic Acid,  $C_5H_9NO_4$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 3$	hkl	$2\theta(^{\circ})$
2.040	8	2 6 1	44.38
2.017M	8	2 2 2	44.91
2.017M		2 7 0	44.91
1.995	3	0 8 1	45.43
1.988	4	3 3 1	45.59
1.953	2	2 3 2	46.47
1.924	3	0 6 2	47.19
1.919	3	1 8 1	47.32
1.902	4	3 4 1	47.79
1.878	4	2 7 1	48.44
1.855M	5	1 6 2	49.07
1.855M		1 9 0	49.07
1.838	1	2 8 0	49.55
1.806	1	3 5 1	50.50
1.803	1	0 9 1	50.59
1.744	3	1 9 1	52.42
1.733	3	4 1 0	52.77
1.729	5	1 7 2	52.90
1.718	4	3 1 2	53.28
1.706M	3	3 6 1	53.68
1.706M		4 2 0	53.68
1.6921	2	3 7 0	54.16
1.6838M	3	2 6 2	54.45
1.6838M		2 9 0	54.45
1.6640	3	1 1 3	55.15
1.6588	3	0 8 2	55.34
1.6505M	3	0 3 3	55.64
1.6505M		4 0 1	55.64
1.6421+	4	4 1 1	55.95
1.6421+		1 2 3	55.95
1.5982	3	1 10 1	57.63
1.5864	2	4 3 1	58.10
1.5425M	2	0 9 2	59.92
1.5425M		0 5 3	59.92
1.5211	2	2 2 3	60.85
1.5055M	1	1 5 3	61.55
1.5055M		0 11 1	61.55

Glycine,  $\alpha$ -C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>

Synonym

1.  $\alpha$ -Aminoacetic acid

CAS registry no.

56-40-6

Sample

The sample from Fisher Scientific Co., Fair Lawn, NJ. was recrystallized from a mixture of water and methanol to which a small amount of ether was added.

Color

Colorless

Structure

Monoclinic, P2<sub>1</sub>/n (14), Z = 4. The structure was determined by Albrecht and Corey [1939] and refined by Marsh [1957].

Lattice constants of this sample

a = 5.4621(12) Å  
b = 11.966(3)  
c = 5.1077(11)  
 $\beta$  = 111.72(2)°

a/b = 0.4565  
c/b = 0.4269

Volume

310.14 Å<sup>3</sup>

Density

(calculated) -.608 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 40.5 (0.014,51)

Reference intensity

I/I<sub>corundum</sub> = 4.6(3)

Polymorphism

$\alpha$ -glycine, the most stable form, is obtained from water at room temperature and below, while  $\beta$ - and  $\gamma$ -glycine are obtained (together with  $\alpha$ -glycine) from mixtures of water with acetic acid at higher temperatures [Hubig, 1958].

Additional pattern

1. PDF card 7-718 [Hanawalt et al., 1938]

References

Albrecht, G. and Corey, R. B. (1939). J. Am. Chem. Soc. 61, 1087.  
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.  
Hubig, W. Z. (1958). Z. Naturforsch. B13, 633.  
Marsh, R. E. (1957). Acta Crystallogr. 10, 814.

CuK $\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C				
Internal standard W, a = 3.16524 Å				
d(Å)	I <sup>rel</sup>	hk $\ell$	$2\theta$ (°)	
$\sigma = \pm 2$				
5.98	9	0 2 0	14.80	
4.670	9	1 1 0	18.99	
4.410	4	0 1 1	20.12	
3.874	1L	1 2 0	22.94	
3.719	15	0 2 1	23.91	
3.523	1L	-1 2 1	25.26	
3.134	6	1 3 0	28.46	
3.053	10	0 3 1	29.23	
2.990	100	0 4 0	29.86	
2.874	1	1 1 1	31.09	
2.654	1L	1 2 1	33.75	
2.532	7	0 4 1	35.42	
2.481	2	2 1 0	36.18	
2.453	4	-2 2 1	36.60	
2.374	1L	0 0 2	37.87	
2.336	1	2 2 0	38.50	
2.327	1	0 1 2	38.67	
2.229	1L	-2 3 1	40.43	
2.205	1	0 2 2	40.90	
2.166	1	1 5 0	41.67	
2.143M	1	-1 3 2	42.14	
2.143M		2 3 0	42.14	
2.105	1	1 4 1	42.94	
2.051	1L	-2 2 2	44.13	
2.039	1	0 3 2	44.40	
2.000	1	-2 4 1	45.30	
1.994	1	0 6 0	45.46	
1.935M	1	-1 4 2	46.91	
1.935M		2 4 0	46.91	
1.915	1	-2 3 2	47.44	
1.874	1L	1 1 2	48.54	
1.859M	1L	2 2 1	48.97	
1.859M		0 4 2	48.97	
1.839	1L	0 6 1	49.54	
1.808	1L	1 2 2	50.43	
1.7998	1L	-3 1 1	50.68	
1.7886	1L	-2 5 1	51.02	
1.7566	1L	2 3 1	52.02	
1.7422M	1L	-1 5 2	52.48	
1.7422M		-3 2 1	52.48	
1.7129	1L	1 3 2	53.45	
1.6988	1L	-1 0 3	53.93	
1.6821	1L	-1 1 3	54.51	
1.6557	1L	-3 3 1	55.45	



Guanidinium Chloride, CH<sub>5</sub>N<sub>3</sub>·HCl

Synonym

1. Guanidine Hydrochloride

CAS registry no.

50-01-1

Sample

The sample was obtained from Mallinckrodt Chemical Works, St. Louis, MO.

Color

Colorless

Structure

Orthorhombic, Pbc<sub>a</sub>(61), Z = 8. The structure was determined by Haas et al. [1965].

Lattice constants of this sample

a = 9.192(2) Å  
b = 13.037(4)  
c = 7.774(2)

a/b = 0.7051  
c/b = 0.5963

Volume

963.6 Å<sup>3</sup>

Density

(calculated) 1.362 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 36.0(0.015,55)

Reference intensity

I/I<sub>corundum</sub> = 0.77(2)

Additional pattern

1. PDF card 3-387 [Theilacker, 1931].

References

Haas, D. J., Harris, D. R., and Mills, H. H. (1965). Acta Crystallogr. 19, 309.  
Theilacker, W. (1931). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 76, 203.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C				
Internal standard W, a = 3.16524 Å				
d(Å)	I <sup>rel</sup> σ = ±1	hkl	2θ(°)	
4.996	3	0 2 1	17.74	
4.591	13	2 0 0	19.32	
4.386	88	1 2 1	20.23	
4.329	16	2 1 0	20.50	
3.884	9	0 0 2	22.88	
3.787	46	2 1 1	23.47	
3.583	50	1 0 2	24.83	
3.448	96	1 1 2	25.82	
3.381	54	2 2 1	26.34	
3.258	29	0 4 0	27.35	
2.968	100	2 0 2	30.08	
2.927	12	2 3 1	30.52	
2.894	5	2 1 2	30.87	
2.783	31	3 1 1	32.14	
2.763	41	1 3 2	32.38	
2.659	75	2 4 0	33.68	
2.497	35	0 4 2	35.93	
2.449M	10	2 3 2	36.66	
2.449M		1 1 3	36.66	
2.407M	11	0 2 3	37.33	
2.407M		3 0 2	37.33	
2.384	6	3 3 1	37.70	
2.368	2	3 1 2	37.97	
2.297	13	4 0 0	39.18	
2.264	5	4 1 0	39.78	
2.223	2	2 1 3	40.54	
2.195	9	2 4 2	41.08	
2.173M	4	4 1 1	41.52	
2.173M		0 6 0	41.52	
2.164	4	1 3 3	41.70	
2.134	3	2 2 3	42.31	
2.106M	11	1 5 2	42.91	
2.106M		3 3 2	42.91	
2.088	9	4 2 1	43.29	
2.040	4	1 6 1	44.36	
2.032	1	4 3 0	44.56	
1.978	3	4 0 2	45.85	
1.966M	5	4 3 1	46.14	
1.966M		2 6 0	46.14	
1.959	7	2 5 2	46.32	
1.957M	5	3 1 3	46.37	
1.957M		4 1 2	46.37	
1.902	6	1 0 4	47.79	
1.894M	6	3 2 3	47.99	
1.894M		4 2 2	47.99	

Guanidinium Chloride,  $\text{CH}_5\text{N}_3\cdot\text{HCl}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 1$	hkl	$2\theta(^{\circ})$
1.881	8	1 1 4	48.35
1.8011M	5	3 3 3	50.64
1.8011M		4 3 2	50.64
1.7683	2	3 5 2	51.65
1.7422	7	1 3 4	52.48
1.7279	5	3 6 1	52.95
1.7046	5	4 1 3	53.73
1.6909M	6	3 4 3	54.20
1.6909M		4 4 2	54.20

Hexamethylenetetramine, C<sub>6</sub>H<sub>12</sub>N<sub>4</sub>

Synonym

1. 1,3,5,7-tetraazatricyclo [3.3.1.1<sup>3,7</sup>]-decane
2. Methenamine

CAS registry no.

100-97-0

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was recrystallized from ethanol. There was one line at  $d = 3.152$  with an intensity of 1 that was not accounted for.

Color

Colorless

Structure

Cubic,  $I\bar{4}3m$  (217),  $Z = 2$ . The structure was determined quantitatively by Becka and Cruickshank [1963].

Lattice constant of this sample

$a = 7.0287(3) \text{ \AA}$

Volume

$347.24 \text{ \AA}^3$

Density

(calculated)  $1.341 \text{ g/cm}^3$

Figure of merit

$F_{22} = 74.3(0.010,29)$

Reference intensity

$I/I_{\text{corundum}} = 3.84(10)$

Additional pattern

1. PDF card 3-135 [Dow Chemical Co., Midland, MI]

Reference

Becka, L. N. and Cruickshank, D. W. J. (1963). Proc. Roy. Soc. Ser. A 273, 435.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$				
$d(\text{Å})$	$I^{\text{rel}}$	hkl	$2\theta(^\circ)$	
$\sigma = \pm 1$				
4.968	100	1 1 0	17.84	
3.517	4	2 0 0	25.30	
2.870	14	2 1 1	31.14	
2.485	2	2 2 0	36.12	
2.224	1L	3 1 0	40.53	
2.0291	6	2 2 2	44.62	
1.8784	4	3 2 1	48.42	
1.6560	1L	4 1 1	55.44	
1.5713	1L	4 2 0	58.71	
1.4984	1	3 3 2	61.87	
1.4346	1L	4 2 2	64.95	
1.3786	1	5 1 0	67.94	
1.2832	1L	5 2 1	73.78	
1.2424	1	4 4 0	76.63	
1.2057	1L	5 3 0	79.42	
1.1715	1L	6 0 0	82.22	
1.1404	1L	6 1 1	84.98	
1.0845	1L	5 4 1	90.52	
1.0595	1L	6 2 2	93.28	
1.0362	1L	6 3 1	96.04	
.9565	1L	7 2 1	107.29	
.8927	1L	7 3 2	119.29	

Hydrazinium Sulfate, (NH<sub>3</sub>)<sub>2</sub>SO<sub>4</sub>

Synonyms

1. Hydrazine sulfate
2. Hydrazonium sulfate

CAS registry no.

10034-93-2

Sample

Hydrazinium sulfate was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was recrystallized from water. The x-ray pattern was run in a humid atmosphere.

Color

Colorless

Structure

Orthorhombic, P<sub>2</sub><sub>1</sub>2<sub>1</sub>2<sub>1</sub> (19), Z = 4. The structure was determined by Nitta et al. [1951] and refined by Jönsson and Hamilton [1970].

Lattice constants of this sample

a = 8.2579(14) Å  
b = 9.178(2)  
c = 5.5386(11)

a/b = 0.8997  
c/b = 0.6035

Volume

419.78 Å<sup>3</sup>

Density

(calculated) 2.059 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 57.4 (0.013,41)

Reference intensity

I/I<sub>corundum</sub> = 1.47(8)

Additional pattern

1. PDF card 4-375 (Inst. of Physics, Univ. College, Cardiff, Wales)

References

- Jönsson, P. G. and Hamilton, W. C. (1970).  
Acta Crystallogr. B26, 536.  
Nitta, I., Sakurai, K., and Tomiie, Y. (1951).  
Acta Crystallogr. 4, 289.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C Internal standard Ag, a = 4.08651 Å			
d(Å)	I <sup>rel</sup> σ = ±5	hkl	θ(°)
6.15	10	1 1 0	14.39
4.602	46	1 0 1	19.27
4.130	100	2 0 0	21.50
4.015	20	1 2 0	22.12
3.768	10	2 1 0	23.59
3.534	62	0 2 1	25.18
3.312	1	2 0 1	26.90
3.250	47	1 2 1	27.42
3.116	43	2 1 1	28.62
3.071	19	2 2 0	29.05
2.769	12	0 0 2	32.30
2.685	17	2 2 1	33.34
2.650	6	0 1 2	33.80
2.636	8	3 1 0	33.98
2.625	9	1 0 2	34.13
2.546	4	1 3 1	35.22
2.525	10	1 1 2	35.53
2.458	6	2 3 0	36.53
2.381	7	3 1 1	37.75
2.361	4	3 2 0	38.09
2.295	3	0 4 0	39.22
2.280	4	1 2 2	39.50
2.246	2	2 3 1	40.11
2.232	9	2 1 2	40.38
2.211	13	1 4 0	40.78
2.172	3	3 2 1	41.54
2.119	1	0 4 1	42.63
2.052M	2	1 4 1	44.09
2.052M		0 3 2	44.09
2.047	2	3 3 0	44.20
2.013	4	4 1 0	44.99
1.993	1	1 3 2	45.47
1.953	2	3 0 2	46.46
1.9100	14	3 1 2	47.57
1.8924	3	4 1 1	48.04
1.8850	6	2 4 1	48.24
1.8382	2	2 3 2	49.55
1.7955	1	3 2 2	50.81
1.7916	1	1 5 0	50.93
1.7824	2	4 2 1	51.21
1.7676M	5	1 1 3	51.67
1.7676M		0 4 2	51.67
1.7622	7	3 4 0	51.84
1.7114	2	4 3 0	53.50
1.6849	2	2 0 3	54.41

Hydrazinium Sulfate,  $(\text{NH}_3)_2\text{SO}_4$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 5$	hkl	$2\theta(^{\circ})$
1.6778M	2	2 5 0	54.66
1.6778M		1 2 3	54.66
1.6579	3	2 1 3	55.37
1.6451	1	3 3 2	55.84
1.6346	3	4 3 1	56.23
1.5821M	2	5 0 1	58.27
1.5821M		2 2 3	58.27
1.5595	3	5 1 1	59.20

Iron Chloride Hydrate (Hydromolysite),  $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$

Synonym

1. Ferric chloride hexahydrate

CAS registry no.

10025-77-1

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was somewhat hygroscopic.

Color

Deep orange yellow

Structure

Monoclinic,  $C2/m$  (12),  $Z = 2$ . The structure of  $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$  was determined by Lind [1961].

Lattice constants of this sample

$a = 11.834(3) \text{ \AA}$

$b = 7.029(2)$

$c = 5.9524(13)$

$\beta = 100.47(2)^\circ$

$a/b = 1.6836$

$c/b = 0.8468$

Volume

$486.8 \text{ \AA}^3$

Density

(calculated)  $1.844 \text{ g/cm}^3$

Figure of merit

$F_{30} = 41.4(0.015, 47)$

Additional pattern

1. PDF card 1-153 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). *Ind. Eng. Chem. Anal. Ed.* **10**, 457.  
Lind, M. D. (1967). *J. Chem. Phys.* **47**, 990.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$				
Internal standard Ag, $a = 4.08651 \text{ \AA}$				
$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 2$	hkl		$2\theta(^\circ)$
6.03	14	1 1 0		14.69
5.866	82	0 0 1		15.09
5.824	100	2 0 0		15.20
4.565	3	-2 0 1		19.43
4.412	5	-1 1 1		20.11
4.015	4	1 1 1		22.12
3.516	4	0 2 0		25.31
3.163	15	-3 1 1		28.19
3.015	2	0 2 1		29.61
2.927	3	0 0 2		30.52
2.909	5	4 0 0		30.71
2.818	2	-4 0 1		31.73
2.782	4	-2 2 1		32.15
2.754	7	3 1 1		32.49
2.736	3	-1 1 2		32.70
2.580	5	2 2 1		34.74
2.540	3	1 1 2		35.31
2.442	13	2 0 2		36.77
2.280	1L	-4 0 2		39.50
2.242	1	4 2 0		40.19
2.203	3	-2 2 2		40.93
2.199	4	-4 2 1		41.02
2.165	1	-1 3 1		41.69
2.060	2	3 1 2		43.92
2.004M	2	2 2 2		45.20
2.004M		3 3 0		45.20
2.001	2	4 2 1		45.28
1.958	5	5 1 1		46.33
1.954	5	-3 3 1		46.44
1.939	3	6 0 0		46.81
1.9096	3	-1 1 3		47.58
1.8979	4	4 0 2		47.89
1.8445	1L	3 3 1		49.37
1.8065	3	1 1 3		50.48
1.7721	2	-6 0 2		51.53
1.7559	1	2 0 3		52.04
1.7117	1L	-2 2 3		53.49
1.7058M	1	0 2 3		53.69
1.7058M		-6 2 1		53.69
1.6982	3	6 2 0		53.95
1.6815	1L	2 4 0		54.53
1.6702	1	4 2 2		54.93

Iron Fluoride Hydrate,  $\beta$ -FeF<sub>3</sub>·3H<sub>2</sub>O

Synonym

1. Ferric trifluoride trihydrate

Sample

The sample was obtained from City Chemical Corp., New York, NY.

Color

Blue gray.

Structure

Tetragonal, P4/n (85), Z = 2. The structure was determined by Teufer [1964].

Lattice constants of this sample

a = 7.8326(5) Å

c = 3.8773(3)

c/a = 0.4950

Volume

237.87 Å<sup>3</sup>

Density

(calculated) 2.330 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 80.9(0.010,36)

Reference intensity

I/I<sub>corundum</sub> = 2.00(4)

Polymorphism

Nielsen [1940] reported another form of FeF<sub>3</sub>·3H<sub>2</sub>O which was colorless and was made by crystallization at a lower temperature than the form studied here.

Additional pattern

1. PDF card 1-202 [Hanawalt et al., 1938]

References

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

Nielsen, A. H. (1940). Z. Anorg. Allgem. Chem., 244, 85.

Teufer, G. (1964). Acta Crystallogr. 17, 1480.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C				
Internal standard W, a = 3.16524 Å				
d(Å)	I <sup>rel</sup>	hkl	2θ(°)	
σ = ±2				
5.542	100	1 1 0	15.98	
3.917	54	2 0 0	22.68	
3.879	14	0 0 1	22.91	
3.476	49	1 0 1	25.61	
3.177	25	1 1 1	28.06	
2.769	28	2 2 0	32.30	
2.600	10	2 1 1	34.47	
2.475	31	3 1 0	36.27	
2.253	1	2 2 1	39.99	
2.1662	1L	3 0 1	41.66	
2.0861	14	3 1 1	43.34	
1.9586	11	4 0 0	46.32	
1.8950	13	3 2 1	47.97	
1.8817	24	1 0 2	48.33	
1.8466	6	3 3 0	49.31	
1.8295	3	1 1 2	49.80	
1.7512	26	4 2 0	52.19	
1.7061	8	4 1 1	53.68	
1.6961	9	2 1 2	54.02	
1.6674	3	3 3 1	55.03	
1.5962	3	4 2 1	57.71	
1.5569	2	3 0 2	59.31	
1.5357	5	5 1 0	60.21	
1.5268	2	3 1 2	60.60	
1.4524	3	4 3 1	64.06	
1.4468	9	3 2 2	64.34	
1.4280	3	5 1 1	65.29	
1.3849	1	4 4 0	67.59	
1.3620	4	5 2 1	68.88	
1.3570	8	4 1 2	69.17	
1.3430	2	5 3 0	70.00	
1.3370	1	3 3 2	70.36	
1.2920	1	0 0 3	73.20	
1.2691	1	5 3 1	74.74	
1.2586	1L	1 1 3	75.47	
1.2385	3	6 2 0	76.92	
1.2275	1L	2 0 3	77.74	
1.2220	1	6 1 1	78.15	
1.2185	4	4 3 2	78.42	
1.2036	2	5 1 2	79.58	
1.1712	1	2 2 3	82.25	
1.1635	4	5 2 2	82.91	
1.1459	1	3 1 3	84.48	

Lanthanum Nickel Platinum,  $\text{LaNi}_{0.25}\text{Pt}_{4.75}$

Sample

The sample was prepared at NBS by Weisman et al. [1975].

Color

Metallic gray

Structure

Hexagonal,  $P6/mmm$  (191),  $Z = 1$ . This phase has the  $\text{CaCu}_5$  type structure. The structure of  $\text{CaCu}_5$  was determined by Haucke [1940].

Lattice constants of this sample

$a = 5.3732(5) \text{ \AA}$

$c = 4.3574(7)$

$c/a = 0.8110$

Volume

$108.95 \text{ \AA}^3$

Density

(calculated)  $16.465 \text{ g/cm}^3$

Figure of merit

$F_{2\theta} = 69.7(0.011, 26)$

References

Haucke, W. (1940). *Z. Anorg. Allg. Chem.* **244**, 17.

Weisman, I. D., Bennett, L. H., McAlister, A. J., and Watson, R. E. (1975). *Phys. Rev. B* **11**, 82.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$			
$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 4$	hkl	$2\theta(^\circ)$
4.655	36	1 0 0	19.05
3.182	10	1 0 1	28.02
2.685	18	1 1 0	33.34
2.327	40	2 0 0	38.66
2.287	100	1 1 1	39.37
2.179	32	0 0 2	41.40
2.0532	54	2 0 1	44.07
1.9730	9	1 0 2	45.96
1.7591	5	2 1 0	51.94
1.6924	7	1 1 2	54.15
1.6312	2	2 1 1	56.36
1.5901	15	2 0 2	57.95
1.5512	4	3 0 0	59.55
1.4608	21	3 0 1	63.65
1.3687	4	2 1 2	68.50
1.3436	13	2 2 0	69.96
1.2774	8	1 1 3	74.17
1.2633	3	3 0 2	75.14
1.2323	6	2 0 3	77.38
1.1632	5	4 0 0	82.94



Lead Bromide, PbBr<sub>2</sub>

CAS registry no.  
10031-22-8

## Sample

The sample originally obtained from National Lead Co. was used. These data replace a very early pattern [Swanson and Fuyat, 1953]. The new measurements have better resolution, improved intensities, and refined lattice parameters.

## Major impurities

Spectrographic analysis showed 0.001 to 0.01% iron and 0.0001 to 0.001% each Ag, Al, Cu, Mg, and Si.

## Color

Colorless

## Structure

Orthorhombic, Pnam (62), Z = 4, isostructural with PbCl<sub>2</sub> [Brækken and Harang, 1928]. The structure was determined by McBride [1967].

## Lattice constants of this sample

a = 8.062(1) Å  
b = 9.5393(13)  
c = 4.7348(6)

a/b = 0.8452  
c/b = 0.4964

## Volume

364.1 Å<sup>3</sup>

## Density

(calculated) 6.695 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 78.8(0.014,38)

## Reference intensity

I/I<sub>corundum</sub> = 1.83(11)

## Additional patterns

1. PDF card 5-608 [Swanson and Fuyat, 1953]
2. Brækken and Harang [1928]
3. Döll and Klemm [1939]
4. Hanawalt, Rinn, and Frevel [1938]

## References

- Brækken, H. and Harang, L. (1928). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 68, 123.  
Döll, W. and Klemm, W. (1939). Z. Anorg, Allg. Chem. 241, 239.  
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.  
McBride, H. D. (1967). Diss. Abstr. B27, 3891.  
Swanson, H. E. and Fuyat, R. K. (1953). Nat. Bur. Stand. U.S. Circ. 539, 2, 47.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup> σ = ±4	hkl	2θ(°)
6.16	3	1 1 0	14.37
4.774	30	0 2 0	18.57
4.239	19	0 1 1	20.94
4.105	56	1 2 0	21.63
4.032	31	2 0 0	22.03
3.751	73	1 1 1	23.70
3.711	8	2 1 0	23.96
3.102	50	1 2 1	28.76
3.081	55	2 2 0	28.96
3.071	56	2 0 1	29.05
2.958	23	1 3 0	30.19
2.924	100	2 1 1	30.55
2.641	90	0 3 1	33.92
2.586	10	3 1 0	34.66
2.580	9	2 2 1	34.74
2.509	8	1 3 1	35.76
2.495	15	2 3 0	35.97
2.385	28	0 4 0	37.69
2.367	45	0 0 2	37.98
2.341	38	3 2 0	38.42
2.286	14	1 4 0	39.38
2.271	42	3 1 1	39.66
2.208M	55	2 3 1	40.83
2.208M		1 1 2	40.83
2.122	5	0 2 2	42.58
2.099	4	3 2 1	43.06
2.052M	18	3 3 0	44.10
2.052M		2 4 0	44.10
2.042	12	2 0 2	44.32
2.016	8	4 0 0	44.92
1.997	2	2 1 2	45.38
1.972	4	4 1 0	45.99
1.8843M	6	2 4 1	48.26
1.8843M		3 3 1	48.26
1.8773	11	2 2 2	48.45
1.8568M	4	4 2 0	49.02
1.8568M		1 5 0	49.02
1.8554	4	4 0 1	49.06
1.8483	6	1 3 2	49.26
1.7834	7	3 4 0	51.18
1.7702	12	0 5 1	51.59
1.7459	2	3 1 2	52.36
1.7291M	14	1 5 1	52.91
1.7291M		4 2 1	52.91
1.7242	10	2 5 0	53.07
1.7185	7	2 3 2	53.26
1.7023	4	4 3 0	53.81
1.6792	9	0 4 2	54.61
1.6688	7	3 4 1	54.98
1.6652	20	3 2 2	55.11

Lead Bromide,  $\text{PbBr}_2$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 4$	hkl	$2\theta(^{\circ})$
1.6448	4	1 4 2	55.85
1.6017	4	4 3 1	57.49
1.5896M	7	5 1 0	57.97
1.5896M		0 6 0	57.97
1.5602	2	1 6 0	59.17
1.5564M	3	0 1 3	59.33
1.5564M		3 5 0	59.33
1.5505M	4	3 3 2	59.58
1.5505M		2 4 2	59.58
1.5390	4	4 4 0	60.07
1.5346	6	4 0 2	60.26
1.5295	7	1 1 3	60.48
1.5277	7	5 2 0	60.56
1.5146	4	4 1 2	61.14
1.5068	15	5 1 1	61.49
1.4793	20	2 6 0	62.76
1.4699	6	2 0 3	63.21
1.4608M	2	4 2 2	63.65
1.4608M		1 5 2	63.65
1.4524	6	2 1 3	64.06
1.4384	1	5 3 0	64.76
1.4247	4	3 4 2	65.46
1.4138	7	0 3 3	66.03
1.4040	2	2 2 3	66.55
1.3938	2	2 5 2	67.10
1.3818	2	4 3 2	67.76
1.3759	2	5 3 1	68.09
1.3470	5	3 1 3	69.76
1.3358	7	5 4 0	70.43
1.3337	7	2 3 3	70.56
1.3196M	5	5 1 2	71.43
1.3196M		0 6 2	71.43
1.3094	5	0 7 1	72.07

Lead Iodate, Pb(IO<sub>3</sub>)<sub>2</sub>

CAS registry no.  
25659-31-8

Sample

The sample was made by adding solid I<sub>2</sub>O<sub>5</sub> to an aqueous solution of Pb(NO<sub>3</sub>)<sub>2</sub>. This was digested by boiling for 1 hour and filtered. The solid was then heated at 300 °C for 2 hours and at 250 °C for 16 hours.

Color

Colorless

Structure

Orthorhombic, Pnaa (56), Z = 4 [Staritzky and Walker, 1956].

Lattice constants of this sample

a = 6.090(2) Å  
b = 16.690(3)  
c = 5.580(2)

a/b = 0.3649  
c/b = 0.3343

Volume

567.2 Å<sup>3</sup>

Density

(calculated) 6.523 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 31.1(0.017,58)

Reference intensity

I/I<sub>corundum</sub> = 11.9(5)

Additional pattern

1. PDF card 11-85 [Staritzky and Walker, 1956]

Reference

Staritzky, E. and Walker, D. I. (1956). Anal. Chem. 28, 914.

d(Å)	I <sup>rel</sup> σ = ±1	hkℓ	2θ(°)
2.999	2	2 1 0	29.77
2.931	1	1 4 1	30.47
2.864	2	0 5 1	31.20
2.784	23	0 6 0	32.12
2.673M	1L	2 0 1	33.50
2.673M		2 3 0	33.50
2.647	1	0 2 2	33.84
2.594	4	1 5 1	34.55
2.546	1L	2 2 1	35.22
2.508	1L	1 1 2	35.77
2.462	1	2 4 0	36.47
2.307	1L	1 3 2	39.01
2.250M	1	2 5 0	40.04
2.250M		2 4 1	40.04
2.194	1L	0 7 1	41.10
2.086M	1L	0 8 0	43.34
2.086M		2 5 1	43.34
2.055	20	2 6 0	44.04
2.043	6	2 1 2	44.31
1.996	1	2 2 2	45.39
1.969	11	0 6 2	46.05
1.930	1L	2 3 2	47.05
1.895	1	3 1 1	47.98
1.877	1L	2 7 0	48.47
1.860M	3	3 2 1	48.94
1.860M		1 8 1	48.94
1.804	9	3 3 1	50.56
1.751	1	2 5 2	52.20
1.735	2	3 4 1	52.70
1.7215	1	2 8 0	53.16
1.6909	19	1 9 1	54.20
1.6707	1	0 8 2	54.91
1.6538	10	2 6 2	55.52
1.6373	1L	1 4 3	56.13
1.5691	1L	1 5 3	58.80
1.5569	1L	2 7 2	59.31
1.5460	1L	1 10 1	59.77
1.5220	1	4 0 0	60.81
1.4643+	1L	0 11 1	63.48
1.4643+		2 8 2	63.48
1.4235	1	1 11 1	65.52
1.4079	1	3 8 1	66.34
1.3905	2	0 12 0	67.28

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Si, a = 5.43088 Å			
d(Å)	I <sup>rel</sup> σ = ±1	hkℓ	2θ(°)
8.36	4	0 2 0	10.57
3.996	2	1 1 1	22.23
3.694	2	1 2 1	24.07
3.309	100	1 3 1	26.92
3.047	15	2 0 0	29.29

Lithium Hydroxide, LiOH

CAS registry no.  
1310-65-2

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, N. J. It contained a small amount of LiOH·H<sub>2</sub>O and was somewhat unstable in air. The d-spacing patterns were run with the sample in vacuum grease, and the intensity patterns run with the sample in Canada Balsam.

Structure

Tetragonal, P4/nmm (129), Z = 2. The structure of LiOH was determined by Ernst [1933].

Lattice constants of this sample

a = 3.5528(5) Å  
c = 4.3476(9)

c/a = 1.2237

Volume

54.88 Å<sup>3</sup>

Density

(calculated) 1.449 g/cm<sup>3</sup>

Figure of merit

F<sub>15</sub> = 63.5(0.013,18)

Additional pattern

1. PDF card 4-708 [Ernst, 1933]

Reference

Ernst, T. (1933). Z. Phys. Chem. Leipzig  
B20, 65.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å			
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)
4.352	43	0 0 1	20.39
2.754	100	1 0 1	32.49
2.514	22	1 1 0	35.69
2.174M	2	1 1 1	41.51
2.174M		0 0 2	41.51
1.8540	6	1 0 2	49.10
1.7760	16	2 0 0	51.41
1.6435M	13	2 0 1	55.90
1.6435M		1 1 2	55.90
1.4919	10	2 1 1	62.17
1.4492	1	0 0 3	64.22
1.3754	1	2 0 2	68.12
1.3418	1	1 0 3	70.07
1.2828	3	2 1 2	73.81
1.2552	4	1 1 3	75.71
1.2068	1	2 2 1	79.33
1.1427	1	3 0 1	84.77

Magnesium Borate, MgB<sub>4</sub>O<sub>7</sub>

CAS registry no.  
12007-62-4

## Sample

The sample was prepared by heating a 1:4 molar mixture of MgCO<sub>3</sub> and H<sub>3</sub>BO<sub>3</sub> at 600 °C for 3 days, followed by heating one hour at 800 °C, and 16 hours at 600 °C with intermittent grinding. There was a very small amount of Mg<sub>2</sub>B<sub>2</sub>O<sub>5</sub> present.

## Color

Colorless

## Structure

Orthorhombic, Pbca (61), Z = 8 [Kuzel, 1964].  
Davis and Knight [1945] reported that this phase had the composition of MgB<sub>2</sub>O<sub>4</sub>.

## Lattice constants of this sample

a = 8.596(2) Å  
b = 13.729(4)  
c = 7.956(2)

a/b = 0.6261  
c/b = 0.5795

## Volume

938.9 Å<sup>3</sup>

## Density

(calculated) 2.540 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 32.8(0.014,64)

## Reference intensity

I/I<sub>corundum</sub> = 0.57(11)

## Additional pattern

1. PDF card 17-927 [Kuzel, 1964]

## References

Davis, H. M. and Knight, M. A. (1945). J. Amer. Ceram. Soc. 28, 100.

Kuzel, H.-J. (1964). Neues Jahrb. Mineral. Monatsh. 1964, 357.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Ag, a = 4.08651 Å			
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)
6.86	21	0 2 0	12.89
5.37	19	1 1 1	16.50
5.196	98	0 2 1	17.05
4.447	81	1 2 1	19.95
4.098	24	2 1 0	21.67
3.976	100	0 0 2	22.34
3.636	37	2 2 0	24.46
3.607M	42	1 0 2	24.66
3.607M		1 3 1	24.66
3.441	64	0 2 2	25.87
3.314	5	2 2 1	26.88
3.194	9	1 2 2	27.91
3.134	34	2 3 0	28.46
2.959	13	1 4 1	30.18
2.916M	29	2 0 2	30.63
2.916M		2 3 1	30.63
2.836	51	1 3 2	31.52
2.683	33	2 4 0	33.37
2.644	8	3 1 1	33.87
2.542	6	2 4 1	35.28
2.485	18	1 5 1	36.12
2.474	21	0 2 3	36.28
2.325M	6	3 0 2	38.70
2.325M		3 3 1	38.70
2.223M	43	2 4 2	40.54
2.223M		2 5 1	40.54
2.203	11	3 2 2	40.93
2.149	10	4 0 0	42.01
2.123	2	4 1 0	42.55
2.074	3	3 3 2	43.61
2.051M	5	4 1 1	44.12
2.051M		4 2 0	44.12
2.001	8	2 5 2	45.29
1.987M	10	0 0 4	45.61
1.987M		4 2 1	45.61
1.958	7	2 6 1	46.34
1.945	16	4 3 0	46.67
1.924M	21	3 4 2	47.19
1.924M		3 5 1	47.19
1.911	7	0 2 4	47.54
1.886	4	2 4 3	48.20
1.872	4	4 1 2	48.60
1.872		3 2 3	48.60
1.861	3	1 5 3	48.89
1.822M	7	4 2 2	50.02
1.822M		4 4 0	50.02
1.789	9	2 1 4	51.02
1.7450M	5	2 2 4	52.39
1.7450M		3 6 1	52.39
1.7227	8	1 7 2	53.12

Magnesium Iodate Hydrate,  $\text{Mg}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$ 

CAS registry no.  
13446-17-8

## Sample

The sample obtained from the Eastman Kodak Co., Rochester, NY, was recrystallized from an aqueous solution at room temperature.

## Color

Colorless

## Structure

Monoclinic,  $P2_1/a$  (14),  $Z = 2$ . It was assumed to be isostructural with  $\text{Co}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$  and  $\beta\text{-Ni}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$  from a comparison of the powder patterns and the cell sizes. The latter compounds were studied by Abrahams et al. [1973]. Preliminary lattice constants for  $\text{Mg}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$  were obtained by the use of the axial ratios given by Groth [1908].

## Lattice constants of this sample

$a = 8.5063(15) \text{ \AA}$   
 $b = 6.6362(15)$   
 $c = 8.3306(12)$   
 $\beta = 100.59(1)^\circ$

$a/b = 1.2818$   
 $c/b = 1.2554$

## Volume

$462.25 \text{ \AA}^3$

## Density

(calculated)  $3.206 \text{ g/cm}^3$

## Figure of merit

$F_{30} = 47.8(0.015, 41)$

## Reference intensity

$I/I_{\text{corundum}} = 2.44(8)$

## Additional pattern

1. PDF card 20-676 [University College, Cardiff, Wales]

## References

Abrahams, S. C., Sherwood, R. C., Bernstein, J. L., and Nassau, K. (1973). *J. Solid State Chem.* 7, 205.  
Groth, P. (1908). *Chemische Krystallographie II* (Engelmann, Leipzig, Germany) p. 120.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$				
Internal standard Si, $a = 5.43088 \text{ \AA}$				
$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 2$	hkl	$2\theta(^\circ)$	
8.18	24	0 0 1	10.81	
5.154	100	0 1 1	17.19	
4.631	13	-1 1 1	19.15	
4.174M	74	2 0 0	21.27	
4.174M		1 1 1	21.27	
4.094	12	0 0 2	21.69	
3.535	8	2 1 0	25.17	
3.478	55	2 0 1	25.59	
3.445	48	-2 1 1	25.84	
3.413	8	-1 1 2	26.09	
3.318	5	0 2 0	26.85	
3.236	13	-2 0 2	27.54	
3.077M	15	2 1 1	29.00	
3.077M		0 2 1	29.00	
3.052	2	1 1 2	29.24	
2.954	30	-1 2 1	30.23	
2.912	4	-2 1 2	30.68	
2.826	4	1 2 1	31.64	
2.728	22	0 0 3	32.80	
2.599	9	2 2 0	34.48	
2.577M	6	-3 1 1	34.78	
2.577M		0 2 2	34.78	
2.570	6	3 1 0	34.88	
2.540	9	-1 1 3	35.31	
2.525	5	0 1 3	35.52	
2.506	5	-2 0 3	35.81	
2.493	6	2 1 2	36.00	
2.397	6	2 2 1	37.49	
2.387	11	1 2 2	37.66	
2.364	3	-3 1 2	38.04	
2.343M	2	-2 1 3	38.39	
2.343M		3 1 1	38.39	
2.316	4	-2 2 2	38.85	
2.311	3	1 1 3	38.94	
2.137M	17	1 3 0	42.26	
2.137M		0 3 1	42.26	
2.114	6	2 0 3	42.74	
2.089M	4	4 0 0	43.27	
2.089M		2 2 2	43.27	
2.046M	4	0 0 4	44.23	
2.046M		1 3 1	44.23	
2.019M	11	-4 1 1	44.85	
2.019M		-4 0 2	44.85	
2.015	11	2 1 3	44.95	
1.994	4	4 1 0	45.46	
1.956M	4	0 1 4	46.39	
1.956M		2 3 0	46.39	
1.941M	4	4 0 1	46.76	
1.941M		-2 3 1	46.76	
1.904	5	-2 1 4	47.72	

Magnesium Iodate Hydrate,  $\text{Mg}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 2$	hkl	$2\theta(^{\circ})$
1.866	1	2 3 1	48.77
1.834	3	1 1 4	49.68
1.7925	2	3 2 2	50.90
1.7619	3	-1 2 4	51.85
1.7425	2	0 2 4	52.47
1.7370	4	4 0 2	52.65
1.7327	4	3 3 0	52.79
1.7236M	7	-4 2 2	53.09
1.7236M		-1 3 3	53.09
1.6801	2	4 1 2	54.58
1.6758	2	4 2 1	54.73
1.6654	2	-3 3 2	55.10
1.6465	2	1 3 3	55.79
1.6298	1	-2 0 5	56.41
1.6190	1	-4 0 4	56.82
1.6092	2	-5 1 2	57.20
1.5901	4	0 1 5	57.95
1.5730	2	-4 1 4	58.64

α-Manganese, Mn

CAS registry no.

7439-96-5

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was annealed in vacuum at 650 °C for 4 hours.

Color

Metallic gray

Structure

Cubic,  $\bar{1}43m$  (217),  $Z = 58$  [Gazzara et al., 1967].

Lattice constant of this sample

$a = 8.9121$  (4) Å

Volume

$707.85$  Å<sup>3</sup>

Density

(calculated)  $7.475$  g/cm<sup>3</sup>

Figure of merit

$F_{30} = 69.9$  (0.012,37)

Polymorphism

There are also β, γ, and δ Mn, the most probable transition temperatures being α ⇌ β, 700 °C; β ⇌ γ, 1079 °C; α ⇌ δ 1143 °C [Sully, 1955].

Additional patterns

1. PDF card 1-1237 [Hanawalt et al., 1938].
2. PDF card 20-180 [Swanson et al., 1969].

References

- Gazzara, C. P., Middleton, R. M., Weiss, R. J., and Hall, E. O. (1967). *Acta Crystallogr.* 22, 859.
- Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). *Ind. Eng. Chem. Anal. Ed.* 10, 457.
- Sully, A. H. (1955). *Manganese* (Butterworth Scientific Publications, London), p. 127.
- Swanson, H. E., McMurdie, H. F., Morris, M. C., and Evans, E. H. (1969). *Nat'l. Bur. Std. U.S. Monogr.* 25, Sec. 7, 142.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)
3.641	1L	2 1 1	24.43
3.153	1	2 2 0	28.28
2.571	3	2 2 2	34.87
2.382	3	3 2 1	37.74
2.227	7	4 0 0	40.48
2.101	100	4 1 1	43.01
1.8994	24	3 3 2	47.85
1.8193	9	4 2 2	50.10
1.7475	14	5 1 0	52.31
1.6274	1	5 2 1	56.50
1.5286	1L	5 3 0	60.52
1.4857	1	6 0 0	62.46
1.4460	1	6 1 1	64.38
1.4088	1L	6 2 0	66.29
1.3754	1L	5 4 1	68.12
1.3435	2	6 2 2	69.97
1.3138	1L	6 3 1	71.79
1.2864	4	4 4 4	73.57
1.2605	7	7 1 0	75.34
1.2125	17	7 2 1	78.88
1.1911	3	6 4 2	80.59
1.1701	2	7 3 0	82.34
1.1317	3	7 3 2	85.79
1.0969	2	8 1 1	89.22
1.0806	1	8 2 0	90.93
1.0652	1	6 5 3	92.63
1.0504	6	8 2 2	94.33
1.0361	1	8 3 1	96.05
1.0223	1L	6 6 2	97.79
1.0091	1	7 5 2	99.52



Mercury Acetate, C<sub>4</sub>H<sub>6</sub>Hg<sub>2</sub>O<sub>4</sub>

## Synonym

1. Mercurous Acetate

## CAS registry no.

631-60-7

## Sample

Hg<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>·2H<sub>2</sub>O was dissolved in water with addition of 25% HNO<sub>3</sub> and treated with a solution of CH<sub>3</sub>CO<sub>2</sub>Na. The precipitate was washed with cold water and dried in a desiccator [Brauer, 1963].

## Color

Colorless

## Structure

Monoclinic, A\*/\*, Z = 2 [Puff et al., 1965].

## Lattice constants of this sample

a = 12.185(3) Å

b = 5.966(2)

c = 5.1867(13)

β = 100.08(2)°

a/b = 2.0424

c/b = 0.8694

## Volume

371.2 Å<sup>3</sup>

## Density

(calculated) 4.645 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 54.5(0.013,42)

## Additional pattern

1. PDF card 19-799 [Puff et al., 1965]

## References

Brauer, G. (1963). Handbook of Preparative Inorganic Chemistry, (Academic Press, New York, NY) p. 1120.

Puff, H., Lorbacher, G., and Skrabs, R. (1965). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 122, 156.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Ag, a = 4.08651 Å			
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)
12.02	100	1 0 0	7.35
6.00	1	2 0 0	14.74
4.001	3	3 0 0	22.20
3.877	11	0 1 1	22.92
3.849	15	-1 1 1	23.09
3.553	2	1 1 1	25.04
3.477	14	-2 1 1	25.60
3.079	1	2 1 1	28.98
3.000	14	4 0 0	29.76
2.894	5	1 2 0	30.87
2.615	4	3 1 1	34.26
2.593	2	-1 0 2	34.57
2.544	1L	-4 1 1	35.25
2.514	3	-2 0 2	35.69
2.399	8	5 0 0	37.46
2.346	2	-3 0 2	38.33
2.233	8	4 1 1	40.35
2.215	2	2 0 2	40.71
2.174	2	-5 1 1	41.51
2.137	1	-4 0 2	42.26
2.115	3	4 2 0	42.72
2.000M	6	6 0 0	45.30
2.000M		3 0 2	45.30
1.956	1	-1 2 2	46.39
1.928	3	5 1 1	47.10
1.924	3	-5 0 2	47.20
1.882	4	-6 1 1	48.32
1.870	3	5 2 0	48.64
1.849	2	-1 3 1	49.23
1.845	2	-3 2 2	49.36
1.8031	1	-2 3 1	50.58
1.7958	1	4 0 2	50.80
1.7769	1	2 2 2	51.38
1.7276	1L	-6 0 2	52.96
1.7141	1L	7 0 0	53.41
1.6602+	2	-1 1 3	55.29
1.6602+		3 2 2	55.29
1.6503M	2	-7 1 1	55.65
1.6503M		-2 1 3	55.65

Mercury Hydroxide Nitrate, Hg(OH)NO<sub>3</sub>

## Synonym

- Mercury oxide nitrate hydrate,  
Hg<sub>2</sub>O(NO<sub>3</sub>)<sub>2</sub>·H<sub>2</sub>O

## Sample

The sample was prepared by dissolving HgNO<sub>3</sub>·H<sub>2</sub>O in a mixture of HNO<sub>3</sub> and H<sub>2</sub>O. The solution was evaporated at room temperature. The first crystals formed were a mixture of phases and were discarded. The second crystals formed were used to obtain the measurements.

## Color

Colorless

## Structure

Monoclinic, P2<sub>1</sub>/n (14), Z = 4. The structure was determined by Ribár et al. [1971].

## Lattice constants of this sample

a = 7.7438(11) Å  
b = 7.1944(11)  
c = 6.5893(11)  
β = 114.28(1)°

a/b = 1.0764  
c/b = 0.9159

## Volume

334.62 Å<sup>3</sup>

## Density

(calculated) 5.550 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 39.1 (0.013,58)

## Reference intensity

I/I<sub>corundum</sub> = 9.2(5)

## Additional pattern

- PDF card 11-189 [Bernstein et al., 1957]

## References

Bernstein, R. B., Pars, H. G., and Blumenthal, D. C. (1957). J. Am. Chem. Soc. 79, 1579.  
Ribár, B., Matković, B., Sljukić, M., and Gabela, F. (1971). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 134, 311.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C				
Internal standard Ag, a = 4.08651 Å				
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)	
5.93	100	-1 0 1	14.93	
4.614	1	0 1 1	19.22	
4.583	2	-1 1 1	19.35	
3.862	33	1 0 1	23.01	
3.526	18	2 0 0	25.24	
3.404	2	1 1 1	26.16	
3.361	2	-2 1 1	26.50	
3.207	32	1 2 0	27.80	
3.088	18	0 2 1	28.89	
3.005	19	0 0 2	29.71	
2.969	19	-2 0 2	30.07	
2.630	3	1 2 1	34.06	
2.612	12	-2 2 1	34.31	
2.582	9	-3 0 1	34.72	
2.454	3	2 1 1	36.59	
2.430M	11	-1 2 2	36.97	
2.430M		-3 1 1	36.97	
2.267	1	-3 1 2	39.73	
2.236	1L	3 1 0	40.30	
2.176	6	-1 0 3	41.47	
2.113	5	2 2 1	42.77	
2.012	4	1 2 2	45.01	
1.991	5	-3 2 2	45.53	
1.984	4	2 3 0	45.70	
1.979	4	-3 0 3	45.82	
1.970	4	3 2 0	46.04	
1.937	1	3 0 1	46.86	
1.930M	2	2 0 2	47.05	
1.930M		0 1 3	47.05	
1.9013	2	-4 0 2	47.80	
1.8704	1	3 1 1	48.64	
1.8547M	4	-4 1 1	49.08	
1.8547M		-2 2 3	49.08	
1.8378	1L	-4 1 2	49.56	
1.7982	3	0 4 0	50.73	
1.7641	1	4 0 0	51.78	
1.7487	3	0 2 3	52.27	
1.7435	2	1 4 0	52.44	
1.7206	3	-1 4 1	53.19	
1.7135	1	4 1 0	53.43	
1.6938M	2	-4 2 1	54.10	
1.6938M		-3 3 2	54.10	
1.6470	1	-2 0 4	55.77	
1.6298	2	1 4 1	56.41	
1.6266	1	-2 4 1	56.53	

Mercury Hydroxide Nitrate,  $\text{Hg}(\text{OH})\text{NO}_3$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 2$	$hkl$	$2\theta(^{\circ})$
1.6025	1	2 4 0	57.46
1.5519	1	-4 2 3	59.52
1.5425	2	0 4 2	59.92
1.5383	2	-2 4 2	60.10
1.5204	1L	-5 0 1	60.88
1.5013	1	0 0 4	61.74
1.4978M	1L	4 1 1	61.90
1.4978M		-2 2 4	61.90
1.4874	1	-5 1 1	62.38
1.4836	1	-4 0 4	62.56
1.4743	1	-5 0 3	63.00
1.4699M	2	0 1 4	63.21
1.4699M		-1 2 4	63.21
1.4608	1	-3 2 4	63.65

Niobium Boride,  $\zeta$ -NbB

CAS registry no.  
12045-19-1

Sample

The sample obtained from the metallurgy Section at NBS was a mixture of  $\zeta$ NbB + Nb.

Color

Metallic gray

Structure

Orthorhombic, Cmc(63), Z = 4. The structure was studied by Andersson and Kiessling [1950] and by Brewer et al., [1951]. It is isostructural with CrB.

Lattice constants of this sample

$a = 3.2973(4) \text{ \AA}$   
 $b = 8.7229(10)$   
 $c = 3.1663(3)$

$a/b = 0.3780$   
 $c/b = 0.3630$

Volume  
 $91.069 \text{ \AA}^3$

Density

(calculated)  $7.565 \text{ g/cm}^3$

Figure of merit

$F_{27} = 74.4(0.0095,38)$

Additional pattern

1. PDF card 29-947 [Spear, K. and Blanks, Pennsylvania State University, University Park, PA].

References

Andersson, L. H. and Kiessling, R. (1950). Acta Chem. Scand. 4, 160.  
Brewer, L., Sawyer, D. L., Templeton, D. H., and Dauben, C. H. (1951). J. Amer. Ceram. Soc. 34, No. 6, 173.

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard Si, $a = 5.43088 \text{ \AA}$			
$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 4$	hkl	$2\theta(^\circ)$
4.363	7	0 2 0	20.34
3.084	46	1 1 0	28.93
2.564	80	0 2 1	34.97
2.209	100	1 1 1	40.81
2.181M	97	1 3 0	41.37
2.181M		0 4 0	41.37
1.7965M	30	1 3 1	50.78
1.7965M		0 4 1	50.78
1.6481	18	2 0 0	55.73
1.5831	13	0 0 2	58.23
1.5418M	2	2 2 0	59.95
1.5418M		1 5 0	59.95
1.4885	1	0 2 2	62.33
1.4540	6	0 6 0	63.98
1.4087	10	1 1 2	66.30
1.3863M	52	2 2 1	67.51
1.3863M		1 5 1	67.51
1.3212	8	0 6 1	71.33
1.3148	10	2 4 0	71.73
1.2808M	27	1 3 2	73.94
1.2808M		0 4 2	73.94
1.2145	6	2 4 1	78.73
1.1656	14	1 7 0	82.73
1.1419	9	2 0 2	84.84
1.1047M	2	2 2 2	88.42
1.1047M		1 5 2	88.42
1.0904+	5	2 6 0	89.89
1.0904+		0 8 0	89.89
1.0707	3	0 6 2	92.01
1.0308+	17	2 6 1	96.71
1.0308+		0 8 1	96.71
1.0283	13	3 3 0	97.03
1.0257	7	0 2 3	97.35
1.0116	8	2 4 2	99.18
.9986	6	1 1 3	100.96

Pentaerythritol, C<sub>5</sub>H<sub>12</sub>O<sub>4</sub>

Synonym

1. 2,2-Bis(hydroxymethyl)-1,3-propanediol

CAS registry no.

115-77-5

Sample

The sample was obtained from Eastman Organic Chemicals, Rochester, NY. It was recrystallized from ethanol.

Color

Colorless

Structure

Tetragonal,  $I\bar{4}$  (82), Z = 2. The structure was determined by Llewellyn et al. [1937] and Nitta and Watanabé [1937] and [1938a]. It was later refined by Shiono et al. [1957], [1958].

Lattice constants of this sample

a = 6.0890(12) Å

c = 8.7481(16)

c/a = 1.4367

Volume

324.34 Å<sup>3</sup>

Density

(calculated) 1.394 g/cm<sup>3</sup>

Figure of merit

F<sub>23</sub> = 58.9(0.012,33)

Reference intensity

I/I<sub>corundum</sub> = 5.33(7)

Polymorphism

There is a cubic high temperature form stable from 179.5 °C to the melting point (260.5 °C). [Nitta and Watanabé, 1938b].

Additional pattern

1. PDF card 3-214 [Dow Chemical Co. Midland, MI]

References

- Llewellyn, F. J., Cox, E. G., and Goodwin, T. H. (1937). J. Chem. Soc. London, 1937, 883.  
 Nitta, I. and Watanabé, T. (1937). Nature London 140, 365.  
 Nitta, I. and Watanabé, T. (1938a). Sci. Pap. Inst. Phys. Chem. Res. Tokyo 34, 1669.  
 Nitta, I. and Watanabé, T. (1938b). Bull. Chem. Soc. Japan 13, 28.  
 Shiono, R., Cruickshank, D. W. J., and Cox, E. G. (1957). Acta Crystallogr. 10, 794.  
 Shiono, R., Cruickshank, D. W. J., and Cox, E. G. (1958). Acta Crystallogr. 11, 387.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup> σ = ±	hkl	2θ(°)
4.998	6	1 0 1	17.73
4.371	100	0 0 2	20.30
4.306	4	1 1 0	20.61
3.068	7	1 1 2	29.08
3.044	4	2 0 0	29.32
2.632	2	1 0 3	34.04
2.601	4	2 1 1	34.46
2.499	3	2 0 2	35.90
2.186	1	0 0 4	41.26
2.153	1	2 2 0	41.93
1.991	2	2 1 3	45.53
1.9506	1	1 1 4	46.52
1.9314	2	2 2 2	47.01
1.7769	1L	2 0 4	51.38
1.7619	1L	3 1 2	51.85
1.6815	1L	1 0 5	54.53
1.6649	1	3 0 3	55.12
1.6591	1	3 2 1	55.33
1.5336	1L	2 2 4	60.30
1.4722	1L	2 1 5	63.10
1.4581	1L	0 0 6	63.78
1.4451	1L	3 1 4	64.42
1.3250	1L	3 0 5	71.09

Phenylhydrazine Hydrochloride, C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>·HCl

Synonym

1. Hydrazinobenzene hydrochloride

CAS registry no.

59-88-1

Sample

The sample was obtained from Eastman Kodak Co., Rochester, NY. One of the lines at  $2\theta = 38.96^\circ$  came only within  $0.06^\circ$  of the calculated value.

Color

Colorless

Structure

Monoclinic, P2<sub>1</sub>/n (14), Z = 4. The structure was studied by Koo [1965].

Lattice constants of this sample

a = 6.066(2) Å

b = 30.641(6)

c = 3.884(2)

$\beta = 100.86(5)^\circ$

a/b = 0.1980

c/b = 0.1268

Volume

709.0 Å<sup>3</sup>

Density

(calculated) 1.355 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 13.0(0.014, 172)

Reference intensity

I/I<sub>corundum</sub> = 1.28(14)

Reference

Koo, O. H. (1965). Bull. Chem. Soc. Jpn. 38, 262.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup> σ = ±3	hkl	2θ(°)
15.30	100	0 2 0	5.77
7.66	22	0 4 0	11.54
5.556	30	1 2 0	15.94
4.706	22	1 4 0	18.84
3.831	90	0 8 0	23.20
3.700	20	0 2 1	24.03
3.524M	8	-1 0 1	25.25
3.524M		1 7 0	25.25
3.507	12	-1 1 1	25.38
3.417	22	0 4 1	26.06
3.224	13	1 8 0	27.65
3.065	33	0 10 0	29.11
2.977	41	2 0 0	29.99
2.924	12	2 2 0	30.55
2.901	4	-1 6 1	30.80
2.703	4	0 8 1	33.11
2.555	33	0 12 0	35.09
2.352	8	2 8 0	38.24
2.310	4	-1 10 1	38.96
2.188	1	0 14 0	41.22
2.185	2	-1 11 1	41.28
2.137M	9	2 2 1	42.26
2.137M		2 10 0	42.26
2.065	3	-2 9 1	43.81
2.034	1	2 11 0	44.51
1.938	8	2 12 0	46.83
1.9160M	3	-3 0 1	47.41
1.9160M		0 16 0	47.41
1.8234M	5	1 16 0	49.98
1.8234M		2 9 1	49.98
1.7616+	2	-1 7 2	51.86
1.7616+		1 14 1	51.86
1.7111	5	0 16 1	53.51
1.6696	1	-3 9 1	54.95
1.6370+	2	3 1 1	56.14
1.6370+		1 18 0	56.14
1.6105	1	2 16 0	57.15
1.6061M	1	-2 15 1	57.32
1.6061M		-1 17 1	57.32
1.5545	1	0 18 1	59.41
1.5323M	2	-3 12 1	60.36
1.5323M		0 20 0	60.36
1.4823M	2	4 2 0	62.62
1.4823M		-3 5 2	62.62
1.4778+	2	-4 2 1	62.83
1.4778+		2 18 0	62.83

Potassium Arsenic Fluoride,  $\text{KAsF}_6$

Synonym

1. Potassium hexafluoroarsenate

CAS registry no.

17029-22-0

Sample

The sample was obtained from Alfa Inorganics, Beverly, MA.

Color

Colorless

Structure

Hexagonal,  $R\bar{3}m$  (166),  $Z = 3$ . The structure was determined by Roof [1955] and refined by Ibers [1956]. It is isostructural with  $\text{NH}_4\text{SbF}_6$ .

Lattice constants of this sample

$a = 7.3780(4) \text{ \AA}$

$c = 7.3095(5)$

$c/a = 0.9907$

Volume

$344.58 \text{ \AA}^3$

Density

(calculated)  $3.296 \text{ g/cm}^3$

Figure of merit

$F_{30} = 100.6(0.009,32)$

Reference intensity

$I/I_{\text{corundum}} = 3.00(8)$

References

Roof, R. B. Jr., (1955). Acta Crystallogr. 8, 739.

Ibers, J. A. (1956). Acta Crystallogr. 9, 967.

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard W, $a = 3.16524 \text{ \AA}$			
$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 2$	hkl	$2\theta(^\circ)$
4.810	69	1 0 1	18.43
3.684	100	1 1 0	24.14
3.170	62	0 1 2	28.13
2.927	14	0 2 1	30.52
2.436	3	0 0 3	36.87
2.405	7	2 0 2	37.36
2.293	4	2 1 1	39.26
2.1287	5	3 0 0	42.43
2.0317	7	1 1 3	44.56
2.0146	50	1 2 2	44.96
1.8445	7	2 2 0	49.37
1.7569	2	1 0 4	52.01
1.7227	5	1 3 1	53.12
1.6035	5	3 0 3	57.42
1.5947	5	3 1 2	57.77
1.5859	6	0 2 4	58.12
1.4707	3	2 2 3	63.17
1.4632	9	0 4 2	63.53
1.4571	12	2 1 4	63.83
1.4370	2	3 2 1	64.83
1.3943	6	4 1 0	67.07
1.3605	4	2 3 2	68.97
1.3293	1	2 0 5	70.83
1.2720	2	1 3 4	74.54
1.2588	1L	0 5 1	75.46
1.2506	1L	1 2 5	76.04
1.2299	3	3 3 0	77.56
1.2181	1	0 0 6	78.45
1.2101	1	4 1 3	79.07
1.2063	3	5 0 2	79.37
1.2028	3	4 0 4	79.65
1.1914	1	2 4 1	80.56
1.1570	2	1 1 6	83.48
1.1466	2	4 2 2	84.41
1.1436	2	3 2 4	84.69
1.1338	1	5 1 1	85.59
1.1279	1	3 1 5	86.15
1.0951	1L	1 5 2	89.40
1.0649	1L	6 0 0	92.66
1.0574	1	3 0 6	93.52
1.0473	1L	0 5 4	94.70
1.0398	1	4 3 1	95.60
1.0352	1L	2 3 5	96.16
1.0307	1L	1 0 7	96.73
1.0231	1L	5 2 0	97.69
1.0165	1L	2 2 6	98.54
1.0093	1L	3 4 2	99.49
1.0074	1L	2 4 4	99.75

Potassium Hydrogen Iodate,  $\gamma$ -KH(IO<sub>3</sub>)<sub>2</sub>

CAS registry no.  
13455-24-8

Sample

A sample labelled KH(IO<sub>3</sub>)<sub>2</sub> was obtained from Fisher Scientific Co., Fair Lawn, N. J. It was recrystallized in water solution with the pH adjusted with I<sub>2</sub>O<sub>5</sub>. This  $\gamma$ -phase decomposes in moist air and minor amounts of another phase may be present. The reflection,  $d = 4.590$  and  $I = 15$  has  $|2\theta_{\text{obs}} - 2\theta_{\text{calc}}| = 0.056^\circ$ .

Color

Colorless

Structure

Monoclinic, P2<sub>1</sub>/c (14), Z = 8 [Argay et al., 1969].

Lattice constants of this sample

$a = 21.853(5) \text{ \AA}$   
 $b = 8.206(3)$   
 $c = 7.031(2)$   
 $\beta = 98.02(3)^\circ$

$a/b = 2.6631$   
 $c/b = 0.8568$

Volume

1249.  $\text{\AA}^3$

Density

(calculated) 4.149 g/cm<sup>3</sup>

Figure of merit

$F_{30} = 16.8(0.018, 97)$

Polymorphism

The monoclinic polymorph,  $\alpha$ -KH(IO<sub>3</sub>)<sub>2</sub>, also has the space group P2<sub>1</sub>/a but a cell volume of 629.6  $\text{\AA}^3$  [Argay et al., 1969].

Additional pattern

1. Argay et al. [1969]

References

Argay, Gy., Naray-Szabo, I., and Peter, E. (1969). J. Therm. Anal. 1, 413.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$			
$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 3$	hkl	$2\theta(^\circ)$
10.87	1L	2 0 0	8.13
6.55	1L	2 1 0	13.50
5.41M	41	3 1 0	16.38
5.41M		4 0 0	16.38
5.32	21	0 1 1	16.66
5.03	5	1 1 1	17.61
4.591	15	2 1 1	19.32
4.526	10	4 1 0	19.60
4.075	5	3 1 1	21.79
4.032	7	1 2 0	22.03
4.005	2	-4 1 1	22.18
3.831M	9	2 2 0	23.20
3.831M		5 1 0	23.20
3.602M	60	6 0 0	24.70
3.602M		4 1 1	24.70
3.530M	20	0 2 1	25.21
3.530M		-1 2 1	25.21
3.481	42	0 0 2	25.57
3.457	45	-2 0 2	25.75
3.268M	100	4 2 0	27.27
3.268M		-3 2 1	27.27
3.186M	44	2 0 2	27.98
3.186M		-2 1 2	27.98
3.142	18	-6 1 1	28.38
3.135	17	-4 0 2	28.45
3.089M	41	7 0 0	28.88
3.089M		3 2 1	28.88
2.978M	5	5 2 0	29.98
2.978M		3 0 2	29.98
2.807	5	-7 1 1	31.85
2.759	1	4 0 2	32.43
2.705	18	8 0 0	33.09
2.649M	19	2 3 0	33.81
2.649M		5 2 1	33.81
2.567M	4	8 1 0	34.92
2.567M		-6 1 2	34.92
2.556M	4	3 3 0	35.08
2.556M		7 1 1	35.08
2.522	2	-8 1 1	35.57
2.432	3	5 1 2	36.93
2.411M	1L	-7 2 1	37.26
2.411M		3 2 2	37.26
2.347	5	6 0 2	38.32
2.313M	3	8 1 1	38.90
2.313M		5 3 0	38.90



Potassium Hydrogen Iodate,  $\gamma$ -KH(IO<sub>3</sub>)<sub>2</sub> - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 3$	hkl	$2\theta(^{\circ})$
2.283	1L	-9 1 1	39.43
2.250	4	7 2 1	40.04
2.163M	2	10 0 0	41.72
2.163M		5 2 2	41.72
2.133M	3	-6 3 1	42.35
2.133M		2 1 3	42.35
2.107	2	9 1 1	42.89
2.092	3	10 1 0	43.22
2.075M	6	2 3 2	43.59
2.075M		9 2 0	43.59
2.057M	28	-9 2 1	43.99
2.057M		3 1 3	43.99
2.054	25	-9 1 2	44.05
2.034	24	-1 2 3	44.51
2.004M	9	8 0 2	45.22
2.004M		-8 2 2	45.22
1.989	4	1 2 3	45.58
1.924+	7	8 3 0	47.20
1.924+		2 4 1	47.20
1.912+	5	-11 1 1	47.52
1.912+		-10 1 2	47.52
1.803	3	12 0 0	50.59
1.783+	9	11 1 1	51.19
1.783+		6 4 0	51.19
1.768	7	0 4 2	51.67
1.763	6	-3 3 3	51.83
1.750	9	5 2 3	52.23
1.729	8	-4 0 4	52.91
1.725	7	2 4 2	53.06
1.717+	4	2 3 3	53.30
1.717+		-4 4 2	53.30
1.701	4	-12 0 2	53.85
1.682	5	2 0 4	54.52
1.679M	4	1 1 4	54.60
1.679M		-5 4 2	54.60
1.669M	5	-10 1 3	54.96
1.669M		11 2 1	54.96
1.6484M	4	-9 2 3	55.72
1.6484M		2 1 4	55.72
1.6338M	7	8 4 0	56.26
1.6338M		-6 4 2	56.26
1.5962+	2	10 2 2	57.71
1.5962+		-10 3 2	57.71
1.5448+	1L	-4 5 1	59.82
1.5448+		6 4 2	59.82

Potassium Hydrogen Oxalate Hydrate,  $C_4H_3KO_8 \cdot 2H_2O$

Synonyms

- Potassium trihydrogen oxalate dihydrate
- Potassium tetroxalate

CAS registry no.  
6100-20-5

Sample  
NBS Standard Reference Material #189.

Color  
Colorless

Structure  
Triclinic,  $P\bar{1}$  (2),  $Z = 2$ . The structure was determined by Haas (1964).

Lattice constants of this sample

$a = 7.031(2) \text{ \AA}$   
 $b = 10.611(4)$   
 $c = 6.367(2)$   
 $\alpha = 101.36(3)^\circ$   
 $\beta = 100.18(2)$   
 $\gamma = 93.82(2)$

$a/b = 0.6626$   
 $c/b = 0.6000$

Volume  
 $455.8 \text{ \AA}^3$

Density  
(calculated)  $1.852 \text{ g/cm}^3$

Figure of merit  
 $F_{30} = 40.6(0.017, 44)$

Reference intensity  
 $I/I_{\text{corundum}} = 1.14(7)$

Additional pattern  
1. PDF card 14-845 [Dow Chemical Co., Midland, Michigan]

Reference  
Haas, D. J. (1964). Acta Crystallogr. 17, 1511.

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 3$	hkl	$2\theta(^\circ)$
4.841	14	0 1 1	18.31
4.767	5	-1 -1 1	18.60
4.451	13	0 -2 1	19.93
4.367	3	-1 2 0	20.32
4.197	3	1 -1 1	21.15
3.943	3	1 2 0	22.53
3.828	2	-1 -2 1	23.22
3.626	1	1 1 1	24.53
3.597	2	0 2 1	24.73
3.458	5	-1 2 1	25.74
3.446	5	0 3 0	25.83
3.440	4	2 0 0	25.88
3.376	3	-2 1 0	26.38
3.321	3	0 -3 1	26.82
3.283	4	-2 0 1	27.14
3.143	100	-2 -1 1	28.37
3.123	76	0 -1 2	28.56
3.064	28	0 0 2	29.12
3.041	7	-1 -1 2	29.35
2.990	7	1 -3 1	29.86
2.963M	7	1 2 1	30.14
2.963M		1 3 0	30.14
2.921	1	0 -2 2	30.58
2.820	8	-1 -2 2	31.71
2.790	27	-2 -2 1	32.05
2.783	22	-1 1 2	32.14
2.757	9	-2 2 1	32.45
2.658	7	2 -2 1	33.69
2.578M	12	0 -3 2	34.77
2.578M		1 -2 2	34.77
2.544	4	-2 0 2	35.25
2.531	7	-2 -1 2	35.44
2.509	5	-1 4 0	35.76
2.483	3	-1 -3 2	36.15
2.442M	20	-1 2 2	36.78
2.442M		1 -4 1	36.78
2.426	6	1 3 1	37.03
2.412	6	1 1 2	37.25
2.394	4	-2 -3 1	37.54
2.384	5	2 -3 1	37.70
2.361	13	-2 3 1	38.08
2.348	8	1 -3 2	38.30
2.342	6	1 4 0	38.40
2.316	3	2 3 0	38.85
2.281	7	2 2 1	39.48
2.257	2	-3 1 1	39.91
2.232	6	-3 -1 1	40.37
2.199	3	-2 2 2	41.01
2.184	5	-3 2 0	41.30
2.146	7	-1 -4 2	42.07

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard W, $a = 3.16524 \text{ \AA}$			
$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 3$	hkl	$2\theta(^\circ)$
6.13	9	0 0 1	14.43
6.04	8	-1 1 0	14.66
5.85	1	0 -1 1	15.14
5.47	1	1 1 0	16.18
5.101	2	-1 0 1	17.37

Potassium Hydrogen Oxalate Hydrate,  $C_4H_3KO_8 \cdot 2H_2O$  - (continued)

$d(\text{\AA})$	$I^{rel}$ $\sigma = \pm 3$	hkl	$2\theta(^{\circ})$
2.100M	2	2 -2 2	43.04
2.100M		0 -5 1	43.04
2.094	3	2 0 2	43.17
2.083	2	-3 -2 1	43.41
2.068M	4	-1 0 3	43.73
2.068M		0 5 0	43.73
2.053	5	0 -2 3	44.07
2.049	3	3 -1 1	44.16
2.040M	3	0 0 3	44.36
2.040M		-1 5 0	44.36
2.015	2	-3 -1 2	44.94
2.009	2	-3 3 0	45.09
1.998	7	3 -2 1	45.35

Potassium Niobium Oxide, KNbO<sub>3</sub>

Synonym

1. Potassium niobate

CAS registry no.

12030-85-2

Sample

The sample was a Johnson Matthey chemical obtained from Ventron Corp., Danvers, MA.

Major impurities

The manufacturer's spectrographic analysis showed  $\approx$  3 ppm silicon.

Color

Colorless

Structure

Orthorhombic, Cm2m (38), Z = 2, iso-structural with the distorted perovskite form of BaTiO<sub>3</sub>. The structure was determined by Katz and Megaw [1954].

Lattice constants of this sample

a = 5.6950(4) Å  
b = 5.7213(3)  
c = 3.9739(2)

a/b = 0.9954  
c/b = 0.6946

Volume

129.48 Å<sup>3</sup>

Density

(calculated) 4.167 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 96.0(0.009,35)

Reference intensity

I/I<sub>corundum</sub> = 5.26(12)

Polymorphism

Potassium niobium oxide crystallizes in three modifications, orthorhombic at room temperature, changing to tetragonal at about 255 °C and cubic near 435 °C [Wood, 1951].

Additional pattern

1. PDF card 9-156 [Wood, priv. comm.]

References

Katz, L. and Megaw, H. D. (1967). Acta Crystallogr. 22, 639.  
Wood, E. A. (1951). Acta Crystallogr. 4, 353.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C				
Internal standard W, a = 3.16524 Å				
d(Å)	I <sup>rel</sup>	hkl	2θ(°)	
σ = ±1				
4.035	47	1 1 0	22.01	
3.973	22	0 0 1	22.36	
2.859	36	0 2 0	31.26	
2.848	46	2 0 0	31.39	
2.832	100	1 1 1	31.57	
2.322	1	0 2 1	38.75	
2.0180	33	2 2 0	44.88	
1.9866	16	0 0 2	45.63	
1.8081	3	1 3 0	50.43	
1.7998	9	2 2 1	50.68	
1.7831	6	1 1 2	51.19	
1.6462	15	1 3 1	55.80	
1.6413	19	3 1 1	55.98	
1.6314	11	0 2 2	56.35	
1.6296	6	2 0 2	56.42	
1.4305	2	0 4 0	65.16	
1.4239	4	4 0 0	65.50	
1.4160	13	2 2 2	65.91	
1.3458M	1	0 4 1	69.83	
1.3458M		3 3 0	69.83	
1.3405	1	4 0 1	70.15	
1.3371	2	1 3 2	70.35	
1.3347	2	3 1 2	70.50	
1.3249	1L	0 0 3	71.10	
1.2782	2	2 4 0	74.12	
1.2746M	7	4 2 0	74.36	
1.2746M		3 3 1	74.36	
1.2586	4	1 1 3	75.47	
1.2169	1L	2 4 1	78.54	
1.2137	1L	4 2 1	78.79	
1.2020	1L	0 2 3	79.71	
1.1610	2	0 4 2	83.13	
1.1576	3	4 0 2	83.43	
1.1221	1L	1 5 0	86.70	
1.1170	1L	5 1 0	87.20	
1.1142	1L	3 3 2	87.47	
1.1075	1L	2 2 3	88.14	
1.0797	1	1 5 1	91.03	
1.0751M	3	5 1 1	91.53	
1.0751M		2 4 2	91.53	
1.0727	3	4 2 2	91.79	
1.0687	3	1 3 3	92.24	
1.0674	2	3 1 3	92.38	
1.0091	1	4 4 0	99.52	
.9934	1L	0 0 4	101.68	

Potassium Niobium Oxide,  $\text{KNbO}_3$  - (continued)

$d(\text{Å})$	$I^{\text{rel}}$	$hkl$	$2\theta(^{\circ})$
	$\sigma = \pm 1$		
.9801	1L	3 5 0	103.62
.9780M	1L	4 4 1	103.93
.9780M		5 3 0	103.93
.9769	1L	1 5 2	104.10
.9738	1L	5 1 2	104.57
.9696	1L	4 0 3	105.20
.9646	1L	1 1 4	105.99
.9534	1L	0 6 0	107.79
.9514	1	3 5 1	108.13
.9494M	2	5 3 1	108.46
.9494M		6 0 0	108.46
.9438	1	3 3 3	109.41
.9381	1	2 0 4	110.40
.9272	1L	0 6 1	112.35
.9231	1L	6 0 1	113.12
.9197	1L	2 4 3	113.76

Potassium Sulfate, K<sub>2</sub>S<sub>2</sub>O<sub>8</sub>

Synonym

1. Potassium persulfate

CAS registry no.

7727-21-1

Sample

The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ. and was recrystallized from an aqueous solution.

Color

Colorless

Structure

Triclinic, Z = 1 (assuming a density near 2.5). The cell was obtained by V. Himes using a single crystal on a diffractometer. The cell was confirmed by the Visser program [1969]. Two somewhat different triclinic cells were reported in the literature [Keen, 1935 and Gerstäcker et al., 1928]. Our data did not index on either of these cells.

Lattice constants of this sample

a = 5.514(2) Å  
 b = 7.038(2)  
 c = 5.116(2)  
 α = 106.11(2)°  
 β = 90.15(3)  
 γ = 106.30(3)

a/b = 0.7835  
 c/b = 0.7269

Volume

182.38 Å<sup>3</sup>

Density

(calculated) 2.461 g/cm<sup>3</sup>  
 (measured) 2.45 g/cm<sup>3</sup>

Figures of merit

F<sub>30</sub> = 34.9(0.016,52)  
 M<sub>20</sub> = 27.3

Reference intensity

I/I<sub>corundum</sub> = 1.31(7)

Additional pattern

1. PDF card 12-483 [Institute of Physics, University College, Cardiff, Wales].

References

Gerstäcker, A., Möller, H., and Reis, A. (1928). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 66, 421.  
 Keen, R. C. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 91, 129.  
 Visser, J. W. (1969). J. Appl. Crystallogr.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Si, a = 5.43088 Å			
d(Å)	I <sup>rel</sup> σ = ±4	hkl	2θ(°)
5.27	2	1 0 0	16.80
4.892	15	0 0 1	18.12
4.847	20	-1 1 0	18.29
4.602	1L	0 -1 1	19.27
3.750	9	-1 0 1	23.71
3.699	38	1 -1 1	24.04
3.603	4	1 1 0	24.69
3.443	52	1 0 1	25.86
3.268	56	-1 -1 1	27.27
3.232M	100	0 2 0	27.58
3.232M		-1 1 1	27.58
3.153	3	0 -2 1	28.28
3.025	11	1 -2 1	29.50
2.736	14	-2 1 0	32.71
2.634M	9	1 1 1	34.01
2.634M		2 0 0	34.01
2.548	10	0 -1 2	35.20
2.466	22	-1 -2 1	36.40
2.419	10	-2 2 0	37.13
2.397	5	0 2 1	37.49
2.358	3	-2 1 1	38.14
2.315	3	1 -1 2	38.87
2.297+	5	-1 0 2	39.18
2.297+		2 -2 1	39.18
2.273M	3	1 -3 1	39.62
2.273M		-1 -1 2	39.62
2.239M	2	2 0 1	40.25
2.239M		-1 3 0	40.25
2.224M	1	0 -3 1	40.52
2.224M		2 1 0	40.52
2.154	3	0 3 0	41.90
2.098	1	0 1 2	43.08
1.995	5	1 2 1	45.42
1.975M	7	-2 3 0	45.91
1.975M		2 -3 1	45.91
1.923	10	1 -3 2	47.22
1.917	4	0 -3 2	47.39
1.881	7	-1 -3 1	48.35
1.858	2	-1 3 1	48.98
1.853	2	2 -2 2	49.14
1.844	1	1 1 2	49.39
1.809	5	-2 -1 2	50.40
1.800	7	2 2 0	50.66
1.753	2	1 -4 1	52.14
1.711	3	3 -2 1	53.51

Potassium Sulfate,  $K_2S_2O_8$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 4$	hkl	$2\theta(^{\circ})$
1.6338M	3	-3 2 1	56.26
1.6338M		-2 -2 2	56.26
1.6154M	8	1 -2 3	56.96
1.6154M		1 -1 3	56.96
1.6138M	4	1 -4 2	57.02
1.6138M		-2 2 2	57.02

Scandium Boride, ScB<sub>2</sub>

CAS registry no.  
12007-34-0

Sample

The sample was obtained from Cerac, Menomonee Falls, WI.

Color

Metallic gray

Structure

Hexagonal, P6/mmm (191) Z = 1. The structure was qualitatively done by Zhuravlev and Stepanova [1958].

Lattice constants of this sample

a = 3.14573(12) Å  
c = 3.5175(2)  
c/a = 1.1182

Volume

30.145 Å<sup>3</sup>

Density

(calculated) 3.667 g/cm<sup>3</sup>

Figure of merit

F<sub>19</sub> = 73.3(0.011,23)

Additional pattern

1. PDF card 11-527 [Zhuravlev and Stepanova, 1958].

References

Zhuravlev, N. N. and Stepanova, A. A. (1958).  
Kristallografiya 3, 83.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)
3.517	17	0 0 1	25.30
2.725	51	1 0 0	32.84
2.153	100	1 0 1	41.92
1.7594	10	0 0 2	51.93
1.5733	18	1 1 0	58.63
1.4774	13	1 0 2	62.85
1.4358	8	1 1 1	64.89
1.3619	5	2 0 0	68.89
1.2703	12	2 0 1	74.66
1.1721M	12	0 0 3	82.17
1.1721M		1 1 2	82.17
1.0768M	8	1 0 3	91.34
1.0768M		2 0 2	91.34
1.0297	3	2 1 0	96.85
.9883	8	2 1 1	102.42
.9401	1L	1 1 3	110.05
.9081	3	3 0 0	116.05
.8885M	6	2 0 3	120.21
.8885M		2 1 2	120.21
.8792M	2	0 0 4	122.35
.8792M		3 0 1	122.35
.8369	2	1 0 4	133.99
.8069	3	3 0 2	145.36



Silver Mercury Iodide,  $\beta$ -Ag<sub>2</sub>HgI<sub>4</sub>

CAS registry no.

7784-03-4

## Sample

The sample was obtained from Ventron Corp.  
(Alfa), Danvers, MA.

## Color

Vivid yellow

## Structure

Tetragonal,  $I\bar{4}$  (82),  $Z = 2$ , pseudocubic.  
The structure of  $\beta$ -Ag<sub>2</sub>HgI<sub>4</sub> was determined by  
Hahn et al. [1955]. A cell with  $c/2$  was  
reported by Ketelaar [1931] and a cell with  
2a was reported by Frevel and North [1950].

## Lattice constants of this sample

a = 6.3302(8) Å

c = 12.624(2)

c/a = 1.9942

## Volume

505.88 Å<sup>3</sup>

## Density

(calculated) 6.069 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 47.1(0.016,41)

## Reference intensity

I/I<sub>corundum</sub> = 5.60(10)

## Polymorphism

Above 60 °C, Ag<sub>2</sub>HgI<sub>4</sub> is cubic [Ketelaar,  
1931]. Otsubo [1966] reports another  
form of Ag<sub>2</sub>HgI<sub>4</sub> as hexagonal and stable  
above 165 °C.

## Additional patterns

1. PDF card 3-0949 [Ketelaar, 1931]
2. PDF card 4-0442 [Frevel and North,  
1950]
3. PDF card 18-1183 [Hahn et al., 1955]

## References

- Frevel, L. K. and North, P. P. (1950). J.  
Appl. Phys. 21, 1038.  
Hahn, H., Frank, G., and Klingler, W. (1955).  
Z. Anorg. Allgem. Chem. 279, 271.  
Ketelaar, J. A. A. (1931). Z. Kristallogr.  
Kristallgeometrie Kristallphys.  
Kristallchem. 80, 192.  
Otsubo, Y., Nitta, A., Kaneko, M., Iwata, Y.,  
and Ueki, A. (1966). Kogyo Kagaku  
Zasshi 69, 1716.

CuK $\alpha_1$ $\lambda = 1.540598$ Å; temp. 25±1 °C			
Internal standard Si, a = 5.43088 Å			
d(Å)	I <sup>rel</sup> $\sigma = \pm 1$	hkl	2 $\theta$ (°)
6.30	3	0 0 2	14.05
5.64	6	1 0 1	15.69
4.471	6	1 1 0	19.84
3.650	100	1 1 2	24.37
3.502	5	1 0 3	25.41
3.163	1L	2 0 0	28.19
3.156	1L	0 0 4	28.25
2.828	5	2 0 2	31.61
2.761	5	2 1 1	32.40
2.578	4	1 1 4	34.77
2.347M	3	2 1 3	38.32
2.347M		1 0 5	38.32
2.236	45	2 0 4	40.31
2.103	2	0 0 6	42.97
2.081	2	3 0 1	43.46
2.002	1	3 1 0	45.27
1.908	19	3 1 2	47.62
1.904	18	1 1 6	47.72
1.884	1	2 1 5	48.26
1.7385	1L	3 2 1	52.60
1.7340	1L	1 0 7	52.75
1.6907	1L	3 1 4	54.21
1.6203	1	3 2 3	56.77
1.5829	3	4 0 0	58.24
1.5782	3	0 0 8	58.43
1.5332	1	2 2 6	60.32
1.5240	1L	4 1 1	60.72
1.5206	1L	2 1 7	60.87
1.4887	1L	1 1 8	62.32
1.4508	4	3 1 6	64.14
1.4416M	2	4 1 3	64.60
1.4416M		3 2 5	64.60
1.3813	1L	4 2 2	67.79
1.3494	1L	3 3 4	69.62
1.3119	1L	4 1 5	71.91
1.2917	4	4 2 4	73.22
1.2901	3	2 2 8	73.32
1.2643	1L	4 0 6	75.07

Sodium Chlorate Hydrate, NaClO<sub>4</sub>·H<sub>2</sub>O

## Synonym

1. Sodium perchlorate hydrate

## CAS registry no.

7791-07-3

## Sample

The sample was recrystallized from reagent material received from the Fisher Scientific Co., Fair Lawn, NJ. The crystals were very unstable, changing readily to the anhydrous phase and back again depending on the atmospheric relative humidity.

\* Because of the sample's instability, the intensities were calculated from the structure data given by Berglund et al. [1975].

## Color

Colorless

## Structure

Monoclinic, C2/c (15), Z = 8. The structure was refined by Berglund et al. [1975].

## Lattice constants of this sample

a = 15.555(3) Å  
b = 5.5436(9)  
c = 11.063(3)  
β = 110.70(2)°

a/b = 2.8059

c/b = 1.9956

## Volume

892.4 Å<sup>3</sup>

## Density

(calculated) 2.091 g/cm<sup>3</sup>

## Figure of merit

F<sub>30</sub> = 26.0 (0.015,78)

## Reference intensity

I/I<sub>corundum</sub> = 1.34 (calculated from the structural data)

## Additional pattern

1. PDF card 28-1071 [Hanawalt et al., 1938]

## References

Berglund, B., Thomas, J. O., and Tellgren, R. (1975). Acta Crystallogr. B31, 1842.  
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

CuKα<sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I*	hkl	2θ(°)
5.18M	44	1 1 0	17.10
5.18M		0 0 2	17.10
4.894	2	-1 1 1	18.11
4.421	6	1 1 1	20.07
3.648+	77	2 0 2	24.38
3.648+		3 1 0	24.38
3.445M	100	1 1 2	25.84
3.445M		-3 1 2	25.84
3.187	5	3 1 1	27.97
2.928	3	-3 1 3	30.51
2.771	9	0 2 0	32.28
2.764	11	-2 0 4	32.36
2.707	3	-5 1 1	33.06
2.666	4	3 1 2	33.59
2.660	3	-5 1 2	33.66
2.592M	1	-2 2 1	34.58
2.592M		2 2 0	34.58
2.585M	1L	0 0 4	34.67
2.585M		-4 0 4	34.67
2.577M	1L	4 0 2	34.78
2.577M		5 1 0	34.78
2.467	1	-5 1 3	36.39
2.443+	5	0 2 2	36.76
2.443+		-2 2 2	36.76
2.437	5	-3 1 4	36.86
2.228	1	3 1 3	40.45
2.205+	16	4 2 0	40.90
2.205+		2 0 4	40.90
2.162	1	0 2 3	41.75
2.063	4	5 1 2	43.85
2.060	3	-7 1 2	43.92
2.040	1	-7 1 1	44.36
2.011	1	-1 1 5	45.04
1.958M	1	-2 2 4	46.33
1.958M		2 2 3	46.33
1.947M	1	6 0 2	46.61
1.947M		7 1 0	46.61
1.885M	2	-6 2 2	48.23
1.885M		-6 2 1	48.23
1.844	1L	1 1 5	49.39
1.825M	7	4 0 4	49.93
1.825M		6 2 0	49.93
1.820M	8	-8 0 4	50.07
1.820M		-1 3 1	50.07
1.811	1L	5 1 3	50.35
1.792	1L	1 3 1	50.92
1.739	2	-3 3 1	52.57
1.724M	9	0 0 6	53.08
1.724M		-6 2 4	53.08
1.722M	8	-6 0 6	53.16

Sodium Chlorate Hydrate  $\text{NaClO}_4 \cdot \text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^*$	hkl	$2\theta(^{\circ})$
1.722M		6 2 1	53.16
1.7040M	1	1 3 2	53.75
1.7040M		-3 3 2	53.75
1.7017M	3	-1 1 6	53.83
1.7017M		-4 2 5	53.83
1.6691	1	3 3 1	54.97
1.6497M	1L	7 1 2	55.67
1.6497M		-1 3 3	55.67
1.5919	1	-8 2 2	57.88
1.5794M	1	3 3 2	58.38
1.5794M		-5 3 2	58.38
1.5514M	1L	9 1 0	59.54
1.5514M		-10 0 2	59.54
1.5254M	1	2 2 5	60.66
1.5254M		4 2 4	60.66
1.5202	2	8 2 0	60.89
1.5126	1L	-9 1 5	61.23
1.5006M	1L	5 3 1	61.77
1.5006M		-5 1 7	61.77
1.4199M	2	3 1 6	65.71
1.4199M		-7 3 2	65.71
1.4162	3	-3 3 5	65.90
1.3860	1	0 4 0	67.53
1.3816M	2	7 3 0	67.77
1.3816M		4 0 6	67.77
1.3734	1	0 4 1	68.23
1.3631	1	-11 1 2	68.82
1.3543+	1	7 1 4	69.33
1.3543+		8 2 2	69.33
1.3385+	1L	-2 4 2	70.27
1.3385+		2 4 1	70.27
1.3342M	1	-11 1 1	70.53
1.3342M		6 2 4	70.53
1.3309M	1	-10 2 4	70.73
1.3309M		-10 2 1	70.73
1.2953M	1	-4 4 2	72.98
1.2953M		4 4 0	72.98

Sodium L(+)-Glutamate Hydrate, C<sub>5</sub>H<sub>8</sub>NNaO<sub>4</sub>·H<sub>2</sub>O

Synonym

1. Monosodium glutamate hydrate
2. Accent

CAS registry no.

142-47-2

Sample

The sample was manufactured by the Ajinomoto Co., Japan, and purchased as a food additive. It was recrystallized from a mixture of water and ethanol.

Color

Colorless

Structure

Orthorhombic, P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>(19), Z = 8. The unit cell and space group were determined by Uno [1952].

Lattice constants of this sample

a = 15.235(3) Å  
 b = 17.937(4)  
 c = 5.667(2)

a/b = 0.8494  
 c/b = 0.3104

Volume

1521.3 Å<sup>3</sup>

Density

(calculated) 1.634 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 45.6(0.014,48)

Reference intensity

I/I<sub>corundum</sub> = 0.35(2)

Additional pattern

1. PDF card 18-1904 [Institute of Physics, University College, Cardiff, Wales]

Reference

Uno, T., (1952). Yokugaku Zasshi (J. Pharm. Soc. Japan) 72, 26.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C				
Internal standard Si, a = 5.43088 Å				
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)	
11.62	3	1 1 0	7.60	
8.95	10	0 2 0	9.87	
7.72	10	1 2 0	11.46	
7.61	4	2 0 0	11.62	
7.02	3	2 1 0	12.60	
5.80	15	2 2 0	15.27	
5.562	5	1 3 0	15.92	
5.024	8	1 1 1	17.64	
4.886	2	3 1 0	18.14	
4.697	4	2 3 0	18.88	
4.519	95	1 2 1	19.63	
4.416	75	3 2 0	20.09	
4.358	39	2 1 1	20.36	
4.298	6	1 4 0	20.65	
4.017	38	2 2 1	22.11	
3.935	24	1 3 1	22.58	
3.860	32	2 4 0	23.02	
3.807	88	4 0 0	23.35	
3.728	33	4 1 0	23.85	
3.589	33	2 3 1	24.79	
3.505	100	4 2 0	25.39	
3.460	17	3 2 1	25.73	
3.402	18	1 4 1	26.17	
3.361	12	3 4 0	26.50	
3.209	24	4 3 0	27.78	
3.175M	74	3 3 1	28.08	
3.175M		2 4 1	28.08	
3.141	19	4 0 1	28.39	
3.096	19	4 1 1	28.81	
2.958	16	1 5 1	30.19	
2.931M	8	1 6 0	30.47	
2.931M		3 5 0	30.47	
2.901	19	4 4 0	30.80	
2.879	37	3 4 1	31.04	
2.802	16	2 5 1	31.91	
2.784+	8	0 0 2	32.12	
2.784+		2 6 0	32.12	
2.715	2	5 3 0	32.97	
2.706	2	1 1 2	33.08	
2.642	9	5 1 1	33.90	
2.633	14	0 6 1	34.02	
2.612M	25	2 0 2	34.30	
2.612M		4 5 0	34.30	
2.593M	29	1 6 1	34.57	
2.593M		3 5 1	34.57	

Sodium L(+)-Glutamate Hydrate,  $C_5H_8NNaO_4 \cdot H_2O$  - (continued)

$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 2$	hkl	$2\theta(^{\circ})$
2.562	7	5 2 1	35.00
2.525M	9	1 7 0	35.53
2.525M		0 3 2	35.53
2.521	9	5 4 0	35.58
2.489M	26	1 3 2	36.06
2.489M		2 6 1	36.06
2.441+	16	6 2 0	36.79
2.441+		3 0 2	36.79
2.362	11	4 5 1	38.06
2.356	12	3 2 2	38.16
2.352	17	4 6 0	38.24
2.338+	9	3 6 1	38.48
2.338+		6 3 0	38.48
2.310	8	6 0 1	38.96
2.301	16	1 7 1	39.11
2.296	17	5 4 1	39.21
2.258M	16	3 3 2	39.90
2.258M		2 4 2	39.90
2.237	24	6 2 1	40.28
2.230	22	4 1 2	40.42
2.227	19	2 7 1	40.48
2.200	12	0 5 2	41.00
2.167	41	4 6 1	41.65
2.144M	6	3 4 2	42.12
2.144M		5 5 1	42.12
2.135	4	5 6 0	42.29
2.126	4	4 7 0	42.49
2.115M	6	3 7 1	42.71
2.115M		7 2 0	42.71
2.060	5	1 8 1	43.92
2.052	9	3 8 0	44.10
2.037	4	0 6 2	44.44
1.994	7	5 6 1	45.46
1.987	5	4 7 1	45.62
1.959	7	7 4 0	46.31

Sodium Hydrogen Oxalate Hydrate,  $C_2HNaO_4 \cdot H_2O$

Synonym

1. Sodium binoxalate hydrate
2. Sodium acid oxalate hydrate

CAS registry no.

16009-94-2

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, N. J. It was recrystallized from a hot aqueous solution to which a small amount of  $H_2C_2O_4$  was added. The sample was mounted in Canada Balsam for the intensity measurements. Since the material exhibited strong cleavage and a tendency to lose  $H_2O$ , the intensity determinations may be subject to some error.

Color

Colorless

Structure

Triclinic,  $P\bar{1}$  (2),  $Z = 2$  [Hendricks, 1935].

Lattice constants of this sample

$a = 6.516(2) \text{ \AA}$   
 $b = 6.675(2)$   
 $c = 5.708(2)$   
 $\alpha = 95.06(4)^\circ$   
 $\beta = 109.96(4)$   
 $\gamma = 75.03(2)$

$a/b = 0.9762$   
 $c/b = 0.8551$

Volume

$225.43 \text{ \AA}^3$

Density

(calculated)  $1.916 \text{ g/cm}^3$

Figure of merit

$F_{30} = 26.2(0.016, 71)$

Additional pattern

1. PDF card 14-755 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). *Ind. Eng. Chem. Anal. Ed.* 10, 457.  
 Hendricks, S. B. (1935). *Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem.* 92, 301.

CuK $\alpha_1$ $\lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1 \text{ }^\circ\text{C}$				
Internal standard W, $a = 3.16524 \text{ \AA}$				
$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 3$	hkl	$2\theta(^\circ)$	
6.44	4	0 1 0	13.73	
5.93	1L	1 0 0	14.92	
5.36	14	0 0 1	16.53	
5.027	3	1 1 0	17.63	
4.862	14	-1 0 1	18.23	
4.318	11	-1 -1 1	20.55	
4.132M	10	0 -1 1	21.49	
4.132M		0 1 1	21.49	
3.919	10	-1 1 0	22.67	
3.226	14	0 2 0	27.63	
3.179	12	1 2 0	28.05	
3.084	4	-2 -1 1	28.93	
2.987	32	2 1 0	29.89	
2.968	100	2 0 0	30.08	
2.683	21	0 0 2	33.37	
2.583	6	-1 2 0	34.70	
2.568	1L	-2 -2 1	34.91	
2.530	7	-2 1 1	35.45	
2.482	24	-1 1 2	36.16	
2.477+	18	0 -1 2	36.24	
2.477+		0 1 2	36.24	
2.442	8	-2 -1 2	36.77	
2.306	3	2 1 1	39.03	
2.256	5	-1 -2 2	39.93	
2.165	8	-3 -1 1	41.69	
2.131M	9	1 1 2	42.39	
2.131M		-1 -3 1	42.39	
2.097	6	-3 0 1	43.10	
2.063+	7	2 2 1	43.84	
2.063+		0 -2 2	43.84	
2.012+	2	-3 -2 1	45.02	
2.012+		-1 2 2	45.02	
1.959	7	-2 2 0	46.32	
1.906	5	3 2 0	47.67	
1.893	1L	-1 0 3	48.01	
1.858M	3	-3 1 1	49.00	
1.858M		-1 -1 3	49.00	
1.835	4	-1 3 1	49.64	
1.780	4	-1 1 3	51.28	
1.7416M	5	-3 -3 1	52.50	
1.7416M		2 3 1	52.50	
1.7270	13	2 0 2	52.98	
1.6852	1L	3 0 1	54.40	
1.6610	9	1 4 0	55.26	
1.6408	2	-3 -3 2	56.00	

Sodium Iodate Hydrate, NaIO<sub>3</sub>·H<sub>2</sub>O

Synonym

1. Sodium iodate monohydrate

CAS registry no.

22451-04-3

Sample

The sample was crystallized by slow evaporation of an aqueous solution of NaIO<sub>3</sub>. The material was somewhat unstable; thus, the intensity measurements may be slightly in error.

Color

Colorless

Structure

Orthorhombic, P22<sub>1</sub>2 (17), Z = 8, assuming a density near 2.5. Indexed by use of the Visser program. The space group was assumed, based on the consideration of the absent reflections.

Lattice constants of this sample

a = 9.065(3) Å  
b = 16.632(5)  
c = 7.638(2)

a/b = 0.5450  
c/b = 0.4592

Volume

1151.6 Å<sup>3</sup>

Density

(calculated) 2.491 g/cm<sup>3</sup>

Figures of merit

F<sub>30</sub> = 18.7(0.013,120)  
M<sub>20</sub> = 12.2

Reference intensity

I/I<sub>corundum</sub> = 2.42(14)

Additional pattern

1. PDF card 1-156 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.  
Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Si, a = 5.43088 Å			
d(Å)	I <sup>rel</sup> σ = ±3	hkl	2θ(°)
6.93	76	0 1 1	12.77
5.836	100	1 0 1	15.17
4.774	25	1 2 1	18.57
3.976	62	2 2 0	22.34
3.792	8	2 1 1	23.44
3.441	84	1 1 2	25.87
3.189	39	2 3 1	27.96
3.021	85	3 0 0	29.55
2.971M	44	3 1 0	30.05
2.971M		1 3 2	30.05
2.919	8	2 0 2	30.60
2.890	19	1 5 1	30.92
2.771M	20	0 6 0	32.28
2.771M		3 1 1	32.28
2.661	25	3 2 1	33.65
2.654M	13	3 3 0	33.74
2.654M		1 6 0	33.74
2.449	4	1 0 3	36.67
2.391	12	2 4 2	37.59
2.345	9	3 1 2	38.35
2.328	3	3 4 1	38.64
2.314	5	0 3 3	38.88
2.279	23	3 2 2	39.51
2.243M	11	0 6 2	40.17
2.243M		1 3 3	40.17
2.201M	4	1 7 1	40.97
2.201M		2 1 3	40.97
2.144	4	2 2 3	42.11
2.112	14	1 4 3	42.78
2.023M	6	4 3 1	44.77
2.023M		0 5 3	44.77
2.017	7	0 7 2	44.91
2.011	7	2 6 2	45.05
1.989	5	4 4 0	45.56
1.969	26	1 7 2	46.05
1.930	7	3 5 2	47.04
1.8976M	4	4 2 2	47.90
1.8976M		0 1 4	47.90
1.8744	10	0 6 3	48.53
1.8469	4	2 5 3	49.30
1.8344	13	2 8 1	49.66
1.8196	4	4 5 1	50.09
1.7708M	11	5 2 0	51.57
1.7708M		1 3 4	51.57
1.7497	9	2 1 4	52.24
1.7355	6	0 4 4	52.70
1.7218	7	2 2 4	53.15
1.6846	8	4 1 3	54.42

Sodium Sulfate Hydrate, Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>·5H<sub>2</sub>O

Synonym

1. Sodium thiosulfate pentahydrate

CAS registry no.

10102-17-7

Sample

The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color

Colorless

Structure

Monoclinic, P2<sub>1</sub>/a (14), Z = 4. The structure of Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>·5H<sub>2</sub>O was determined by Taylor and Beevers [1952].

Lattice constants of this sample

a = 7.5361(14) Å

b = 21.595(6)

c = 5.9503(12)

β = 103.80(2)°

a/b = 0.3490

c/b = 0.2755

Volume

940.4 Å<sup>3</sup>

Density

(calculated) 1.753 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 52.3(0.012,47)

Additional pattern

1. PDF card 13-528 [University College, Cardiff, Wales]

Reference

Taylor, P. G. and Beevers, C. A. (1952). Acta Crystallogr. 5, 341.

CuKα<sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I <sup>rel</sup> σ = ±1	hkl	2θ(°)
10.79	4	0 2 0	8.19
6.93	5	1 1 0	12.76
6.05	19	1 2 0	14.62
5.775	32	0 0 1	15.33
5.580	24	0 1 1	15.87
5.401	100	0 4 0	16.40
5.125	15	1 3 0	17.29
5.024	20	-1 1 1	17.64
4.665	19	-1 2 1	19.01
4.507	23	0 3 1	19.68
4.339	5	1 4 0	20.45
4.205	28	-1 3 1	21.11
4.010	4	1 1 1	22.15
3.945	11	0 4 1	22.52
3.823	31	1 2 1	23.25
3.660	35	2 0 0	24.30
3.601	16	0 6 0	24.70
3.552	25	1 3 1	25.05
3.490	16	-2 0 1	25.50
3.446	27	-2 1 1	25.83
3.324	46	-2 2 1	26.80
3.258M	2	2 3 0	27.35
3.258M		1 4 1	27.35
3.141	35	-2 3 1	28.39
3.031	2	2 4 0	29.45
2.957	60	-1 6 1	30.20
2.911	35	-1 1 2	30.69
2.864	37	0 1 2	31.20
2.843	34	1 7 0	31.44
2.794M	55	2 5 0	32.01
2.794M		0 2 2	32.01
2.721M	10	0 7 1	32.89
2.721M		-1 3 2	32.89
2.648	1	-1 7 1	33.82
2.613	9	2 3 1	34.29
2.586	8	-2 0 2	34.66
2.566	6	2 6 0	34.94
2.548	6	0 4 2	35.20
2.532	7	1 8 0	35.42
2.506	13	-2 6 1	35.80
2.489	8	2 4 1	36.06
2.451	47	-3 1 1	36.64
2.428M	20	-1 5 2	36.99
2.428M		1 2 2	36.99
2.355	16	1 3 2	38.19
2.335M	3	-3 3 1	38.52
2.335M		-2 4 2	38.52
2.275	6	-1 6 2	39.58
2.263	10	1 4 2	39.81
2.218M	19	-2 5 2	40.65



Sodium Sulfate Hydrate,  $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$	hkl	$2\theta(^{\circ})$
	$\sigma = \pm 1$		
2.218M		0 9 1	40.65
2.160M	7	0 10 0	41.78
2.160M		1 5 2	41.78
2.144	3	-3 5 1	42.12
2.137	4	-2 8 1	42.25
2.124	3	3 5 0	42.53
2.100	10	-2 6 2	43.03
2.091	10	-3 2 2	43.23
2.070M	9	1 10 0	43.69
2.070M		1 9 1	43.69
2.036	17	-3 6 1	44.47
2.007M	7	2 2 2	45.13
2.007M		2 9 0	45.13
1.994M	6	3 3 1	45.44
1.994M		-1 10 1	45.44
1.978	6	-2 9 1	45.85
1.951	3	-1 2 3	46.51
1.9111+	11	-1 3 3	47.54
1.9111+		-3 5 2	47.54
1.8961M	3	0 2 3	47.94
1.8961M		1 11 0	47.94
1.8784	3	-4 0 1	48.42
1.8604+	4	0 3 3	48.92
1.8604+		2 10 0	48.92
1.8466M	7	2 5 2	49.31
1.8466M		0 9 2	49.31
1.8371	18	-2 10 1	49.58
1.8098	10	3 8 0	50.38

Strontium Bromate Hydrate, Sr(BrO<sub>3</sub>)<sub>2</sub>·H<sub>2</sub>O

CAS registry no.  
10022-52-3

Sample  
The sample was made by reaction between SrCO<sub>3</sub>  
and H<sub>2</sub>BrO<sub>3</sub>.

Color  
Colorless

Structure  
Monoclinic, P2<sub>1</sub>/n (14), Z = 4. The cell was  
obtained from axial ratios of Groth [1908],  
assuming Z = 4 and using a density of 3.778 as  
quoted by Groth [1908]. The space group was  
assumed from the peak absences.

Lattice constants of this sample

a = 9.375(2) Å  
b = 7.6205(12)  
c = 8.877(2)  
β = 91.86(2)°

a/b = 1.2302  
c/b = 1.1648

Volume  
633.8 Å<sup>3</sup>

Density  
(calculated) 3.788 g/cm<sup>3</sup>

Figure of merit  
F<sub>30</sub> = 35.3(0.012,74)

Reference intensity  
I/I<sub>corundum</sub> = 2.7(2)

Reference  
Groth, P. (1908). Chemische Kristallographie  
II, (Wilhelm Engelmann, Leipzig, Germany)  
p. 113.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup> σ = ±3	hkl	2θ(°)
5.91	6	1 1 0	14.97
5.779	33	0 1 1	15.32
4.687	4	2 0 0	18.92
4.434	23	0 0 2	20.01
3.836	12	0 1 2	23.17
3.811	32	0 2 0	23.32
3.681	6	-2 1 1	24.16
3.586	31	-1 1 2	24.81
3.515	20	1 1 2	25.32
3.293	32	-1 2 1	27.06

d(Å)	I <sup>rel</sup> σ = ±3	hkl	2θ(°)
3.275	39	-2 0 2	27.21
3.171	47	2 0 2	28.12
2.956	47	2 2 0	30.21
2.891M	100	0 2 2	30.91
2.891M		3 1 0	30.91
2.757	3	0 1 3	32.45
2.484	5	-2 2 2	36.13
2.453	13	1 3 0	36.60
2.445	13	0 3 1	36.72
2.438	11	2 2 2	36.83
2.409	2	-2 1 3	37.30
2.345+	5	2 1 3	38.36
2.345+		-3 2 1	38.36
2.316	16	3 2 1	38.85
2.281	4	-1 2 3	39.47
2.254	2	1 2 3	39.97
2.217	25	0 0 4	40.66
2.188	8	-4 1 1	41.23
2.173	4	-2 3 1	41.52
2.156M	8	4 1 1	41.86
2.156M		2 3 1	41.86
2.138	3	1 3 2	42.23
2.099M	6	-3 1 3	43.07
2.099M		3 2 2	43.07
2.063	1	1 1 4	43.85
2.044	2	4 0 2	44.27
1.9160+	4	2 1 4	47.41
1.9160+		0 2 4	47.41
1.8931	5	-3 2 3	48.02
1.8237	9	1 4 1	49.97
1.8189	11	5 1 0	50.11
1.8145	10	-3 3 2	50.24
1.7876	19	3 3 2	51.05
1.7651	10	2 4 0	51.75
1.7591	10	4 1 3	51.94
1.7509	11	0 4 2	52.20
1.7343+	7	3 1 4	52.74
1.7343+		-2 4 1	52.74
1.7020	9	-5 1 2	53.82
1.6832	1	4 3 1	54.47
1.6649	7	5 1 2	55.12
1.6514	2	-1 3 4	55.61
1.6341M	4	4 2 3	56.25
1.6341M		2 4 2	56.25
1.6043	2	-3 4 1	57.39
1.5921	3	4 3 2	57.87
1.5829	2	-1 4 3	58.24
1.5617M	2	2 3 4	59.11
1.5617M		6 0 0	59.11
1.5077+	7	2 2 5	61.45
1.5077+		5 3 0	61.45
1.4774	2	4 4 0	62.85

Strontium Chromium Oxide, SrCr<sub>2</sub>O<sub>7</sub>

Synonym

1. Strontium dichromate

Sample

The sample was prepared by heating SrCr<sub>2</sub>O<sub>7</sub>·3H<sub>2</sub>O at 130 °C for 18 hours, followed by heating at 150 °C for 24 hours.

Color

Deep orange yellow

Structure

Tetragonal, P<sub>4</sub><sub>2</sub>/nmc (137), Z = 8, isostructural with PbCr<sub>2</sub>O<sub>7</sub>. The structure of SrCr<sub>2</sub>O<sub>7</sub> was determined by Wilhelmi [1967].

Lattice constants of this sample

a = 11.1925(7) Å

c = 9.4833(11) Å

c/a = 0.8473

Volume

1188.0 Å<sup>3</sup>

Density

(calculated) 3.395 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 72.4(0.010,41)

Reference intensity

I/I<sub>corundum</sub> = 2.35(8)

Additional pattern

1. PDF card 20-1191 [Wilhelmi, 1967]

Reference

Wilhelmi, K.-A. (1967). Ark. Kemi 26, 149.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Si, a = 5.43088 Å			
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)
7.91	2	1 1 0	11.17
7.24	2	1 0 1	12.22
5.601	5	2 0 0	15.81
4.739	3	0 0 2	18.71
4.423	11	2 1 1	20.06
4.070	4	1 1 2	21.82
3.955	2	2 2 0	22.46
3.619	68	2 0 2	24.58
3.538	4	3 1 0	25.15
3.474	25	3 0 1	25.62
3.443	5	2 1 2	25.86
3.315	100	3 1 1	26.87
3.040M	32	1 0 3	29.36
3.040M		2 2 2	29.36
2.950	15	3 2 1	30.27
2.931	11	3 0 2	30.47
2.836	3	3 1 2	31.52
2.796	2	4 0 0	31.98
2.751	1	2 0 3	32.52
2.673	2	2 1 3	33.50
2.636	2	3 3 0	33.98
2.609	1	4 1 1	34.34
2.596	2	3 2 2	34.52
2.503	9	4 2 0	35.85
2.420	7	4 2 1	37.12
2.413	9	3 0 3	37.24
2.357M	11	3 1 3	38.15
2.357M		4 1 2	38.15
2.305	6	3 3 2	39.04
2.2145M	12	3 2 3	40.71
2.2145M		4 2 2	40.71
2.1944	7	5 1 0	41.10
2.1787	15	4 3 1	41.41
2.1388	3	5 1 1	42.22
2.0948	1	4 0 3	43.15
2.0304	29	5 2 1	44.59
2.0011	3	3 0 4	45.28
1.9779	2	4 4 0	45.84
1.9195	8	5 3 0	47.32
1.8835	1	3 2 4	48.28
1.8813	2	5 3 1	48.34
1.8654	8	6 0 0	48.78
1.8264M	13	4 3 3	49.89
1.8264M		4 4 2	49.89
1.8088	1	4 0 4	50.41

Strontium Chromium Oxide, SrCr<sub>2</sub>O<sub>7</sub> - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 2$	hkl	$2\theta(^{\circ})$
1.8038	2	5 1 3	50.56
1.7795	6	5 3 2	51.30
1.7635	5	3 3 4	51.80
1.7367M	2	5 2 3	52.66
1.7367M		6 0 2	52.66
1.7203	4	4 2 4	53.20
1.6909	4	3 0 5	54.20
1.6585	2	6 2 2	55.35
1.6432	1	6 3 1	55.91
1.6185	4	3 2 5	56.84
1.5904	1	6 1 3	57.94
1.5829	2	7 1 0	58.24
1.5770	2	7 0 1	58.48
1.5547	1	4 1 5	59.40
1.5502	1L	1 1 6	59.59
1.5316	1L	6 4 1	60.39
1.5175	3	7 2 1	61.01
1.5150	1L	7 0 2	61.12
1.5015	1	7 1 2	61.73
1.4699	2	7 3 0	63.21
1.4524	6	7 3 1	64.06

Strontium Chromium Oxide Hydrate, SrCr<sub>2</sub>O<sub>7</sub>·3H<sub>2</sub>O

Synonym

1. Strontium dichromate trihydrate

Sample

The sample was prepared by adding SrCrO<sub>4</sub> to a saturated solution of CrO<sub>3</sub>. Large red crystals formed slowly.

Color

Unground, deep reddish brown. Ground, deep orange.

Structure

Monoclinic, P<sub>2</sub><sub>1</sub>/c (14), Z = 4. The crystallographic information was obtained on a single crystal diffractometer by V. Himes. The cell parameters were confirmed by the Visser program [1969] and by axial ratios given by Groth [1908], assuming Z = 4 and a density near 2.6.

Lattice constants of this sample

a = 8.3583(12) Å  
 b = 14.023(2)  
 c = 7.574(2)  
 β = 91.95(2)°

a/b = 0.5960  
 c/b = 0.5401

Volume

887.22 Å<sup>3</sup>

Density

(calculated) 2.678 g/cm<sup>3</sup>

Figures of merit

F<sub>30</sub> = 74.8 (0.010,40)  
 M<sub>20</sub> = 38.4

Reference intensity

I/I<sub>corundum</sub> = 1.04(5)

References

Groth, P. (1908). *Chemische Krystallographie* II (Wilhelm Engelmann, Leipzig, Germany) p. 593.  
 Visser, J. W. (1969). *J. Appl. Crystallogr.* 2, 89.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Si, a = 5.43088 Å			
d(Å)	I <sup>rel</sup>	hkl	2θ(°)
σ = ±3			
8.35	31	1 0 0	10.59
7.18	9	1 1 0	12.31
7.02	8	0 2 0	12.60
6.67	4	0 1 1	13.27
5.368	9	1 2 0	16.50
5.286	25	-1 1 1	16.76
5.142M	10	0 2 1	17.23
5.142M		1 1 1	17.23
4.425	21	-1 2 1	20.05
4.337	20	1 2 1	20.46
4.178	100	2 0 0	21.25
4.079	23	1 3 0	21.77
4.001	68	2 1 0	22.20
3.980	70	0 3 1	22.32
3.784	45	0 0 2	23.49
3.652	25	0 1 2	24.35
3.614	25	-1 3 1	24.61
3.589M	10	2 2 0	24.79
3.589M		-2 1 1	24.79
3.504	45	0 4 0	25.40
3.388	21	-1 1 2	26.28
3.307	4	1 1 2	26.94
3.282	3	-2 2 1	27.15
3.230	17	1 4 0	27.59
3.208	35	2 2 1	27.79
3.181	7	0 4 1	28.03
3.128	4	-1 2 2	28.51
3.061	3	1 2 2	29.15
2.987	13	-1 4 1	29.89
2.958	14	1 4 1	30.19
2.907	13	-2 3 1	30.73
2.856M	15	2 3 1	31.29
2.856M		-2 0 2	31.29
2.785	20	3 0 0	32.11
2.752	7	1 3 2	32.51
2.731	6	3 1 0	32.76
2.706	20	2 1 2	33.08
2.686	9	2 4 0	33.33
2.657	10	1 5 0	33.70
2.597	15	-3 1 1	34.51
2.567	13	2 2 2	34.92
2.541	9	3 1 1	35.29
2.500	3	1 5 1	35.89
2.473M	7	-1 4 2	36.30
2.473M		-3 2 1	36.30

Strontium Chromium Oxide Hydrate,  $\text{SrCr}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$	hkl	$2\theta(^{\circ})$
	$\sigma = \pm 3$		
2.425	20	3 2 1	37.04
2.393	30	3 3 0	37.56
2.359	3	1 1 3	38.11
2.338	3	0 6 0	38.48
2.302M	9	-1 2 3	39.10
2.302M		-3 3 1	39.10
2.263M	1	1 2 3	39.80
2.263M		3 3 1	39.80
2.233	4	0 6 1	40.36
2.212M	5	2 5 1	40.75
2.212M		-2 4 2	40.75
2.186	4	-1 5 2	41.26
2.1662+	25	2 4 2	41.66
2.1662+		-2 1 3	41.66
2.1036M	16	3 2 2	42.96
2.1036M		2 1 3	42.96
2.0879	10	4 0 0	43.30
2.0648	2	4 1 0	43.81
2.0492M	13	-3 3 2	44.16
2.0492M		0 4 3	44.16
2.0103	12	-4 1 1	45.06
2.0028M	21	-1 4 3	45.24
2.0028M		4 2 0	45.24
1.9767M	32	1 4 3	45.87
1.9767M		3 5 0	45.87
1.9622	5	2 6 1	46.23
1.9376M	24	0 7 1	46.85
1.9376M		2 3 3	46.85

Thiosemicarbazide, CH<sub>5</sub>N<sub>3</sub>S

Synonym

1. Hydrazinecarbothioamide

CAS registry no.

79-19-6

Sample

The sample was obtained from J. T. Baker Co., Phillipsburg, NJ. It was re-crystallized from ethanol.

Color

Colorless

Structure

Triclinic, P $\bar{1}$  (2), Z = 2. The structure was determined by Andreetti et al. [1970].

Lattice constants of this sample

a = 6.0266(12) Å

b = 7.327(2)

c = 4.9353(15)

$\alpha$  = 103.00(2)°

$\beta$  = 96.33(2)

$\gamma$  = 77.21(2)

a/b = 0.8225

c/b = 0.6736

Volume

206.65 Å<sup>3</sup>

Density

(calculated) 1.465 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 40.9(0.015,50)

Reference intensity

I/I<sub>corundum</sub> = 2.56(11)

Additional pattern

1. PDF card 24-1952 [Institute of Physics, University College, Cardiff, Wales]

Reference

Andreetti, G. D., Domiano, P., Gasparri, G. F., Nardelli, M., and Sgarabotto, P. (1970). Acta Crystallogr. B26, 1005.

CuK $\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup>	hkl	2 $\theta$ (°)
$\sigma = \pm 2$			
5.86	5	1 0 0	15.11
5.021	18	1 1 0	17.65
4.797	13	0 0 1	18.48
4.399	5	0 -1 1	20.17
4.100	4	-1 1 0	21.66
3.619	36	0 1 1	24.58
3.497	11	0 2 0	25.45
3.309	1	1 2 0	26.92
3.245	11	1 -1 1	27.46
3.163	100	1 1 1	28.19
3.082	7	-1 -2 1	28.95
3.008	8	-1 1 1	29.68
2.931	6	2 0 0	30.47
2.767	1L	-1 2 0	32.33
2.685	1	-2 -1 1	33.35
2.582	1	0 2 1	34.71
2.548	2	1 -2 1	35.19
2.527	4	-2 1 0	35.49
2.512	1	2 2 0	35.71
2.472	3	1 2 1	36.31
2.437M	2	-2 -2 1	36.86
2.437M		2 0 1	36.86
2.333	2	1 3 0	38.56
2.291	1L	0 -3 1	39.29
2.271M	1L	-1 0 2	39.66
2.271M		-1 2 1	39.66
2.202M	2	0 -2 2	40.95
2.202M		-1 -2 2	40.95
2.173	2	1 0 2	41.52
2.143	1	1 -1 2	42.13
2.138	1L	0 1 2	42.23
2.051	2	-2 2 0	44.13
2.037	1	2 3 0	44.44
2.008	2	-2 -1 2	45.11
1.990	1	3 1 0	45.54
1.985	2	1 -3 1	45.66
1.945M	1	1 -2 2	46.66
1.945M		0 3 1	46.66
1.929	1L	1 3 1	47.06
1.925	1L	-3 -1 1	47.18

Thiosemicarbazide, CH<sub>5</sub>N<sub>3</sub>S - (continued)

d(Å)	I <sup>rel</sup>	hkl	2θ(°)
	σ = ±2		
1.877M	1L	0 -3 2	48.47
1.877M		3 2 0	48.47
1.859	2	-3 -2 1	48.95
1.836	1	-2 2 1	49.61
1.811	1	0 2 2	50.35
1.8025	1	2 0 2	50.60
1.7906	1	-3 1 0	50.96
1.7724M	2	3 0 1	51.52
1.7724M		-1 3 1	51.52
1.7594+	4	-2 -3 2	51.93
1.7594+		1 2 2	51.93
1.7315	2	2 1 2	52.83
1.7034	1L	-1 2 2	53.77
1.6907M	1L	-2 -4 1	54.21
1.6907M		-3 -3 1	54.21
1.6741M	1	3 -1 1	54.79
1.6741M		3 3 0	54.79
1.6541	1L	3 2 1	55.51
1.6219M	1	-1 -1 3	56.71
1.6219M		2 -2 2	56.71



Thiourea, CH<sub>4</sub>N<sub>2</sub>S

Synonym

1. Thiocarbamide

CAS registry no.

62-56-6

Sample

The sample was obtained from J. T. Baker Chemical Co., Phillipsburg, NJ. It was recrystallized from ethanol.

Color

Colorless

Structure

Orthorhombic, Pnma (62), Z = 4. The structure was first determined by Demeny and Nitta, [1928]. It was later refined by Truter [1957].

Lattice constants of this sample

a = 7.6644(12) Å

b = 8.5591(12)

c = 5.4925(8)

a/b = 0.8955

c/b = 0.6417

Volume

360.31 Å<sup>3</sup>

Density

(calculated) 1.403 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 66.3(0.009,49)

Reference intensity

I/I<sub>corundum</sub> = 0.91(3)

Additional pattern

1. PDF card 9-790 [Morse and Baun, Wright Patterson Air Force Base, Ohio]

References

Demeny, L. and Nitta, I. (1928). Bull. Chem. Soc. Japan 3, 128.

Truter, M. R. (1957). Acta Crystallogr. 10, 786.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C				
Internal standard W, a = 3.16524 Å				
d(Å)	I <sup>rel</sup>	hkl	2θ(°)	
σ = ±2				
4.624	9	0 1 1	19.18	
4.467	70	1 0 1	19.86	
4.279	100	0 2 0	20.74	
3.834	61	2 0 0	23.18	
3.498	53	2 1 0	25.44	
3.142	65	2 0 1	28.38	
3.089	66	1 2 1	28.88	
2.951	24	2 1 1	30.26	
2.855	45	2 2 0	31.31	
2.747	8	0 0 2	32.57	
2.532M	28	2 2 1	35.43	
2.532M		0 3 1	35.43	
2.475	31	1 1 2	36.26	
2.405	1	1 3 1	37.36	
2.317	9	3 0 1	38.83	
2.2885	3	2 3 0	39.34	
2.1598	7	2 1 2	41.79	
2.1393	2	0 4 0	42.21	
2.1116	5	2 3 1	42.79	
2.0369	8	3 2 1	44.44	
1.9291	14	1 4 1	47.07	
1.9164M	5	4 0 0	47.40	
1.9164M		1 3 2	47.40	
1.8683	9	2 4 0	48.70	
1.8271	8	3 1 2	49.87	
1.7902	7	0 1 3	50.97	
1.7695M	11	4 1 1	51.61	
1.7695M		2 4 1	51.61	
1.7487	3	4 2 0	52.27	
1.7135	1	3 2 2	53.43	
1.6883	1	0 4 2	54.29	
1.6665	1L	4 2 1	55.06	
1.6440	4	1 2 3	55.88	
1.6346	2	0 5 1	56.23	
1.6219	3	2 1 3	56.71	
1.5716M	3	3 4 1	58.70	
1.5716M		4 0 2	58.70	
1.5643	4	3 3 2	59.00	

Tin Chloride Hydrate,  $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$

Synonym

1. Stannous chloride dihydrate

CAS registry no.

10025-69-1

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ.

Color

Colorless

Structure

Monoclinic,  $P2_1/c$  (14),  $Z = 4$ . The structure of  $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$  was determined by Grdenic and Kamenar [1960].

Lattice constants of this sample

$a = 9.318(3) \text{ \AA}$

$b = 7.2571(14)$

$c = 8.973(2)$

$\beta = 114.89(2)^\circ$

$a/b = 1.2840$

$c/b = 1.2365$

Volume

$550.4 \text{ \AA}^3$

Density

(calculated)  $2.723 \text{ g/cm}^3$

Figure of merit

$F_{30} = 49.4 (0.012, 49)$

Reference intensity

$I/I_{\text{corundum}} = 1.50(2)$

Additional pattern

1. PDF card 20-1292 [University of Leeds, Leeds, England]

Reference

Grdenic, D. and Kamenar, B. (1960). Proc. Chem. Soc. 1960, 312.

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$ ; temp. $25 \pm 1^\circ \text{C}$			
Internal standard Si, $a = 5.43088 \text{ \AA}$			
$d(\text{Å})$	$I^{\text{rel}}$ $\sigma = \pm 8$	hkl	$2\theta(^\circ)$
8.43	59	1 0 0	10.48
5.511	100	1 1 0	16.07
5.414	8	0 1 1	16.36
5.279	4	-1 1 1	16.78
4.483	1	-1 0 2	19.79
4.227	11	2 0 0	21.00
4.068M	19	1 1 1	21.83
4.068M		0 0 2	21.83
3.902	4	-2 1 1	22.77
3.810	53	-1 1 2	23.33
3.655	81	2 1 0	24.33
3.628	13	0 2 0	24.52
3.551	12	0 1 2	25.06
3.402	43	-2 1 2	26.17
3.334	8	1 2 0	26.72
3.181	8	1 0 2	28.03
2.953	6	2 1 1	30.24
2.912	5	1 1 2	30.68
2.819M	28	-1 2 2	31.72
2.819M		3 0 0	31.72
2.754M	20	-3 1 2	32.49
2.754M		2 2 0	32.49
2.709	60	0 2 2	33.04
2.642	34	-2 2 2	33.90
2.627	22	3 1 0	34.10
2.541	6	0 1 3	35.29
2.461	14	2 0 2	36.48
2.420	4	-3 1 3	37.12
2.392	19	1 2 2	37.57
2.327	24	1 3 0	38.67
2.318M	25	0 3 1	38.82
2.318M		-4 0 2	38.82
2.303	25	-3 2 2	39.09
2.253	2	3 1 1	39.99
2.238	10	-2 0 4	40.26
2.225	2	3 2 0	40.51
2.206M	2	-4 1 2	40.87
2.206M		1 1 3	40.87
2.171	3	1 3 1	41.57
2.138	7	-2 1 4	42.24
2.130M	20	-3 0 4	42.41
2.130M		-1 3 2	42.41
2.113	4	4 0 0	42.75
2.100	25	2 3 0	43.04
2.079	4	0 3 2	43.50
2.048	12	-2 3 2	44.18
2.035M	3	2 2 2	44.49
2.035M		0 0 4	44.49
1.960	10	0 1 4	46.29
1.953M	12	-4 2 2	46.47

Tin Chloride Hydrate,  $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$  - (continued)

$d(\text{\AA})$	$I^{\text{rel}}$ $\sigma = \pm 8$	hkl	$2\theta(^{\circ})$
1.953M		1 2 3	46.47
1.924M	4	-4 0 4	47.19
1.924M		1 3 2	47.19
1.905M	9	-3 3 1	47.71
1.905M		-2 2 4	47.71
1.894	10	3 1 2	47.99
1.8766M	4	-1 3 3	48.47
1.8766M		2 1 3	48.47
1.8618M	8	-4 1 4	48.88
1.8618M		-4 2 3	48.88
1.8357M	9	-3 2 4	49.62
1.8357M		3 3 0	49.62
1.8264	17	4 2 0	49.89
1.8142	17	0 4 0	50.25
1.8061M	14	0 3 3	50.49
1.8061M		-5 1 2	50.49
1.7734	8	1 4 0	51.49
1.7610M	6	-3 3 3	51.88
1.7610M		-5 1 1	51.88
1.7246	8	2 3 2	53.06

Zirconium Silicide, ZrSi<sub>2</sub>

CAS registry no.  
12039-90-6

Sample

The sample was prepared at NBS by R. F. Walker and S. Y. Holley. The sample had a small amount of ZrO<sub>2</sub> and Si present.

Major impurities

>1% Hf; 0.1 to 1.0 % Al; 0.01 to 0.1% each Fe, Ni, and Ti; and 0.001 to 0.01% each Ca, Cr, and Mn.

Structure

Orthorhombic, Cmc<sub>2</sub>m (63), Z = 4 [Seyfarth, 1928]. The structure was redetermined by Schachner et al. [1954] and by Vaughn and Bracuti [1958].

Lattice constants of this sample

a = 3.6958(3) Å  
b = 14.7514(9)  
c = 3.6654(3)

a/b = 0.2505  
c/b = 0.2485

Volume

199.83 Å<sup>3</sup>

Density

(calculated) 4.899 g/cm<sup>3</sup>

Figure of merit

F<sub>30</sub> = 81.8(0.009,40)

Additional pattern

1. PDF card 10-236 [Cotter et al., 1956].

References

Cotter, P. G., Kohn, J. A., and Potter, R. A. (1956). J. Amer. Ceram. Soc. 39, 11.  
Schachner, H., Nowotny, H., and Kudielka, H. (1954). Monatsh. Chem. 85, 1140.  
Seyfarth, H. (1928). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 67, 295.  
Vaughn, P. A. and Bracuti, A. (1958). Diss. Abstr. B. 19, 1217.

CuKα <sub>1</sub> λ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I <sup>rel</sup> σ = ±2	hkl	2θ(°)
7.37	4	0 2 0	12.00
3.685	9	0 4 0	24.13
3.586	15	1 1 0	24.81
3.283	32	0 2 1	27.14
2.954	15	1 3 0	30.23
2.601	1	0 4 1	34.46
2.564	10	1 1 1	34.97
2.458	15	0 6 0	36.53
2.300	100	1 3 1	39.14
2.0417	14	0 6 1	44.33
1.9518	1	1 5 1	46.49
1.8480	11	2 0 0	49.27
1.8434	7	0 8 0	49.40
1.8330	14	0 0 2	49.70
1.7782	1L	0 2 2	51.34
1.6519	2	2 4 0	55.59
1.6473	7	0 8 1	55.76
1.6381	7	1 7 1	56.10
1.6322	6	1 1 2	56.32
1.6102	7	2 2 1	57.16
1.5576	4	1 3 2	59.28
1.4982	6	1 9 0	61.88
1.4772	4	2 6 0	62.86
1.4692	5	0 6 2	63.24
1.4346	6	1 5 2	64.95
1.3867	2	1 9 1	67.49
1.3704	6	2 6 1	68.40
1.3050	1	2 8 0	72.35
1.3016	5	2 0 2	72.57
1.2603	1	1 11 0	75.35
1.2296M	3	2 8 1	77.58
1.2296M		0 12 0	77.58
1.2269	3	2 4 2	77.78
1.2051	1	0 2 3	79.46
1.1923	2	1 11 1	80.49
1.1655	1	0 12 1	82.74
1.1641	1	3 1 1	82.86
1.1602M	3	1 9 2	83.20
1.1602M		0 4 3	83.20
1.1502	2	2 6 2	84.09
1.1361	6	3 3 1	85.38
1.1291	4	1 3 3	86.04
1.0998	1L	2 10 1	88.92
1.0942	1L	0 6 3	89.50
1.0849	1L	1 13 0	90.47
1.0631	1	2 8 2	92.87
1.0538	1	0 14 0	93.94
1.0386	1	1 11 2	95.75

INORGANIC NAMES

	Vol. or	Page		Vol. or	Page
	Sec.			Sec.	
Aluminum, Al .....	1	11	Ammonium aluminum selenate hydrate,		
Aluminum antimony, AlSb .....	4	72	NH <sub>4</sub> Al(SeO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	9m	6
Aluminum bismuth oxide, Al <sub>4</sub> Bi <sub>2</sub> O <sub>9</sub> ..	11m	5	Ammonium aluminum sulfate,		
Aluminum borate, Al <sub>18</sub> B <sub>4</sub> O <sub>33</sub> .....	17m	5	NH <sub>4</sub> Al(SO <sub>4</sub> ) <sub>2</sub> .....	10m	5
Aluminum chloride, AlCl <sub>3</sub> .....	9m	61	Ammonium aluminum sulfate hydrate		
Aluminum chloride hydrate			(tschermigite), NH <sub>4</sub> Al(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O	6	3
(chloraluminite), AlCl <sub>3</sub> ·6H <sub>2</sub> O.....	7	3	Ammonium azide, NH <sub>4</sub> N <sub>3</sub> .....	9	4
Aluminum copper, Al <sub>4</sub> Cu <sub>9</sub> .....	11m	79	Ammonium beryllium fluoride,		
Aluminum fluoride hydroxide silicate,			(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub> .....	3m	5
topaz, Al <sub>2</sub> (F,OH) <sub>2</sub> SiO <sub>4</sub> .....	1m	4	Ammonium borate hydrate,		
Aluminum iron antimony oxide, bahianite,			NH <sub>4</sub> B <sub>5</sub> O <sub>8</sub> ·4H <sub>2</sub> O .....	17m	7
Al <sub>5.66</sub> Fe <sub>0.09</sub> Sb <sub>2.95</sub> O <sub>16</sub> .....	16m	87	Ammonium boron fluoride, NH <sub>4</sub> BF <sub>4</sub> ...	3m	6
Aluminum iron oxide, AlFeO <sub>3</sub> .....	15m	7	Ammonium bromide, NH <sub>4</sub> Br .....	2	49
Aluminum lithium, Al <sub>4</sub> Li <sub>9</sub> .....	10m	98	Ammonium cadmium bromide, (NH <sub>4</sub> ) <sub>4</sub> CdBr <sub>6</sub>	15m	9
Aluminum nickel, AlNi.....	6m	82	Ammonium cadmium chloride, NH <sub>4</sub> CdCl <sub>3</sub>	5m	6
Aluminum nitride, AlN .....	12m	5	Ammonium cadmium sulfate,		
Aluminum nitrate hydrate,			(NH <sub>4</sub> ) <sub>2</sub> Cd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	7m	5
Al(NO <sub>3</sub> ) <sub>3</sub> ·9H <sub>2</sub> O .....	11m	6	Ammonium cadmium sulfate hydrate,		
Aluminum oxide (corundum), α-Al <sub>2</sub> O <sub>3</sub>	9	3	(NH <sub>4</sub> ) <sub>2</sub> Cd(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	8m	5
Aluminum oxide hydrate (boehmite),			Ammonium calcium sulfate,		
α-Al <sub>2</sub> O <sub>3</sub> ·H <sub>2</sub> O .....	3	38	(NH <sub>4</sub> ) <sub>2</sub> Ca <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	8m	7
Aluminum oxide hydrate, diaspore,			Ammonium chlorate, NH <sub>4</sub> ClO <sub>4</sub>		
β-Al <sub>2</sub> O <sub>3</sub> ·H <sub>2</sub> O .....	3	41	(orthorhombic) .....	7	6
Aluminum phosphate, Al(PO <sub>3</sub> ) <sub>3</sub> .....	2m	3	Ammonium chloride (salammoniac),		
Aluminum phosphate (berlinite),			NH <sub>4</sub> Cl .....	1	59
AlPO <sub>4</sub> (trigonal) .....	10	3	Ammonium chromium sulfate hydrate,		
Aluminum phosphate, AlPO <sub>4</sub>			NH <sub>4</sub> Cr(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	6	7
(orthorhombic) .....	10	4	Ammonium cobalt (II) chloride,		
Aluminum plutonium, Al <sub>3</sub> Pu .....	15m	77	NH <sub>4</sub> CoCl <sub>3</sub> .....	6m	5
Aluminum rhenium, AlRe .....	15m	79	Ammonium cobalt fluoride, NH <sub>4</sub> CoF <sub>3</sub>	8m	9
Aluminum rhenium, Al <sub>12</sub> Re .....	15m	80	Ammonium copper bromide hydrate,		
Aluminum rhodium, AlRh .....	15m	82	(NH <sub>4</sub> ) <sub>2</sub> CuBr <sub>4</sub> ·2H <sub>2</sub> O .....	10m	6
Aluminum ruthenium, AlRu .....	15m	83	Ammonium copper chloride, NH <sub>4</sub> CuCl <sub>3</sub>	7m	7
Aluminum ruthenium, Al <sub>6</sub> Ru .....	15m	84	Ammonium copper chloride hydrate,		
Aluminum samarium, AlSm <sub>2</sub> .....	15m	86	(NH <sub>4</sub> ) <sub>2</sub> CuCl <sub>4</sub> ·2H <sub>2</sub> O .....	12m	6
Aluminum samarium, AlSm <sub>3</sub> .....	15m	88	Ammonium copper fluoride, NH <sub>4</sub> CuF <sub>3</sub>	11m	8
Aluminum samarium, Al <sub>2</sub> Sm .....	15m	90	Ammonium gallium sulfate hydrate,		
Aluminum samarium, Al <sub>3</sub> Sm .....	15m	91	NH <sub>4</sub> Ga(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	6	9
Aluminum silicate (mullite),			Ammonium germanium fluoride,		
Al <sub>6</sub> Si <sub>2</sub> O <sub>13</sub> .....	3m	3	(NH <sub>4</sub> ) <sub>2</sub> GeF <sub>6</sub> .....	6	8
Aluminum sulfate, Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	15m	8	Ammonium hydrogen arsenate,		
Aluminum technetium, Al <sub>6</sub> Tc .....	15m	93	NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub> .....	16m	9
Aluminum terbium, Al <sub>2</sub> Tb .....	15m	95	Ammonium hydrogen carbonate		
Aluminum terbium, Al <sub>2</sub> Tb <sub>3</sub> .....	15m	96	(teschemacherite), (NH <sub>4</sub> )HCO <sub>3</sub> .....	9	5
Aluminum thorium uranium, Al <sub>6</sub> ThU ..	15m	98	Ammonium hydrogen phosphate,		
Aluminum tungsten, Al <sub>5</sub> W, δ-phase ..	15m	100	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> .....	4	64
Aluminum tungsten oxide, Al <sub>2</sub> (WO <sub>4</sub> ) <sub>3</sub>	11m	7	Ammonium iodate, NH <sub>4</sub> IO <sub>3</sub> .....	10m	7
Aluminum vanadium, Al <sub>10</sub> V .....	15m	102	Ammonium iodide, NH <sub>4</sub> I .....	4	56
Aluminum vanadium, Al <sub>10.25</sub> V .....	15m	104	Ammonium iridium chloride,		
Aluminum vanadium, Al <sub>23</sub> V <sub>4</sub> .....	15m	106	(NH <sub>4</sub> ) <sub>2</sub> IrCl <sub>6</sub> .....	8	6
Aluminum vanadium, Al <sub>45</sub> V <sub>7</sub> , α'-phase	15m	108	Ammonium iron chloride hydrate,		
Aluminum ytterbium, Al <sub>2</sub> Yb .....	15m	111	(NH <sub>4</sub> ) <sub>2</sub> FeCl <sub>5</sub> ·H <sub>2</sub> O .....	14m	7
Aluminum yttrium, Al <sub>3</sub> Y .....	15m	112	Ammonium iron fluoride, (NH <sub>4</sub> ) <sub>3</sub> FeF <sub>6</sub>	9m	9
Ammonium aluminum fluoride,			Ammonium iron sulfate, NH <sub>4</sub> Fe(SO <sub>4</sub> ) <sub>2</sub>	10m	8
(NH <sub>4</sub> ) <sub>3</sub> AlF <sub>6</sub> .....	9m	5	Ammonium iron sulfate hydrate,		
			NH <sub>4</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	6	10
			Ammonium lead chloride, (NH <sub>4</sub> ) <sub>2</sub> PbCl <sub>6</sub>	11m	10
			Ammonium magnesium aluminum fluoride,		
			NH <sub>4</sub> MgAlF <sub>6</sub> .....	10m	9
			Ammonium magnesium chromium oxide		
			hydrate, (NH <sub>4</sub> ) <sub>2</sub> Mg(CrO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O ....	8m	10
			Ammonium magnesium phosphate hydrate		
			(struvite), NH <sub>4</sub> MgPO <sub>4</sub> ·6H <sub>2</sub> O .....	3m	41
			Ammonium manganese chloride hydrate,		
			(NH <sub>4</sub> ) <sub>2</sub> MnCl <sub>4</sub> ·2H <sub>2</sub> O .....	11m	11

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

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A mineral name in ( ) indicates a synthetic sample.

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Ammonium manganese(II) fluoride, NH <sub>4</sub> MnF <sub>3</sub> .....	5m	8		Antimony gadolinium, GdSb.....	4m 42
Ammonium manganese sulfate, (NH <sub>4</sub> ) <sub>2</sub> Mn <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	7m	8		Antimony gallium, GaSb.....	6 30
Ammonium manganese sulfate hydrate, (NH <sub>4</sub> ) <sub>2</sub> Mn(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	8m	12		Antimony gold (aurostibite), AuSb <sub>2</sub>	7 18
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Ammonium molybdenum oxide phosphate hydrate, (NH <sub>4</sub> ) <sub>3</sub> (MoO <sub>3</sub> ) <sub>12</sub> PO <sub>4</sub> ·4H <sub>2</sub> O ..	8	10		Antimony(III) iodide, SbI <sub>3</sub> .....	6 16
Ammonium nickel(II) chloride, NH <sub>4</sub> NiCl <sub>3</sub> .....	6m	6		Antimony iron titanium oxide hydroxide, derbylite, SbFe <sub>4</sub> Ti <sub>3</sub> O <sub>13</sub> (OH).....	16m 89
Ammonium nickel chromium oxide hydrate, (NH <sub>4</sub> ) <sub>2</sub> Ni(CrO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O ....	8m	16		Antimony lanthanum, LaSb.....	4m 42
Ammonium nickel sulfate hydrate, (NH <sub>4</sub> ) <sub>2</sub> Ni(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	17m	9		Antimony neodymium, NdSb.....	4m 43
Ammonium nitrate (nitrammite), NH <sub>4</sub> NO <sub>3</sub> .....	7	4		Antimony(III) oxide (senarmontite), Sb <sub>2</sub> O <sub>3</sub> (cubic) .....	3 31
Ammonium osmium bromide, (NH <sub>4</sub> ) <sub>2</sub> OsBr <sub>6</sub>	3	71		Antimony(III) oxide, valentinite, Sb <sub>2</sub> O <sub>3</sub> (orthorhombic) .....	10 6
Ammonium osmium chloride, (NH <sub>4</sub> ) <sub>2</sub> OsCl <sub>6</sub> .....	1m	6		Antimony(IV) oxide (cervantite), Sb <sub>2</sub> O <sub>4</sub> .....	10 8
Ammonium palladium chloride, (NH <sub>4</sub> ) <sub>2</sub> PdCl <sub>4</sub> .....	6	6		Antimony(V) oxide, Sb <sub>2</sub> O <sub>5</sub> .....	10 10
Ammonium palladium chloride, (NH <sub>4</sub> ) <sub>2</sub> PdCl <sub>6</sub> .....	8	7		Antimony oxide, Sb <sub>6</sub> O <sub>13</sub> .....	16m 14
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Ammonium potassium iron chloride hydrate (kremersite), (NH <sub>4</sub> ,K) <sub>2</sub> FeCl <sub>5</sub> ·H <sub>2</sub> O .....	14m	8		Antimony selenide, Sb <sub>2</sub> Se <sub>3</sub> .....	3m 7
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Ammonium sulfate (mascagnite), (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> .....	9	8		Antimony telluride, Sb <sub>2</sub> Te <sub>3</sub> .....	3m 8
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				Barium cadmium chloride hydrate, BaCdCl <sub>4</sub> ·4H <sub>2</sub> O.....	15m 14
				Barium calcium nitrate, Ba <sub>2.25</sub> Ca <sub>.75</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m 38
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Barium carbonate, BaCO <sub>3</sub> (cubic) at 1075 °C .....	10	11	Beryllium aluminum silicate, beryl, Be <sub>3</sub> Al <sub>2</sub> (SiO <sub>3</sub> ) <sub>6</sub> .....	9	13
Barium chlorate, Ba(ClO <sub>3</sub> ) <sub>2</sub> .....	16m	17	Beryllium calcium iron magnesium aluminum phosphate hydroxide hydrate, roscherite (monoclinic), Be <sub>2</sub> Ca(Fe <sub>.3</sub> Mg <sub>.7</sub> ) <sub>2</sub> Al <sub>.67</sub> (PO <sub>4</sub> ) <sub>3</sub> (OH) <sub>3</sub> ·2H <sub>2</sub> O	16m	96
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Barium chlorate hydrate, Ba(ClO <sub>3</sub> ) <sub>2</sub> ·H <sub>2</sub> O .....	8m	21	Beryllium calcium oxide, Be <sub>17</sub> Ca <sub>12</sub> O <sub>29</sub> .....	7m	89
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Barium lead chloride, BaPbCl <sub>4</sub> .....	11m	13	Bismuth, Bi .....	3	20
Barium lead nitrate, Ba <sub>.33</sub> Pb <sub>.67</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m	40	Bismuth bromide oxide, BiOBr .....	8	14
Barium lead nitrate, Ba <sub>.67</sub> Pb <sub>.33</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m	40	Bismuth cerium, BiCe .....	4m	46
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Barium nitrate (nitrobarite), Ba(NO <sub>3</sub> ) <sub>2</sub> .....	11m	14	Bismuth fluoride, BiF <sub>3</sub> .....	1m	7
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Barium oxide, BaO .....	9m	63	Bismuth(III) iodide, BiI <sub>3</sub> .....	6	20
Barium oxide, BaO <sub>2</sub> .....	6	18	Bismuth iodide oxide, BiOI .....	9	16
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Barium silicate (sanbornite), β-BaSi <sub>2</sub> O <sub>5</sub> .....	13m	10	Bismuth phosphate, BiPO <sub>4</sub> (trigonal)	3m	13
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Barium silicate, Ba <sub>2</sub> Si <sub>3</sub> O <sub>8</sub> .....	13m	13	Bismuth sulfide (bismuthinite), Bi <sub>2</sub> S <sub>3</sub> .....	5m	13
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Barium silicate, Ba <sub>3</sub> Si <sub>5</sub> O <sub>13</sub> .....	13m	17	Bismuth telluride (tellurobis- muthite), Bi <sub>2</sub> Te <sub>3</sub> .....	3m	16
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Barium strontium nitrate, Ba <sub>.50</sub> Sr <sub>.50</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m	42	Boron oxide, B <sub>2</sub> O <sub>3</sub> , phase 1 .....	10m	70
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Barium sulfate (baryte), BaSO <sub>4</sub> .....	10m	12	Cadmium ammine chloride, Cd(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub> .....	10m	14
Barium sulfide, BaS .....	7	8	Cadmium borate, CdB <sub>4</sub> O <sub>7</sub> .....	16m	24
Barium thiosulfate hydrate, BaS <sub>2</sub> O <sub>3</sub> ·H <sub>2</sub> O .....	16m	20	Cadmium bromate hydrate, Cd(BrO <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O .....	17m	14
Barium tin oxide, BaSnO <sub>3</sub> .....	3m	11	Cadmium bromide, CdBr <sub>2</sub> .....	9	17
Barium titanium oxide, BaTiO <sub>3</sub> .....	3	45	Cadmium bromide chloride, CdBrCl ..	11m	15
Barium titanium silicate (fresnoite), Ba <sub>2</sub> TiSi <sub>2</sub> O <sub>8</sub> .....	9m	14	Cadmium carbonate (otavite), CdCO <sub>3</sub>	7	11
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Cadmium fluoride, CdF <sub>2</sub> .....	10m	15	Calcium fluoride (fluorite), CaF <sub>2</sub> ..	1	69
Cadmium iron oxide, CdFe <sub>2</sub> O <sub>4</sub> .....	9m	16	Calcium fluoride phosphate		
Cadmium lanthanum, CdLa .....	5m	63	(fluorapatite), Ca <sub>5</sub> F(PO <sub>4</sub> ) <sub>3</sub> .....	3m	22
Cadmium manganese oxide, CdMn <sub>2</sub> O <sub>4</sub> ..	10m	16	Calcium fluoride phosphate hydrate,		
Cadmium molybdenum oxide, CdMoO <sub>4</sub> ..	6	21	CaFPO <sub>3</sub> ·2H <sub>2</sub> O .....	15m	24
Cadmium nitrate hydrate,			Calcium gallium germanium oxide,		
Cd(NO <sub>3</sub> ) <sub>2</sub> ·4H <sub>2</sub> O .....	7m	93	Ca <sub>3</sub> Ga <sub>2</sub> (GeO <sub>4</sub> ) <sub>3</sub> .....	10	18
Cadmium oxide, CdO .....	2	27	Calcium hydrogen phosphate hydrate,		
Cadmium oxide, CdO (ref. standard)	8m	2	Ca <sub>8</sub> H <sub>2</sub> (PO <sub>4</sub> ) <sub>6</sub> ·5H <sub>2</sub> O .....	13m	21
Cadmium phosphate, Cd <sub>2</sub> P <sub>2</sub> O <sub>7</sub> .....	16m	26	Calcium hydrogen phosphate sulfate		
Cadmium phosphate, Cd <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> .....	16m	27	hydrate, Ca <sub>2</sub> HPO <sub>4</sub> SO <sub>4</sub> ·4H <sub>2</sub> O .....	16m	109
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Cadmium selenide (cadmoselite),			Ca(OH) <sub>2</sub> .....	1	58
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Cadmium silicate, Cd <sub>3</sub> SiO <sub>5</sub> .....	13m	20	Calcium iodate hydrate,		
Cadmium sulfate, CdSO <sub>4</sub> .....	3m	20	Ca(IO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	14m	13
Cadmium sulfate hydrate,			Calcium iron germanium oxide,		
3CdSO <sub>4</sub> ·8H <sub>2</sub> O .....	6m	8	Ca <sub>3</sub> Fe <sub>2</sub> (GeO <sub>4</sub> ) <sub>3</sub> .....	10	19
Cadmium sulfate hydrate, CdSO <sub>4</sub> ·H <sub>2</sub> O	6m	10	Calcium iron silicate (andradite),		
Cadmium sulfide (greenockite), CdS	4	15	Ca <sub>2</sub> Fe <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> .....	9	22
Cadmium telluride, CdTe .....	3m	21	Calcium iron silicate		
Cadmium titanium oxide, CdTiO <sub>3</sub> ....	15m	21	hydroxide, julgoldite,		
Cadmium tungsten oxide, CdWO <sub>4</sub> .....	2m	8	Ca <sub>2</sub> Fe <sub>3</sub> Si <sub>3</sub> O <sub>10</sub> (OH,O) <sub>2</sub> (OH) <sub>2</sub> .....	10m	72
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Calcium aluminum germanium oxide,			Ca <sub>33</sub> Pb <sub>67</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m	44
Ca <sub>3</sub> Al <sub>2</sub> (GeO <sub>4</sub> ) <sub>3</sub> .....	10	15	Calcium lead nitrate,		
Calcium aluminum hydroxide,			Ca <sub>67</sub> Pb <sub>33</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m	44
Ca <sub>3</sub> Al <sub>2</sub> (OH) <sub>12</sub> .....	11m	16	Calcium magnesium silicate		
Calcium aluminum iron oxide			(diopside), CaMg(SiO <sub>3</sub> ) <sub>2</sub> .....	5m	17
(brownmillerite), Ca <sub>4</sub> Al <sub>2</sub> Fe <sub>2</sub> O <sub>10</sub> ....	16m	28	Calcium molybdenum oxide		
Calcium aluminum oxide, Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> ..	5	10	(powellite), CaMoO <sub>4</sub> .....	6	22
Calcium aluminum oxide (mayenite),			Calcium nitrate, Ca(NO <sub>3</sub> ) <sub>2</sub> .....	7	14
Ca <sub>12</sub> Al <sub>14</sub> O <sub>33</sub> .....	9	20	Calcium oxide (lime), CaO .....	1	43
Calcium aluminum sulfate hydrate			Calcium oxide (lime), CaO		
(ettringite), Ca <sub>6</sub> Al <sub>2</sub> S <sub>3</sub> O <sub>18</sub> ·3H <sub>2</sub> O ..	8	3	(calculated pattern).....	14m	49
Calcium borate, CaB <sub>2</sub> O <sub>4</sub> .....	15m	136	Calcium oxide phosphate, Ca <sub>4</sub> O(PO <sub>4</sub> ) <sub>2</sub>	12m	17
Calcium borate hydrate,			Calcium phosphate, β-Ca <sub>2</sub> P <sub>2</sub> O <sub>7</sub> .....	7m	95
hexahydroborite, Ca[B(OH) <sub>4</sub> ] <sub>2</sub> ·2H <sub>2</sub> O	16m	104	Calcium platinum oxide, Ca <sub>4</sub> PtO <sub>6</sub> ...	10m	18
Calcium boride, CaB <sub>6</sub> .....	16m	29	Calcium selenide, CaSe .....	5m	64
Calcium bromide, CaBr <sub>2</sub> .....	11m	70	Calcium strontium nitrate,		
Calcium bromide hydrate, CaBr <sub>2</sub> ·6H <sub>2</sub> O	8	15	Ca <sub>33</sub> Sr <sub>67</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m	46
Calcium carbonate (aragonite),			Calcium strontium nitrate,		
CaCO <sub>3</sub> (orthorhombic).....	3	53	Ca <sub>67</sub> Sr <sub>33</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m	46
Calcium carbonate (aragonite),			Calcium sulfate (anhydrite), CaSO <sub>4</sub>	4	65
CaCO <sub>3</sub> (orthorhombic, calculated			Calcium sulfate hydrate (gypsum),		
pattern) .....	14m	44	CaSO <sub>4</sub> ·2H <sub>2</sub> O .....	17m	16
Calcium carbonate (calcite),			Calcium sulfide (oldhamite), CaS ..	7	15
CaCO <sub>3</sub> (hexagonal) .....	2	51	Calcium telluride, CaTe .....	4m	50
Calcium chloride (hydrophilite),			Calcium tin oxide, CaSnO <sub>3</sub> .....	17m	18
CaCl <sub>2</sub> .....	11m	18	Calcium titanium oxide		
Calcium chloride fluoride, CaClF ..	10m	17	(perovskite), CaTiO <sub>3</sub> .....	9m	17
Calcium chloride hydrate,			Calcium tungsten oxide, Ca <sub>3</sub> WO <sub>6</sub> ....	9m	19
CaCl <sub>2</sub> ·4H <sub>2</sub> O .....	11m	73	Calcium tungsten oxide, scheelite,		
Calcium chloride hydrate			CaWO <sub>4</sub> .....	6	23
(antarcticite), CaCl <sub>2</sub> ·6H <sub>2</sub> O .....	12m	16	Carbon, diamond, C .....	2	5
Calcium chromium germanium oxide,			Cerium arsenate, CeAsO <sub>4</sub> .....	4m	8
Ca <sub>3</sub> Cr <sub>2</sub> (GeO <sub>4</sub> ) <sub>3</sub> .....	10	16	Cerium(III) chloride, CeCl <sub>3</sub> .....	1m	8
Calcium chromium iron titanium			Cerium cobalt, CeCo <sub>2</sub> .....	13m	50
oxide, loveringite, Ca <sub>72</sub> RE <sub>33</sub> (Y,			Cerium cobalt, Ce <sub>24</sub> Co <sub>11</sub> .....	13m	51
Th,U,Pb) <sub>05</sub> Ti <sub>12</sub> . <sub>48</sub> Fe <sub>3</sub> . <sub>38</sub> Cr <sub>2</sub> . <sub>24</sub>			Cerium copper, CeCu <sub>6</sub> .....	7m	99
Mg. <sub>92</sub> Zr. <sub>58</sub> Al. <sub>39</sub> V. <sub>21</sub> Mn. <sub>04</sub> O <sub>38</sub> .....	16m	106	Cerium(III) fluoride, CeF <sub>3</sub> .....	8	17
Calcium chromium oxide (chromatite),			Cerium gallium, CeGa <sub>2</sub> .....	13m	54
CaCrO <sub>4</sub> .....	7	13	Cerium magnesium, CeMg .....	5m	65
Calcium chromium oxide, Ca <sub>3</sub> (CrO <sub>4</sub> ) <sub>2</sub>	15m	22	Cerium magnesium, CeMg <sub>3</sub> .....	13m	56



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Cerium nickel, CeNi <sub>2</sub> .....	13m	58	Cesium magnesium chromium oxide hydrate, Cs <sub>2</sub> Mg(CrO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	8m	29
Cerium niobium titanium oxide (aeschnite), CeNbTiO <sub>6</sub> .....	3m	24	Cesium magnesium sulfate hydrate, Cs <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	7m	18
Cerium nitrate hydrate, Ce(NO <sub>3</sub> ) <sub>3</sub> ·6H <sub>2</sub> O .....	17m	20	Cesium manganese fluoride, CsMnF <sub>3</sub>	10m	21
Cerium nitride, CeN .....	4m	51	Cesium manganese sulfate hydrate, Cs <sub>2</sub> Mn(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	7m	20
Cerium(IV) oxide (cerianite), CeO <sub>2</sub>	1	56	Cesium mercury chloride, CsHgCl <sub>3</sub> ..	7m	22
Cerium phosphide, CeP .....	4m	52	Cesium nickel(II) chloride, CsNiCl <sub>3</sub>	6m	12
Cerium thallium, CeTl .....	13m	59	Cesium nickel sulfate hydrate, Cs <sub>2</sub> Ni(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	7m	23
Cerium thallium, Ce <sub>3</sub> Tl .....	13m	60	Cesium nitrate, CsNO <sub>3</sub> .....	9	25
Cerium(III) vanadium oxide, CeVO <sub>4</sub>	1m	9	Cesium osmium(IV) bromide, Cs <sub>2</sub> OsBr <sub>6</sub>	2m	10
Cerium zinc, CeZn .....	5m	65	Cesium osmium chloride, Cs <sub>2</sub> OsCl <sub>6</sub> ..	2m	11
Cerium zinc, CeZn <sub>3</sub> .....	14m	50	Cesium platinum bromide, Cs <sub>2</sub> PtBr <sub>6</sub> .	8	19
Cerium zinc, CeZn <sub>5</sub> .....	14m	53	Cesium platinum chloride, Cs <sub>2</sub> PtCl <sub>6</sub>	5	14
Cerium zinc, Ce <sub>2</sub> Zn <sub>17</sub> .....	14m	55	Cesium platinum fluoride, Cs <sub>2</sub> PtF <sub>6</sub> .	6	27
Cesium aluminum sulfate hydrate, CsAl(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	6	25	Cesium selenium bromide, Cs <sub>2</sub> SeBr <sub>6</sub> ..	8	20
Cesium antimony fluoride, CsSbF <sub>6</sub> ..	4m	9	Cesium silicon fluoride, Cs <sub>2</sub> SiF <sub>6</sub> ..	5	19
Cesium beryllium fluoride, CsBeF <sub>3</sub>	9m	69	Cesium strontium chloride, CsSrCl <sub>3</sub>	6m	13
Cesium boron fluoride, CsBF <sub>4</sub> .....	8	22	Cesium sulfate, Cs <sub>2</sub> SO <sub>4</sub> .....	7	17
Cesium bromate, CsBrO <sub>3</sub> .....	8	18	Cesium tellurium bromide, Cs <sub>2</sub> TeBr <sub>6</sub>	9	24
Cesium bromide, CsBr .....	3	49	Cesium tin chloride, Cs <sub>2</sub> SnCl <sub>6</sub> .....	5	16
Cesium cadmium bromide, CsCdBr <sub>3</sub> (hexagonal) .....	10m	20	Cesium vanadium sulfate hydrate, CsV(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	1m	11
Cesium cadmium chloride, CsCdCl <sub>3</sub> (hexagonal) .....	5m	19	Cesium zinc sulfate hydrate, Cs <sub>2</sub> Zn(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	7m	25
Cesium calcium chloride, CsCaCl <sub>3</sub> ..	5m	21	Chromium, Cr .....	5	20
Cesium calcium fluoride, CsCaF <sub>3</sub> .....	8m	25	Chromium boride, ζ-CrB .....	17m	22
Cesium calcium sulfate, Cs <sub>2</sub> Ca <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	7m	12	Chromium chloride, CrCl <sub>2</sub> .....	11m	77
Cesium cerium chloride, Cs <sub>2</sub> CeCl <sub>6</sub> ..	14m	58	Chromium chloride, CrCl <sub>3</sub> .....	17m	23
Cesium chlorate, CsClO <sub>3</sub> .....	8	20	Chromium chloride hydrate, CrCl <sub>3</sub> ·6H <sub>2</sub> O	16m	31
Cesium chlorate, CsClO <sub>4</sub> , (orthorhombic) .....	1m	10	Chromium cobalt niobium, CoCrNb ...	15m	140
Cesium chloride, CsCl .....	2	44	Chromium cobalt silicide, Co <sub>9</sub> Cr <sub>15</sub> Si <sub>6</sub> .....	14m	62
Cesium chromium oxide, Cs <sub>2</sub> CrO <sub>4</sub> ....	3m	25	Chromium cobalt tantalum, CoCrTa ..	15m	142
Cesium chromium sulfate hydrate, CsCr(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	8	21	Chromium fluoride, CrF <sub>2</sub> .....	10m	81
Cesium cobalt(II) chloride, CsCoCl <sub>3</sub>	6m	11	Chromium fluoride, Cr <sub>2</sub> F <sub>5</sub> .....	7m	108
Cesium cobalt chloride, Cs <sub>2</sub> CoCl <sub>4</sub> ..	11m	19	Chromium(III) fluoride hydrate, CrF <sub>3</sub> ·3H <sub>2</sub> O .....	5m	25
Cesium copper(II) chloride, CsCuCl <sub>3</sub>	5m	22	Chromium iridium, Cr <sub>3</sub> Ir .....	6m	14
Cesium copper chloride, Cs <sub>2</sub> CuCl <sub>4</sub> ..	11m	20	Chromium iron oxide, Cr <sub>1.3</sub> Fe <sub>0.7</sub> O <sub>3</sub> .....	17m	24
Cesium copper sulfate hydrate, Cs <sub>2</sub> Cu(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	7m	14	Chromium oxide, CrO <sub>3</sub> .....	17m	25
Cesium fluoride, CsF .....	3m	26	Chromium(III) oxide, Cr <sub>2</sub> O <sub>3</sub> .....	5	22
Cesium gallium sulfate hydrate, CsGa(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	8	23	Chromium phosphate, α-CrPO <sub>4</sub> .....	2m	12
Cesium germanium fluoride, Cs <sub>2</sub> GeF <sub>6</sub>	5	17	Chromium phosphate, β-CrPO <sub>4</sub> .....	9	26
Cesium iodate, CsIO <sub>3</sub> .....	15m	26	Chromium phosphate hydrate, CrPO <sub>4</sub> ·6H <sub>2</sub> O .....	15m	27
Cesium iodide, CsI .....	4	47	Chromium rhodium, Cr <sub>3</sub> Rh .....	6m	15
Cesium iodine bromide, CsI <sub>2</sub> Br .....	7m	103	Chromium silicide, Cr <sub>3</sub> Si .....	6	29
Cesium iodine chloride, CsI <sub>2</sub> Cl .....	3	50	Chromium sulfate, Cr <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	16m	33
Cesium iron chloride hydrate, Cs <sub>2</sub> FeCl <sub>5</sub> ·H <sub>2</sub> O .....	14m	14	Cobalt, Co (cubic) .....	4m	10
Cesium iron sulfate hydrate, Cs <sub>2</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	7m	16	Cobalt aluminum oxide, CoAl <sub>2</sub> O <sub>4</sub> .....	9	27
Cesium iron sulfate hydrate, CsFe(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	6	28	Cobalt ammine iodide, Co(NH <sub>3</sub> ) <sub>6</sub> I <sub>3</sub> ..	10m	83
Cesium lead(II) chloride, CsPbCl <sub>3</sub> (tetragonal) .....	5m	24	Cobalt antimony oxide, CoSb <sub>2</sub> O <sub>6</sub> ....	5m	26
Cesium lead fluoride, CsPbF <sub>3</sub> .....	8m	26	Cobalt arsenide, CoAs <sub>2</sub> .....	4m	10
Cesium lithium cobalt cyanide, CsLiCo(CN) <sub>6</sub> .....	10m	79	Cobalt arsenide (skutterudite), CoAs <sub>3</sub> .....	10	21
Cesium lithium fluoride, CsLiF <sub>2</sub> ...	7m	105	Cobalt borate, Co <sub>3</sub> (BO <sub>3</sub> ) <sub>2</sub> .....	12m	20
Cesium magnesium chromium oxide, Cs <sub>2</sub> Mg <sub>2</sub> (CrO <sub>4</sub> ) <sub>3</sub> .....	8m	27	Cobalt bromide hydrate, CoBr <sub>2</sub> ·6H <sub>2</sub> O	12m	21
			Cobalt(II) carbonate (sphaero- cobaltite), CoCO <sub>3</sub> .....	10	24
			Cobalt chlorate hydrate, Co(ClO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	3m	28
			Cobalt chloride hydrate, CoCl <sub>2</sub> ·2H <sub>2</sub> O	11m	22
			Cobalt chloride hydrate, CoCl <sub>2</sub> ·6H <sub>2</sub> O	11m	23

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Cobalt chromium oxide, $\text{CoCr}_2\text{O}_4$ ....	9m	21	Cobalt(II) oxide, $\text{CoO}$ .....	9	28
Cobalt copper tin, $\text{CoCu}_2\text{Sn}$ .....	14m	64	Cobalt(II,III) oxide, $\text{Co}_3\text{O}_4$ .....	9	29
Cobalt dysprosium, $\text{Co}_2\text{Dy}$ .....	13m	63	Cobalt phosphate, $\text{Co}(\text{PO}_3)_2$ .....	13m	23
Cobalt erbium, $\text{Co}_2\text{Er}$ .....	13m	64	Cobalt phosphide, $\text{CoP}$ .....	14m	83
Cobalt erbium, $\text{Co}_7\text{Er}_2$ .....	13m	65	Cobalt phosphide, $\text{CoP}_3$ .....	14m	85
Cobalt fluoride, $\text{CoF}_2$ .....	10m	85	Cobalt platinum, $\text{CoPt}$ (disordered)	15m	167
Cobalt fluoride hydrate, $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$	11m	24	Cobalt platinum, $\text{CoPt}$ (ordered) ...	15m	168
Cobalt gadolinium, $\text{CoGd}_3$ .....	13m	68	Cobalt platinum, $\text{CoPt}_3$		
Cobalt gadolinium, $\text{Co}_2\text{Gd}$ .....	13m	71	(disordered) .....	15m	169
Cobalt gadolinium, $\text{Co}_7\text{Gd}_2$ .....	13m	72	Cobalt platinum, $\text{CoPt}_3$ (ordered)...	15m	170
Cobalt gallium hafnium, $\text{Co}_2\text{GaHf}$ ...	14m	65	Cobalt plutonium, $\text{CoPu}_2$ .....	14m	87
Cobalt gallium manganese, $\text{Co}_2\text{GaMn}$	13m	75	Cobalt plutonium, $\text{CoPu}_3$ .....	15m	171
Cobalt gallium niobium,			Cobalt plutonium, $\text{CoPu}_6$ .....	14m	89
$\text{Co}_{1.5}\text{Ga}_{0.5}\text{Nb}$ .....	15m	144	Cobalt plutonium, $\text{Co}_2\text{Pu}$ .....	14m	91
Cobalt gallium niobium, $\text{Co}_2\text{GaNb}$ ...	14m	66	Cobalt plutonium, $\text{Co}_3\text{Pu}$ .....	14m	92
Cobalt gallium oxide, $\text{CoGa}_2\text{O}_4$ ....	10	27	Cobalt plutonium, $\text{Co}_{17}\text{Pu}_2$ .....	14m	94
Cobalt gallium tantalum,			Cobalt praseodymium, $\text{Co}_2\text{Pr}$ .....	14m	97
$\text{Co}_{1.5}\text{Ga}_{0.5}\text{Ta}$ .....	15m	146	Cobalt rhodium sulfide, $\text{Co}_8\text{RhS}_8$ ....	14m	98
Cobalt gallium tantalum, $\text{Co}_2\text{GaTa}$	13m	76	Cobalt ruthenium sulfide, $\text{Co}_8\text{RuS}_8$ ..	14m	100
Cobalt gallium titanium, $\text{Co}_2\text{GaTi}$ ..	13m	77	Cobalt samarium, $\text{Co}_2\text{Sm}$ .....	15m	173
Cobalt gallium vanadium, $\text{Co}_2\text{GaV}$ ...	13m	78	Cobalt samarium, $\text{Co}_5\text{Sm}$ .....	13m	90
Cobalt germanium, $\text{Co}_3\text{Ge}_2$ .....	14m	67	Cobalt silicate, $\text{Co}_2\text{SiO}_4$		
Cobalt germanium, $\text{Co}_5\text{Ge}_7$ .....	15m	148	(orthorhombic) .....	4m	11
Cobalt germanium hafnium,			Cobalt silicon fluoride hydrate,		
$\text{Co}_{16}\text{Ge}_7\text{Hf}_6$ .....	14m	69	$\text{CoSiF}_6 \cdot 6\text{H}_2\text{O}$ .....	3m	27
Cobalt germanium manganese,			Cobalt sulfate, $\beta\text{-CoSO}_4$ .....	2m	14
$\text{Co}_2\text{GeMn}$ .....	13m	79	Cobalt tantalum silicide,		
Cobalt germanium niobium,			$\text{Co}_{16}\text{Ta}_6\text{Si}_7$ .....	14m	102
$\text{Co}_{1.5}\text{Ge}_{0.5}\text{Nb}$ .....	15m	150	Cobalt thorium, $\text{Co}_{17}\text{Th}_2$ .....	12m	64
Cobalt germanium niobium,			Cobalt tin, $\text{Co}_3\text{Sn}_2$ .....	13m	92
$\text{Co}_{16}\text{Ge}_7\text{Nb}_6$ .....	14m	71	Cobalt tin oxide, $\text{Co}_2\text{SnO}_4$ .....	15m	30
Cobalt germanium oxide, $\text{Co}_2\text{GeO}_4$ ...	10	27	Cobalt tin vanadium, $\text{Co}_2\text{SnV}$ .....	15m	174
Cobalt germanium tantalum,			Cobalt tin zirconium, $\text{Co}_2\text{SnZr}$ ....	15m	175
$\text{Co}_{1.5}\text{Ge}_{0.5}\text{Ta}$ .....	15m	152	Cobalt titanium oxide, $\text{CoTiO}_3$ ....	4m	13
Cobalt germanium tantalum,			Cobalt titanium silicide,		
$\text{Co}_{16}\text{Ge}_7\text{Ta}_6$ .....	14m	73	$\text{Co}_{16}\text{Ti}_6\text{Si}_7$ .....	14m	104
Cobalt germanium titanium, $\text{Co}_2\text{GeTi}$	13m	80	Cobalt tungsten oxide, $\text{CoWO}_4$ .....	4m	13
Cobalt hafnium tin, $\text{Co}_2\text{HfSn}$ .....	14m	75	Cobalt vanadium silicide, $\text{Co}_2\text{VSi}$ ..	15m	176
Cobalt holmium, $\text{Co}_2\text{Ho}$ .....	14m	76	Copper, $\text{Cu}$ .....	1	15
Cobalt holmium, $\text{Co}_9 \cdot 2\text{Ho}_{12}$ .....	15m	154	Copper ammine selenate,		
Cobalt hydroxide, $\beta\text{-Co}(\text{OH})_2$ .....	15m	29	$\text{Cu}(\text{NH}_3)_4\text{SeO}_4$ .....	10m	87
Cobalt indium, $\text{CoIn}_3$ .....	13m	81	Copper ammine sulfate hydrate,		
Cobalt iodide, $\text{CoI}_2$ .....	4m	52	$\text{Cu}(\text{NH}_3)_4\text{SO}_4 \cdot \text{H}_2\text{O}$ .....	10m	90
Cobalt iron arsenide			Copper antimony oxide, $\text{CuSb}_2\text{O}_6$ ....	5m	27
(safflorite), $\text{CoFeAs}_4$ .....	10	28	Copper arsenate (tripplite),		
Cobalt iron oxide, $\text{CoFe}_2\text{O}_4$ .....	9m	22	$\text{CuAs}_2\text{O}_4$ .....	16m	120
Cobalt iron sulfide, $\text{Co}_3\text{FeS}_8$ .....	14m	77	Copper(I) bromide, $\text{CuBr}$ .....	4	36
Cobalt iron vanadium,			Copper(I) chloride (nantokite),		
$\text{Co}_{4.35}\text{Fe}_{13.47}\text{V}_{12.18}$ .....	14m	79	$\text{CuCl}$ .....	4	35
Cobalt lanthanum, $\text{CoLa}_3$ .....	13m	83	Copper fluoride hydrate, $\text{CuF}_2 \cdot 2\text{H}_2\text{O}$	11m	25
Cobalt lutetium, $\text{Co}_2\text{Lu}$ .....	13m	86	Copper hydrogen phosphite hydrate,		
Cobalt magnesium, $\text{Co}_2\text{Mg}$ .....	15m	156	$\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ .....	11m	83
Cobalt manganese silicide, $\text{Co}_2\text{MnSi}$	14m	81	Copper hydroxide carbonate,		
Cobalt mercury thiocyanate,			azurite, $\text{Cu}_3(\text{OH})_2(\text{CO}_3)_2$ .....	10	30
$\text{Co}[\text{Hg}(\text{CNS})_4]$ .....	2m	13	Copper hydroxide carbonate		
Cobalt molybdenum, $\text{Co}_2\text{Mo}$ .....	14m	82	(malachite), $\text{Cu}_2(\text{OH})_2\text{CO}_3$ .....	10	31
Cobalt molybdenum, $\text{Co}_2\text{Mo}_3$ .....	15m	158	Copper hydroxide phosphate		
Cobalt molybdenum, $\text{Co}_7\text{Mo}_6$ .....	15m	160	(libethenite), $\text{Cu}_2(\text{OH})\text{PO}_4$ .....	17m	30
Cobalt molybdenum silicide,			Copper(I) iodide (marshite), $\text{CuI}$ ..	4	38
$\text{Co}_3\text{Mo}_2\text{Si}$ .....	15m	162	Copper lead hydroxide sulfate,		
Cobalt neodymium, $\text{Co}_2\text{Nd}$ .....	13m	87	linarite, $\text{CuPb}(\text{OH})_2(\text{SO}_4)$ .....	16m	34
Cobalt nickel tin,			Copper(I) oxide (cuprite), $\text{Cu}_2\text{O}$ ...	2	23
$\text{Co}_{.75}\text{Ni}_{.75}\text{Sn}_{.75}$ .....	13m	88	Copper(II) oxide (tenorite), $\text{CuO}$ ..	1	49
Cobalt niobium silicide, $\text{Co}_3\text{Nb}_4\text{Si}_7$	15m	164	Copper phosphate, $\text{Cu}(\text{PO}_3)_2$ .....	14m	15
Cobalt niobium tin, $\text{Co}_2\text{NbSn}$ .....	15m	166	Copper phosphate, $\alpha\text{-Cu}_2\text{P}_2\text{O}_7$ .....	7m	113
Cobalt nitrate hydrate,			Copper sulfate (chalcocyanite),		
$\alpha\text{-Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ .....	12m	22	$\text{CuSO}_4$ .....	3m	29

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Copper(II) sulfide (covellite), CuS	4	13	Germanium oxide, GeO <sub>2</sub>		
Copper uranium oxide, CuUO <sub>4</sub> .....	10m	93	(tetragonal) (high form) .....	8	28
Dichlorotetraaquo chromium (III)			Gold, Au .....	1	33
chloride dihydrate, [Cr(H <sub>2</sub> O) <sub>4</sub> Cl <sub>2</sub> ]			Gold chloride, AuCl .....	16m	37
Cl·2H <sub>2</sub> O .....	16m	31	Gold(I) cyanide, AuCN .....	10	33
Dysprosium arsenate, DyAsO <sub>4</sub> .....	3m	30	Gold holmium, AuHo.....	5m	68
Dysprosium arsenide, DyAs .....	4m	53	Gold magnesium, AuMg.....	6m	83
Dysprosium gallium oxide,			Gold niobium, AuNb <sub>3</sub> .....	6m	16
Dy <sub>3</sub> Ga <sub>5</sub> O <sub>12</sub> .....	2m	15	Gold potassium cyanide, AuK(CN) <sub>2</sub> ..	8m	36
Dysprosium gold, DyAu .....	5m	66	Gold tin, AuSn .....	7	19
Dysprosium nitride, DyN .....	4m	53	Gold titanium, AuTi <sub>3</sub> .....	6m	17
Dysprosium oxide, Dy <sub>2</sub> O <sub>3</sub> .....	9	30	Gold vanadium, AuV <sub>3</sub> .....	6m	18
Dysprosium silver, DyAg .....	5m	66	Hafnium, Hf .....	3	18
Dysprosium telluride, DyTe .....	4m	54	Holmium arsenate, HoAsO <sub>4</sub> .....	3m	34
Dysprosium vanadium oxide, DyVO <sub>4</sub> ..	4m	15	Holmium fluoride, HoF <sub>3</sub> .....	10m	23
Erbium arsenate, ErAsO <sub>4</sub> .....	3m	31	Holmium nitride, HoN .....	4m	58
Erbium arsenide, ErAs .....	4m	54	Holmium oxide, Ho <sub>2</sub> O <sub>3</sub> .....	9	32
Erbium gallium oxide, Er <sub>3</sub> Ga <sub>5</sub> O <sub>12</sub> ...	1m	12	Holmium selenide, HoSe .....	4m	59
Erbium manganese oxide, ErMnO <sub>3</sub> ....	2m	16	Holmium silver, HoAg .....	5m	68
Erbium nitride, ErN .....	4m	55	Holmium vanadium oxide, HoVO <sub>4</sub> .....	4m	18
Erbium oxide, Er <sub>2</sub> O <sub>3</sub> .....	8	25	Hydrazinium sulfate, (NH <sub>3</sub> ) <sub>2</sub> SO <sub>4</sub> .....	17m	38
Erbium phosphate, ErPO <sub>4</sub> .....	9	31	Hydrogen amidosulfate, H <sub>2</sub> NSO <sub>3</sub> H .....	7	54
Erbium silver, ErAg .....	5m	67	Hydrogen arsenate, H <sub>5</sub> As <sub>3</sub> O <sub>10</sub> .....	7m	84
Erbium telluride, ErTe .....	4m	55	Hydrogen borate, β-HBO <sub>2</sub> (monoclinic)	9m	71
Erbium vanadium oxide, ErVO <sub>4</sub> .....	5m	29	Hydrogen borate (metaborite),		
Europium arsenate, EuAsO <sub>4</sub> .....	3m	32	HBO <sub>2</sub> (cubic) .....	4m	27
Europium(III) chloride, EuCl <sub>3</sub> .....	1m	13	Hydrogen iodate, HIO <sub>3</sub> .....	5	28
Europium chloride oxide, EuClO ....	1m	13	Hydrogen iodate, HI <sub>3</sub> O <sub>8</sub> .....	8m	104
Europium gallium oxide,			Hydrogen phosphate hydrate,		
Eu <sub>3</sub> Ga <sub>5</sub> O <sub>12</sub> .....	2m	17	H <sub>3</sub> PO <sub>4</sub> ·0.5H <sub>2</sub> O .....	12m	56
Europium nitride, EuN .....	4m	56	Hydrogen tellurate, H <sub>6</sub> TeO <sub>6</sub> .....	12m	34
Europium oxide, EuO .....	4m	56	Indium, In .....	3	12
Europium phosphate, EuPO <sub>4</sub> .....	11m	26	Indium arsenide, InAs.....	3m	35
Europium(III) vanadium oxide, EuVO <sub>4</sub>	4m	16	Indium oxide, In <sub>2</sub> O <sub>3</sub> .....	5	26
Gadolinium arsenate, GdAsO <sub>4</sub> .....	4m	17	Indium phosphate, InPO <sub>4</sub> .....	8	29
Gadolinium arsenide, GdAs .....	4m	57	Indium sulfide, In <sub>2</sub> S <sub>3</sub> .....	11m	30
Gadolinium chloride hydrate,			Iodine, I <sub>2</sub> .....	3	16
GdCl <sub>3</sub> ·6H <sub>2</sub> O .....	7m	118	Iridium, Ir.....	4	9
Gadolinium chloride oxide, GdClO ..	1m	17	Iridium niobium, IrNb <sub>3</sub> .....	6m	19
Gadolinium fluoride, GdF <sub>3</sub> .....	1m	14	Iridium oxide, IrO <sub>2</sub> .....	4m	19
Gadolinium gallium oxide,			Iridium titanium, IrTi <sub>3</sub> .....	6m	20
Gd <sub>3</sub> Ga <sub>5</sub> O <sub>12</sub> .....	2m	18	Iridium vanadium, IrV <sub>3</sub> .....	6m	21
Gadolinium indium, GdIn .....	5m	67	Iron, α-Fe .....	4	3
Gadolinium nitride, GdN .....	4m	57	Iron arsenide, FeAs .....	1m	19
Gadolinium oxide, Gd <sub>2</sub> O <sub>3</sub> .....	1m	16	Iron arsenide (loellingite), FeAs <sub>2</sub>	10	34
Gadolinium silver, GdAg .....	6m	87	Iron bromide, FeBr <sub>2</sub> .....	4m	59
Gadolinium titanium oxide, Gd <sub>2</sub> TiO <sub>5</sub>	8m	32	Iron carbonate, siderite, FeCO <sub>3</sub> ...	15m	32
Gadolinium vanadium oxide, GdVO <sub>4</sub> ..	5m	30	Iron chloride hydrate, FeCl <sub>2</sub> ·2H <sub>2</sub> O	11m	32
Gallium, Ga .....	2	9	Iron chloride hydrate (hydromolysite),		
Gallium arsenide, GaAs .....	3m	33	FeCl <sub>3</sub> ·6H <sub>2</sub> O .....	17m	40
Gallium lutetium oxide, Ga <sub>5</sub> Lu <sub>3</sub> O <sub>12</sub>	2m	22	Iron fluoride hydrate, FeF <sub>2</sub> ·4H <sub>2</sub> O	11m	90
Gallium magnesium, Ga <sub>2</sub> Mg .....	12m	48	Iron fluoride hydrate, β-FeF <sub>3</sub> ·3H <sub>2</sub> O .	17m	41
Gallium magnesium, Ga <sub>5</sub> Mg <sub>2</sub> .....	12m	51	Iron hydroxide sulfate hydrate,		
Gallium neodymium oxide, Ga <sub>5</sub> Nd <sub>3</sub> O <sub>12</sub>	1m	34	butlerite, Fe(OH)SO <sub>4</sub> ·2H <sub>2</sub> O .....	10m	95
Gallium oxide, α-Ga <sub>2</sub> O <sub>3</sub> .....	4	25	Iron iodide, FeI <sub>2</sub> .....	4m	60
Gallium phosphate (α-quartz type),			Iron(II,III) oxide (magnetite),		
GaPO <sub>4</sub> .....	8	27	Fe <sub>3</sub> O <sub>4</sub> .....	5m	31
Gallium phosphate hydrate,			Iron phosphate, FePO <sub>4</sub> .....	15m	33
GaPO <sub>4</sub> ·2H <sub>2</sub> O .....	8m	34	Iron phosphate hydrate (vivianite),		
Gallium samarium oxide, Ga <sub>5</sub> Sm <sub>3</sub> O <sub>12</sub>	1m	42	Fe <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O .....	16m	38
Gallium ytterbium oxide, Ga <sub>5</sub> Yb <sub>3</sub> O <sub>12</sub>	1m	49	Iron sulfate, Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	16m	39
Gallium yttrium oxide, Ga <sub>5</sub> Y <sub>3</sub> O <sub>12</sub> ...	1m	50	Iron sulfate hydrate (melanterite),		
Germanium, Ge .....	1	18	FeSO <sub>4</sub> ·7H <sub>2</sub> O.....	8m	38
Germanium iodide, GeI <sub>2</sub> .....	4m	58	Iron sulfide (pyrite), FeS <sub>2</sub> .....	5	29
Germanium(IV) iodide, GeI <sub>4</sub> .....	5	25	Iron thorium, Fe <sub>17</sub> Th <sub>2</sub> .....	12m	67
Germanium oxide, GeO <sub>2</sub> (hexagonal)			Iron titanium oxide (ilmenite),		
(low form) .....	1	51	FeTiO <sub>3</sub> .....	15m	34
			Lanthanum arsenate, LaAsO <sub>4</sub> .....	3m	36

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Lanthanum arsenide, LaAs .....	4m	60	Lithium barium fluoride, LiBaF <sub>3</sub> ...	5m	35
Lanthanum borate, LaBO <sub>3</sub> .....	1m	20	Lithium beryllium fluoride, Li <sub>2</sub> BeF <sub>4</sub>	7m	126
Lanthanum chloride, LaCl <sub>3</sub> .....	1m	20	Lithium borate, Li <sub>2</sub> B <sub>4</sub> O <sub>7</sub> .....	8m	114
Lanthanum chloride oxide, LaClO ...	7	22	Lithium bromide, LiBr .....	4	30
Lanthanum fluoride, LaF <sub>3</sub> .....	7	21	Lithium calcium aluminum boron		
Lanthanum magnesium, LaMg.....	5m	69	hydroxy silicate, liddicoatite,		
Lanthanum nickel platinum,			Ca(Li,Al) <sub>3</sub> Al <sub>6</sub> B <sub>3</sub> Si <sub>6</sub> O <sub>27</sub> (O,OH) <sub>3</sub> (OH,F)	16m	42
LaNi <sub>0.25</sub> Pt <sub>4.75</sub> .....	17m	42	Lithium carbonate, Li <sub>2</sub> CO <sub>3</sub> .....	8m	42
Lanthanum niobium titanium oxide,			Lithium chlorate hydrate,		
LaNbTiO <sub>6</sub> .....	3m	37	LiClO <sub>4</sub> ·3H <sub>2</sub> O .....	8	34
Lanthanum nitrate hydrate,			Lithium chloride, LiCl .....	1	62
La(NO <sub>3</sub> ) <sub>3</sub> ·6H <sub>2</sub> O .....	8m	40	Lithium chromium oxide hydrate,		
Lanthanum nitride, LaN .....	4m	61	Li <sub>2</sub> CrO <sub>4</sub> ·2H <sub>2</sub> O .....	16m	44
Lanthanum oxide, La <sub>2</sub> O <sub>3</sub> .....	3	33	Lithium fluoride, LiF .....	1	61
Lanthanum phosphide, LaP .....	5m	69	Lithium gallium oxide, LiGaO <sub>2</sub> .....	10m	31
Lanthanum selenide, LaSe .....	4m	61	Lithium hydroxide, LiOH .....	17m	46
Lanthanum titanium oxide, La <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub>	15m	35	Lithium hydroxide hydrate, LiOH·H <sub>2</sub> O	11m	92
Lanthanum zinc, LaZn .....	5m	70	Lithium iodate, LiIO <sub>3</sub> (hexagonal)	7	26
Lead, Pb .....	1	34	Lithium iodate, LiIO <sub>3</sub> (tetragonal)	10m	33
Lead borate, PbB <sub>4</sub> O <sub>7</sub> .....	4m	19	Lithium molybdenum oxide, Li <sub>2</sub> MoO <sub>4</sub>		
Lead bromide, PbBr <sub>2</sub> .....	17m	43	(trigonal) .....	1m	23
Lead bromide chloride, PbBrCl .....	11m	33	Lithium niobium oxide, LiNbO <sub>3</sub> .....	6m	22
Lead bromide fluoride, PbBrF .....	10m	25	Lithium nitrate, LiNO <sub>3</sub> .....	7	27
Lead bromide hydroxide, PbBr(OH) ..	16m	40	Lithium oxide, Li <sub>2</sub> O .....	1m	25
Lead bromide oxide, Pb <sub>3</sub> O <sub>2</sub> Br <sub>2</sub> .....	5m	32	Lithium phosphate hydrate,		
Lead carbonate (cerussite), PbCO <sub>3</sub>	2	56	Li <sub>3</sub> P <sub>3</sub> O <sub>9</sub> ·3H <sub>2</sub> O .....	2m	20
Lead chloride (cotunnite), PbCl <sub>2</sub> ..	12m	23	Lithium phosphate, low form		
Lead chloride fluoride (matlockite),			(lithiophosphate), Li <sub>3</sub> PO <sub>4</sub> .....	4m	21
PbClF .....	13m	25	Lithium phosphate, high form,		
Lead chromium oxide, Pb <sub>2</sub> CrO <sub>5</sub> .....	14m	16	Li <sub>3</sub> PO <sub>4</sub> .....	3m	39
Lead fluoride, α-PbF <sub>2</sub>			Lithium potassium sulfate, KLiSO <sub>4</sub>	3m	43
(orthorhombic) .....	5	31	Lithium rubidium fluoride, LiRbF <sub>2</sub>	7m	128
Lead fluoride, β-PbF <sub>2</sub> (cubic) .....	5	33	Lithium selenide, Li <sub>2</sub> Se .....	10m	100
Lead fluoride iodide, PbFI .....	10m	26	Lithium silicate, Li <sub>2</sub> SiO <sub>3</sub> .....	14m	19
Lead hydrogen arsenate (schultenite),			Lithium silver bromide,		
PbHAsO <sub>4</sub> .....	14m	18	Li <sub>2</sub> Ag <sub>.8</sub> Br .....	12m	55
Lead hydrogen phosphate, PbHPO <sub>4</sub> ....	15m	37	Lithium silver bromide,		
Lead hydroxide phosphate,			Li <sub>.4</sub> Ag <sub>.6</sub> Br .....	12m	55
Pb <sub>5</sub> OH(PO <sub>4</sub> ) <sub>3</sub> .....	8	33	Lithium silver bromide,		
Lead iodate, Pb(IO <sub>3</sub> ) <sub>2</sub> .....	17m	45	Li <sub>.6</sub> Ag <sub>.4</sub> Br .....	12m	55
Lead(II) iodide, PbI <sub>2</sub> .....	5	34	Lithium silver bromide,		
Lead molybdenum oxide (wulfenite),			Li <sub>.8</sub> Ag <sub>.2</sub> Br .....	12m	55
PbMoO <sub>4</sub> .....	7	23	Lithium sodium aluminum fluoride,		
Lead nitrate, Pb(NO <sub>3</sub> ) <sub>2</sub> .....	5	36	cryolithionite, Li <sub>3</sub> Na <sub>3</sub> Al <sub>2</sub> F <sub>12</sub> .....	9m	23
Lead oxide (litharge), PbO (red,			Lithium sodium sulfate, LiNaSO <sub>4</sub> ...	6m	24
tetragonal).....	2	30	Lithium sulfate, Li <sub>2</sub> SO <sub>4</sub> .....	6m	26
Lead oxide (massicot), PbO (yellow,			Lithium sulfate hydrate,		
orthorhombic).....	2	32	Li <sub>2</sub> SO <sub>4</sub> ·H <sub>2</sub> O .....	4m	22
Lead(II,III) oxide (minium), Pb <sub>3</sub> O <sub>4</sub>	8	32	Lithium sulfide, Li <sub>2</sub> S .....	10m	101
Lead oxide sulfate, Pb <sub>5</sub> O <sub>5</sub> SO <sub>4</sub> .....	10m	27	Lithium tantalum oxide, LiTaO <sub>3</sub> .....	14m	20
Lead selenide (clausthalite), PbSe	5	38	Lithium telluride, Li <sub>2</sub> Te .....	10m	102
Lead strontium nitrate,			Lithium tin oxide, Li <sub>2</sub> SnO <sub>3</sub> .....	16m	45
Pb <sub>.33</sub> Sr <sub>.67</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m	53	Lithium tungsten oxide, Li <sub>2</sub> WO <sub>4</sub>		
Lead strontium nitrate,			(trigonal) .....	1m	25
Pb <sub>.67</sub> Sr <sub>.33</sub> (NO <sub>3</sub> ) <sub>2</sub> .....	12m	53	Lithium tungsten oxide hydrate,		
Lead sulfate (anglesite), PbSO <sub>4</sub> ...	3	67	Li <sub>2</sub> WO <sub>4</sub> ·0.5H <sub>2</sub> O .....	2m	20
Lead sulfide (galena), PbS.....	2	18	Lithium uranium fluoride, LiUF <sub>5</sub> ...	7m	131
Lead tin oxide, Pb <sub>2</sub> SnO <sub>4</sub> .....	10m	29	Lutetium arsenate, LuAsO <sub>4</sub> .....	5m	36
Lead titanium oxide (macedonite),			Lutetium manganese oxide, LuMnO <sub>3</sub> ..	2m	23
PbTiO <sub>3</sub> .....	5	39	Lutetium nitride, LuN .....	4m	62
Lead tungsten oxide (stolzite),			Lutetium oxide, Lu <sub>2</sub> O <sub>3</sub> .....	1m	27
PbWO <sub>4</sub> (tetragonal).....	5m	34	Lutetium vanadium oxide, LuVO <sub>4</sub> ....	5m	37
Lead uranium oxide, Pb <sub>3</sub> UO <sub>6</sub> .....	8m	109	Magnesium, Mg .....	1	10
Lithium aluminum fluoride,			Magnesium aluminum oxide (spinel),		
α-Li <sub>3</sub> AlF <sub>6</sub> .....	8m	111	MgAl <sub>2</sub> O <sub>4</sub> .....	9m	25
Lithium arsenate, Li <sub>3</sub> AsO <sub>4</sub> .....	2m	19	Magnesium aluminum silicate (low		
Lithium azide, LiN <sub>3</sub> .....	8m	113	cordierite), Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub>		
			(orthorhombic) .....	1m	28

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Magnesium aluminum silicate (indialite) $Mg_2Al_4Si_5O_{18}$ (hexagonal) .....	1m	29	Magnesium sulfate hydrate (epsomite), $MgSO_4 \cdot 7H_2O$ .....	7	30
Magnesium aluminum silicate (pyrope), $Mg_3Al_2(SiO_4)_2$ .....	4m	24	Magnesium sulfide, $MgS$ .....	7	31
Magnesium borate, $MgB_4O_7$ .....	17m	47	Magnesium sulfite hydrate, $MgSO_3 \cdot 6H_2O$ .....	9m	26
Magnesium borate, $Mg_2B_2O_5$ (triclinic) .....	4m	25	Magnesium tin, $Mg_2Sn$ .....	5	41
Magnesium bromide, $MgBr_2$ .....	4m	62	Magnesium tin oxide, $Mg_2SnO_4$ .....	10m	37
Magnesium bromide hydrate, $MgBr_2 \cdot 6H_2O$ .....	11m	35	Magnesium titanium oxide (geikielite), $MgTiO_3$ .....	5	43
Magnesium carbonate (magnesite), $MgCO_3$ .....	7	28	Magnesium titanium oxide, $Mg_2TiO_4$ .....	12m	25
Magnesium cerium nitrate hydrate, $Mg_3Ce_2(NO_3)_{12} \cdot 24H_2O$ .....	10	20	Magnesium tungsten oxide, $MgWO_4$ ...	13m	27
Magnesium chlorate hydrate, $Mg(ClO_4)_2 \cdot 6H_2O$ .....	7m	30	Manganese, $\alpha$ -Mn (calculated pattern)	7m	142
Magnesium chloride (chloro- magnesite), $MgCl_2$ .....	11m	94	Manganese, $\alpha$ -Mn .....	17m	50
Magnesium chloride hydrate, $MgCl_2 \cdot 12H_2O$ .....	7m	135	Manganese aluminum oxide (galaxite), $MnAl_2O_4$ .....	9	35
Magnesium chloride hydrate (bischofite), $MgCl_2 \cdot 6H_2O$ .....	11m	37	Manganese bromide, $MnBr_2$ .....	4m	63
Magnesium chromium oxide (magnesiochromite), $MgCr_2O_4$ .....	9	34	Manganese(II) carbonate (rhodochrosite), $MnCO_3$ .....	7	32
Magnesium chromium oxide hydrate, $MgCrO_4 \cdot 5H_2O$ .....	15m	39	Manganese chloride (scacchite), $MnCl_2$ .....	8m	43
Magnesium fluoride (sellaite), $MgF_2$	4	33	Manganese chloride hydrate, $MnCl_2 \cdot 2H_2O$ .....	11m	38
Magnesium fluoride silicate (humite), $Mg_7F_2Si_3O_{12}$ .....	1m	30	Manganese chloride hydrate, $MnCl_2 \cdot 4H_2O$ .....	9m	28
Magnesium fluoride silicate (norbergite), $Mg_3F_2SiO_4$ .....	10	39	Manganese cobalt oxide, $MnCo_2O_4$ ...	9m	30
Magnesium gallium oxide, $MgGa_2O_4$ ..	10	36	Manganese fluoride, $MnF_2$ .....	10m	105
Magnesium germanium oxide, $Mg_2GeO_4$ (cubic) .....	10	37	Manganese iodide, $MnI_2$ .....	4m	63
Magnesium germanium oxide, $Mg_2GeO_4$ (orthorhombic) .....	10	38	Manganese iron oxide (jacobsite), $MnFe_2O_4$ .....	9	36
Magnesium hydrogen phosphate hydrate, newberyite, $MgHPO_4 \cdot 3H_2O$	7m	139	Manganese(II) oxide (manganosite), $MnO$ .....	5	45
Magnesium hydroxide (brucite), $Mg(OH)_2$ .....	6	30	Manganese oxide (pyrolusite), $\beta$ - $MnO_2$	10m	39
Magnesium iodate hydrate, $Mg(IO_3)_2 \cdot 4H_2O$ .....	17m	48	Manganese oxide (bixbyite), $\alpha$ - $Mn_2O_3$	11m	95
Magnesium iron hydroxide carbonate hydrate, pyroaurite, $Mg_6Fe_2(OH)_{16}CO_3 \cdot 4H_2O$ (rhomb.)....	10m	104	Manganese oxide (hausmannite), $Mn_3O_4$ .....	10m	38
Magnesium iron hydroxide carbonate hydrate, sjögrenite, $Mg_6Fe_2(OH)_{16}CO_3 \cdot 4H_2O$ , (hexag.) ...	10m	103	Manganese oxide hydroxide, groutite, $\alpha$ - $MnOOH$ .....	11m	97
Magnesium lanthanum nitrate hydrate, $Mg_3La_2(NO_3)_{12} \cdot 24H_2O$ .....	1m	22	Manganese phosphate, $Mn(PO_3)_2$ .....	14m	21
Magnesium manganese oxide, $MgMn_2O_4$	10m	35	Manganese phosphate, $Mn_2P_2O_7$ .....	15m	41
Magnesium mercury, $MgHg$ .....	6m	84	Manganese phosphate, $Mn_3(PO_4)_2$ ...	16m	47
Magnesium molybdenum oxide, $MgMoO_4$	7m	28	Manganese selenide, $MnSe$ .....	10	41
Magnesium nickel oxide, $MgNiO_2$ ...	10m	36	Manganese sulfate hydrate (szmikite), $MnSO_4 \cdot H_2O$ .....	16m	49
Magnesium oxide (periclase), $MgO$ ..	1	37	Manganese sulfide (alabandite), $\alpha$ - $MnS$ .....	4	11
Magnesium phosphate, $Mg(PO_3)_2$ .....	13m	26	Manganese titanium oxide (pyrophanite), $MnTiO_3$ .....	15m	42
Magnesium phosphate, $\alpha$ - $Mg_2P_2O_7$ ...	9m	73	Manganese(II) tungsten oxide (huebnerite), $MnWO_4$ .....	2m	24
Magnesium selenide, $MgSe$ .....	5m	70	Manganese vanadium oxide, $Mn_2V_2O_7$	9m	75
Magnesium selenite hydrate, $MgSeO_3 \cdot 6H_2O$ .....	8m	116	Mercury amide chloride, $HgNH_2Cl$ ...	10m	40
Magnesium silicate, enstatite, $MgSiO_3$ .....	6	32	Mercury ammine chloride, $Hg(NH_3)_2Cl_2$ .....	11m	39
Magnesium silicate (forsterite), $Mg_2SiO_4$ .....	1	83	Mercury bromate, $Hg(BrO_3)_2$ .....	10m	107
Magnesium sulfate hydrate (kieserite), $MgSO_4 \cdot H_2O$ .....	16m	46	Mercury bromide, $HgBr_2$ .....	10m	110
			Mercury bromide, $Hg_2Br_2$ .....	7	33
			Mercury chloride, $HgCl_2$ .....	13m	29
			Mercury chloride (calomel), $Hg_2Cl_2$ .....	13m	30
			Mercury chloride sulfide, $\alpha$ - $Hg_3Cl_2S_2$ .....	8m	118
			Mercury(II) cyanide, $Hg(CN)_2$ .....	6	35
			Mercury(II) fluoride, $HgF_2$ .....	2m	25
			Mercury hydroxide nitrate, $Hg(OH)NO_3$ .....	17m	52
			Mercury(I) iodide, $HgI$ .....	4	49
			Mercury(II) iodide, $HgI_2$ (tetragonal)	7m	32

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Mercury(II) oxide (montroydite), HgO.....	9	39	Osmium titanium, OsTi .....	6m	85
Mercury(II) selenide (tiemannite), HgSe .....	7	35	Palladium, Pd .....	1	21
Mercury sulfate, HgSO <sub>4</sub> .....	16m	50	Palladium hydride, PdH <sub>0.706</sub> .....	5m	72
Mercury sulfate, Hg <sub>2</sub> SO <sub>4</sub> .....	16m	52	Palladium oxide, PdO .....	4	27
Mercury(II) sulfide (cinnabar), HgS (hexagonal) .....	4	17	Palladium selenium (palladseite), Pd <sub>17</sub> Se <sub>15</sub> .....	16m	139
Mercury(II) sulfide (metacinnabar), HgS (cubic) .....	4	21	Palladium vanadium, PdV <sub>3</sub> .....	6m	32
Molybdenum, Mo .....	1	20	Phosphorus bromide, PBr <sub>7</sub> .....	7m	150
Molybdenum arsenide, Mo <sub>2</sub> As <sub>3</sub> .....	10m	115	Phosphorus oxide (stable form I), P <sub>2</sub> O <sub>5</sub> (orthorhombic) .....	9m	86
Molybdenum osmium, Mo <sub>3</sub> Os .....	6m	28	Phosphorus oxide (stable form II), P <sub>2</sub> O <sub>5</sub> (orthorhombic) .....	9m	88
Molybdenum oxide (molybdate), MoO <sub>3</sub> Molybdenum sulfide (molybdenite), MoS <sub>2</sub> .....	3	30	Phosphorus oxide (metastable form), P <sub>4</sub> O <sub>10</sub> (rhombohedral) .....	9m	91
Neodymium arsenate, NdAsO <sub>4</sub> .....	4m	28	Platinum, Pt .....	1	31
Neodymium arsenide, NdAs .....	4m	64	Platinum titanium, PtTi <sub>3</sub> .....	6m	33
Neodymium borate, NdBO <sub>3</sub> .....	1m	32	Platinum vanadium, PtV <sub>3</sub> .....	6m	34
Neodymium chloride, NdCl <sub>3</sub> .....	1m	33	Plutonium arsenide, PuAs .....	4m	65
Neodymium chloride oxide, NdOCl....	8	37	Plutonium phosphide, PuP .....	4m	65
Neodymium fluoride, NdF <sub>3</sub> .....	8	36	Plutonium telluride, PuTe .....	4m	66
Neodymium oxide, Nd <sub>2</sub> O <sub>3</sub> .....	4	26	Potassium aluminum sulfate, KAl(SO <sub>4</sub> ) <sub>2</sub> .....	9m	31
Neodymium phosphate, NdPO <sub>4</sub> .....	11m	40	Potassium aluminum sulfate hydrate (potash alum), KAl(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O ...	6	36
Neodymium selenide, NdSe.....	5m	71	Potassium arsenic fluoride, KAsF <sub>6</sub> .....	17m	57
Neodymium silver, NdAg.....	5m	71	Potassium barium chromium oxide, K <sub>2</sub> Ba(CrO <sub>4</sub> ) <sub>2</sub> .....	14m	23
Neodymium vanadium oxide, NdVO <sub>4</sub> ...	4m	30	Potassium barium iron titanium oxide, K <sub>1.16</sub> Ba <sub>0.72</sub> Fe <sub>0.36</sub> Ti <sub>5.58</sub> O <sub>13</sub>	16m	147
Neptunium nitride, NpN .....	4m	64	Potassium barium molybdenum oxide, K <sub>2</sub> Ba(MoO <sub>4</sub> ) <sub>2</sub> .....	14m	24
Nickel, Ni .....	1	13	Potassium barium nickel nitrite, K <sub>2</sub> BaNi(NO <sub>2</sub> ) <sub>6</sub> .....	9m	32
Nickel aluminum oxide, NiAl <sub>2</sub> O <sub>4</sub> ....	9	42	Potassium borate hydroxide hydrate, K <sub>2</sub> B <sub>4</sub> O <sub>5</sub> (OH) <sub>4</sub> ·2H <sub>2</sub> O .....	15m	46
Nickel arsenide (rammelsbergite), NiAs <sub>2</sub> .....	10	42	Potassium boron hydride, KBH <sub>4</sub> .....	9	44
Nickel arsenic sulfide (gersdorffite), NiAsS .....	1m	35	Potassium bromate, KBrO <sub>3</sub> .....	7	38
Nickel bromide, NiBr <sub>2</sub> .....	10m	119	Potassium bromide, KBr .....	1	66
Nickel(II) carbonate, NiCO <sub>3</sub> (trigonal) .....	1m	36	Potassium bromide chloride, KBr <sub>0.5</sub> Cl <sub>0.5</sub> .....	8m	46
Nickel chloride, NiCl <sub>2</sub> .....	9m	81	Potassium bromide iodide, KBr <sub>.33</sub> I <sub>.67</sub> .....	11m	44
Nickel chloride hydrate, NiCl <sub>2</sub> ·6H <sub>2</sub> O .....	11m	42	Potassium bromide iodide, KBr <sub>.67</sub> I <sub>.33</sub> .....	11m	45
Nickel fluoride, NiF <sub>2</sub> .....	10m	121	Potassium cadmium fluoride, KCdF <sub>3</sub> Potassium cadmium sulfate, K <sub>2</sub> Cd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	8m	47
Nickel fluoride hydrate, NiF <sub>2</sub> ·4H <sub>2</sub> O	11m	43	Potassium calcium carbonate (fairchildite), K <sub>2</sub> Ca(CO <sub>3</sub> ) <sub>2</sub> .....	7m	34
Nickel gallium oxide, NiGa <sub>2</sub> O <sub>4</sub> .....	10	45	Potassium calcium chloride, KCaCl <sub>3</sub> Potassium calcium fluoride, KCaF <sub>3</sub> Potassium calcium magnesium sulfate, K <sub>2</sub> CaMg(SO <sub>4</sub> ) <sub>3</sub> .....	8m	48
Nickel germanium oxide, Ni <sub>2</sub> GeO <sub>4</sub> ...	9	43	Potassium calcium nickel nitrite, K <sub>2</sub> CaNi(NO <sub>2</sub> ) <sub>6</sub> .....	7m	36
Nickel iron oxide (trevorite), NiFe <sub>2</sub> O <sub>4</sub> .....	10	44	Potassium calcium sulfate, K <sub>2</sub> Ca <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	8m	49
Nickel nitrate hydrate, Ni(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	12m	26	Potassium calcium sulfate hydrate (syngenite), K <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub> ·H <sub>2</sub> O .....	7m	37
Nickel(II) oxide (bunsenite), NiO	1	47	Potassium cerium fluoride, β-KCeF <sub>4</sub> Potassium chlorate, KClO <sub>3</sub> .....	14m	25
Nickel phosphate, Ni(PO <sub>3</sub> ) <sub>2</sub> .....	14m	22	Potassium chlorate, KClO <sub>4</sub> .....	12m	59
Nickel phosphide, Ni <sub>12</sub> P <sub>5</sub> .....	9m	83	Potassium chlorate (sylvite), KCl	3m	42
Nickel silicon fluoride hydrate, NiSiF <sub>6</sub> ·6H <sub>2</sub> O .....	8	38	Potassium chloride (sylvite), KCl	6	43
Nickel sulfate, NiSO <sub>4</sub> .....	2m	26	Potassium chromium oxide, K <sub>3</sub> CrO <sub>8</sub> ..	1	65
Nickel sulfate hydrate (retgersite), NiSO <sub>4</sub> ·6H <sub>2</sub> O .....	7	36	Potassium chromium oxide (lopezite), K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> .....	3m	44
Nickel sulfide, millerite, NiS ....	1m	37		15m	47
Nickel tungsten oxide, NiWO <sub>4</sub> .....	2m	27			
Nickel yttrium, Ni <sub>3</sub> Y .....	10m	123			
Niobium boride, ζ-NbB .....	17m	54			
Niobium chloride oxide, NbCl <sub>3</sub> O ....	7m	148			
Niobium osmium, Nb <sub>3</sub> Os.....	6m	30			
Niobium platinum, Nb <sub>3</sub> Pt.....	6m	31			
Niobium silicide, NbSi <sub>2</sub> .....	8	39			
Niobium silicide, α-Nb <sub>5</sub> Si <sub>3</sub> .....	15m	43			
Niobium silicide, β-Nb <sub>5</sub> Si <sub>3</sub> .....	15m	44			
Osmium, Os .....	4	8			

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Potassium chromium oxide sulfate, K <sub>2</sub> (CrO <sub>4</sub> ) <sub>33</sub> (SO <sub>4</sub> ) <sub>67</sub> .....	12m	28	Potassium manganese oxide, KMnO <sub>4</sub>	7	42
Potassium chromium oxide sulfate, K <sub>2</sub> (CrO <sub>4</sub> ) <sub>67</sub> (SO <sub>4</sub> ) <sub>33</sub> .....	12m	27	Potassium manganese(II) sulfate (manganolangbeinite), K <sub>2</sub> Mn <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	6m	43
Potassium chromium sulfate, KCr(SO <sub>4</sub> ) <sub>2</sub> .....	16m	58	Potassium molybdenum oxide, K <sub>2</sub> MoO <sub>4</sub>	15m	53
Potassium chromium sulfate hydrate, KCr(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O .....	6	39	Potassium molybdenum oxide phos- phate hydrate, K <sub>3</sub> (MoO <sub>3</sub> ) <sub>12</sub> PO <sub>4</sub> ·4H <sub>2</sub> O	8	43
Potassium cobalt(II) fluoride, KCoF <sub>3</sub> .....	6m	37	Potassium nickel fluoride, KNiF <sub>3</sub>	7m	42
Potassium cobalt fluoride, K <sub>2</sub> CoF <sub>4</sub>	11m	46	Potassium nickel fluoride, K <sub>2</sub> NiF <sub>4</sub>	10m	45
Potassium cobalt nitrite, K <sub>3</sub> Co(NO <sub>2</sub> ) <sub>6</sub> .....	9	45	Potassium nickel(II) sulfate, K <sub>2</sub> Ni <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	6m	46
Potassium cobalt(II) sulfate, K <sub>2</sub> Co <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	6m	35	Potassium niobium fluoride, K <sub>2</sub> NbF <sub>7</sub>	8m	120
Potassium copper chloride, KCuCl <sub>3</sub>	7m	41	Potassium niobium oxide, KNbO <sub>3</sub> ....	17m	62
Potassium copper chloride hydrate (mitscherlichite), K <sub>2</sub> CuCl <sub>4</sub> ·2H <sub>2</sub> O ..	9m	34	Potassium nitrate (niter), KNO <sub>3</sub> ...	3	58
Potassium copper(II) fluoride, KCuF <sub>3</sub> .....	6m	38	Potassium nitrite, KNO <sub>2</sub> .....	9m	38
Potassium cyanate, KCNO .....	7	39	Potassium nitrosyl ruthenium chloride, K <sub>2</sub> NORuCl <sub>5</sub> .....	16m	61
Potassium cyanide, KCN .....	1	77	Potassium oxide, K <sub>2</sub> O .....	10m	125
Potassium fluoride, KF .....	1	64	Potassium platinum bromide, K <sub>2</sub> PtBr <sub>6</sub>	8	40
Potassium germanium fluoride, K <sub>2</sub> GeF <sub>6</sub> .....	6	41	Potassium platinum chloride, K <sub>2</sub> PtCl <sub>6</sub> .....	13m	34
Potassium hydrogen arsenate, KH <sub>2</sub> AsO <sub>4</sub> .....	1m	38	Potassium platinum fluoride, K <sub>2</sub> PtF <sub>6</sub> .....	6	42
Potassium hydrogen iodate, KH(IO <sub>3</sub> ) <sub>2</sub> .....	17m	58	Potassium rhenium chloride, K <sub>2</sub> ReCl <sub>6</sub>	2m	28
Potassium hydrogen phosphate, KH <sub>2</sub> PO <sub>4</sub> .....	3	69	Potassium rhenium oxide, KReO <sub>4</sub> ....	8	41
Potassium hydroxide, KOH at 300 °C	4m	66	Potassium rubidium chloride, K <sub>0.5</sub> Rb <sub>0.5</sub> Cl .....	8m	76
Potassium iodate, KIO <sub>3</sub> .....	15m	48	Potassium rubidium chromium oxide, KRbCrO <sub>4</sub> .....	12m	29
Potassium iodate, KIO <sub>4</sub> .....	7	41	Potassium ruthenium chloride, K <sub>2</sub> RuCl <sub>6</sub> .....	10	46
Potassium iodide, KI .....	1	68	Potassium ruthenium oxide chloride hydrate, K <sub>4</sub> Ru <sub>2</sub> OCl <sub>10</sub> ·H <sub>2</sub> O .....	10	47
Potassium iron chloride hydrate (erythrosiderite), K <sub>2</sub> FeCl <sub>5</sub> ·H <sub>2</sub> O ...	14m	27	Potassium selenate, K <sub>2</sub> SeO <sub>4</sub> .....	9m	41
Potassium iron cyanide, K <sub>3</sub> Fe(CN) <sub>6</sub>	9m	35	Potassium selenide, K <sub>2</sub> Se .....	10m	126
Potassium iron(II) fluoride, KFeF <sub>3</sub>	6m	39	Potassium selenium bromide, K <sub>2</sub> SeBr <sub>6</sub>	8	41
Potassium iron fluoride, K <sub>3</sub> FeF <sub>6</sub> ...	9m	37	Potassium silicon fluoride (hieratite), K <sub>2</sub> SiF <sub>6</sub> .....	5	50
Potassium iron sulfate (yavapaiite), KFe(SO <sub>4</sub> ) <sub>2</sub> .....	16m	59	Potassium silver cyanide, KAg(CN) <sub>2</sub>	8m	78
Potassium lead chloride, KPb <sub>2</sub> Cl <sub>5</sub> ..	13m	33	Potassium sodium aluminum fluoride (elpasolite), K <sub>2</sub> NaAlF <sub>6</sub> .....	9m	43
Potassium lead chromium oxide, K <sub>2</sub> Pb(CrO <sub>4</sub> ) <sub>2</sub> .....	14m	28	Potassium sodium bromide, K <sub>2</sub> Na <sub>8</sub> Br .....	12m	62
Potassium lead molybdenum oxide, K <sub>2</sub> Pb(MoO <sub>4</sub> ) <sub>2</sub> .....	14m	29	Potassium sodium bromide, K <sub>4</sub> Na <sub>6</sub> Br .....	12m	62
Potassium lead phosphate, K <sub>2</sub> Pb(PO <sub>3</sub> ) <sub>4</sub> .....	15m	50	Potassium sodium bromide, K <sub>6</sub> Na <sub>4</sub> Br .....	12m	62
Potassium lead selenate, K <sub>2</sub> Pb(SeO <sub>4</sub> ) <sub>2</sub> .....	15m	52	Potassium sodium bromide, K <sub>8</sub> Na <sub>2</sub> Br .....	12m	62
Potassium lead sulfate (palmierite), K <sub>2</sub> Pb(SO <sub>4</sub> ) <sub>2</sub> .....	14m	30	Potassium sodium chloride, K <sub>2</sub> Na <sub>8</sub> Cl .....	12m	63
Potassium magnesium chloride hydrate (carnallite), KMgCl <sub>3</sub> ·6H <sub>2</sub> O	8m	50	Potassium sodium chloride, K <sub>4</sub> Na <sub>6</sub> Cl .....	12m	63
Potassium magnesium chromium oxide, K <sub>2</sub> Mg <sub>2</sub> (CrO <sub>4</sub> ) <sub>3</sub> .....	8m	52	Potassium sodium chloride, K <sub>6</sub> Na <sub>4</sub> Cl .....	12m	63
Potassium magnesium fluoride, KMgF <sub>3</sub>	6m	42	Potassium sodium chloride, K <sub>8</sub> Na <sub>2</sub> Cl .....	12m	63
Potassium magnesium fluoride, K <sub>2</sub> MgF <sub>4</sub> .....	10m	42	Potassium sodium sulfate, K <sub>67</sub> Na <sub>1.33</sub> SO <sub>4</sub> .....	6m	48
Potassium magnesium selenate hydrate, K <sub>2</sub> Mg(SeO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	10m	43	Potassium sodium sulfate, KNaSO <sub>4</sub> ..	6m	50
Potassium magnesium sulfate (langbeinite), K <sub>2</sub> Mg <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .....	6m	40	Potassium sodium sulfate (aphthitalite), K <sub>3</sub> Na(SO <sub>4</sub> ) <sub>2</sub> .....	6m	52
Potassium magnesium sulfate hydrate (picromerite), K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	8m	54	Potassium strontium chromium oxide, K <sub>2</sub> Sr(CrO <sub>4</sub> ) <sub>2</sub> .....	15m	57
Potassium manganese(II) fluoride, KMnF <sub>3</sub> .....	6m	45	Potassium strontium selenate, K <sub>2</sub> Sr(SeO <sub>4</sub> ) <sub>2</sub> .....	15m	58
			Potassium strontium sulfate (kalistrontite), K <sub>2</sub> Sr(SO <sub>4</sub> ) <sub>2</sub> .....	14m	31

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Potassium sulfate, $K_2S_2O_7$ .....	9m	99	Rubidium copper sulfate hydrate, $Rb_2Cu(SO_4)_2 \cdot 6H_2O$ .....	8m	61
Potassium sulfate, $K_2S_2O_8$ .....	17m	64	Rubidium fluoride, $RbF$ .....	8m	63
Potassium sulfate (arcanite), $K_2SO_4$	3	62	Rubidium iodate, $RbIO_3$ .....	15m	62
Potassium sulfide, $K_2S$ .....	10m	127	Rubidium iodate, $RbIO_4$ .....	2m	31
Potassium telluride, $K_2Te$ .....	10m	128	Rubidium iodide, $RbI$ .....	4	43
Potassium thiocyanate, $KCNS$ .....	8	44	Rubidium iron chloride hydrate, $Rb_2FeCl_5 \cdot H_2O$ .....	14m	33
Potassium tin chloride, $K_2SnCl_6$ ...	6	38	Rubidium iron sulfate hydrate, $Rb_2Fe(SO_4)_2 \cdot 6H_2O$ .....	8m	64
Potassium titanium fluoride, $K_2TiF_6$	7	40	Rubidium lead chromium oxide, $Rb_2Pb(CrO_4)_2$ .....	14m	34
Potassium tungsten oxide, $K_2WO_4$ ...	11m	47	Rubidium lead molybdenum oxide, $Rb_2Pb(MoO_4)_2$ .....	15m	63
Potassium vanadium oxide, $KV_3O_8$ ...	8m	56	Rubidium magnesium chromium oxide, $Rb_2Mg_2(CrO_4)_3$ .....	8m	66
Potassium zinc bromide hydrate, $KZnBr_3 \cdot 2H_2O$ .....	11m	104	Rubidium magnesium chromium oxide hydrate, $Rb_2Mg(CrO_4)_2 \cdot 6H_2O$ .....	8m	68
Potassium zinc fluoride, $KZnF_3$ ....	5	51	Rubidium magnesium sulfate, $Rb_2Mg_2(SO_4)_3$ .....	7m	50
Potassium zinc fluoride, $K_2ZnF_4$ ...	10m	46	Rubidium magnesium sulfate hydrate, $Rb_2Mg(SO_4)_2 \cdot 6H_2O$ .....	8m	70
Potassium zinc iodide hydrate, $KZnI_3 \cdot 2H_2O$ .....	11m	107	Rubidium manganese(II) fluoride, $RbMnF_3$ .....	5m	44
Potassium zinc sulfate, $K_2Zn_2(SO_4)_3$	6m	54	Rubidium manganese sulfate, $Rb_2Mn_2(SO_4)_3$ .....	7m	52
Potassium zinc sulfate hydrate, $K_2Zn(SO_4)_2 \cdot 6H_2O$ .....	7m	43	Rubidium nickel(II) chloride, $RbNiCl_3$ .....	6m	58
Potassium zinc vanadium oxide hydrate, $K_2Zn_2V_{10}O_{28} \cdot 16H_2O$ .....	3m	45	Rubidium nickel sulfate, $Rb_2Ni_2(SO_4)_3$ .....	8m	72
Potassium zirconium fluoride, $K_3ZrF_7$ .....	9	46	Rubidium nickel sulfate hydrate, $Rb_2Ni(SO_4)_2 \cdot 6H_2O$ .....	8m	74
Praseodymium arsenate, $PrAsO_4$ .....	4m	32	Rubidium nitrate, $RbNO_3$ (trigonal)	5m	45
Praseodymium arsenide, $PrAs$ .....	4m	67	Rubidium platinum chloride, $Rb_2PtCl_6$ .....	5	53
Praseodymium chloride, $PrCl_3$ .....	1m	39	Rubidium platinum fluoride, $Rb_2PtF_6$	6	48
Praseodymium chloride oxide, $PrOCl$	9	47	Rubidium selenate, $Rb_2SeO_4$ .....	9m	44
Praseodymium fluoride, $PrF_3$ .....	5	52	Rubidium silicon fluoride, $Rb_2SiF_6$	6	49
Praseodymium sulfide, $PrS$ .....	4m	67	Rubidium strontium chloride, $RbSrCl_3$ .....	7m	54
Praseodymium vanadium oxide, $PrVO_4$	5m	40	Rubidium strontium chromium oxide, $Rb_2Sr(CrO_4)_2$ .....	15m	64
Praseodymium zinc, $PrZn$ .....	5m	72	Rubidium strontium sulfate, $Rb_2Sr(SO_4)_2$ .....	15m	65
Rhenium, $Re$ .....	2	13	Rubidium sulfate, $Rb_2SO_4$ .....	8	48
Rhodium, $Rh$ .....	3	9	Rubidium tellurium bromide, $Rb_2TeBr_6$ .....	8	46
Rhodium vanadium, $RhV_3$ .....	6m	56	Rubidium tellurium chloride, $Rb_2TeCl_6$ .....	8	48
Rubidium aluminum sulfate hydrate, $RbAl(SO_4)_2 \cdot 12H_2O$ .....	6	44	Rubidium tin chloride, $Rb_2SnCl_6$ ...	6	46
Rubidium amide, $RbNH_2$ .....	5m	73	Rubidium zinc fluoride, $RbZnF_3$ ....	7m	57
Rubidium barium chromium oxide, $Rb_2Ba(CrO_4)_2$ .....	14m	32	Rubidium zinc sulfate hydrate, $Rb_2Zn(SO_4)_2 \cdot 6H_2O$ .....	7m	55
Rubidium barium molybdenum oxide, $Rb_2Ba(MoO_4)_2$ .....	15m	59	Ruthenium, $Ru$ .....	4	5
Rubidium bromate, $RbBrO_3$ .....	8	45	Ruthenium titanium, $RuTi$ .....	6m	86
Rubidium bromide, $RbBr$ .....	7	43	Samarium arsenate, $SmAsO_4$ .....	4m	33
Rubidium cadmium chloride, high form, $RbCdCl_3$ (tetragonal) .....	5m	43	Samarium arsenide, $SmAs$ .....	4m	68
Rubidium cadmium chloride, low form, $RbCdCl_3$ (orthorhombic)	5m	41	Samarium chloride, $SmCl_3$ .....	1m	40
Rubidium cadmium sulfate, $Rb_2Cd_2(SO_4)_3$ .....	7m	45	Samarium chloride oxide, $SmOCl$ ....	1m	43
Rubidium calcium chloride, $RbCaCl_3$	7m	47	Samarium fluoride, $SmF_3$ .....	1m	41
Rubidium calcium fluoride, $RbCaF_3$	8m	57	Samarium oxide, $Sm_2O_3$ (cubic) ....	4m	34
Rubidium calcium sulfate, $Rb_2Ca_2(SO_4)_3$ .....	7m	48	Samarium silver, $SmAg$ .....	5m	73
Rubidium chlorate, $RbClO_3$ .....	8	47	Samarium tin oxide, $Sm_2Sn_2O_7$ .....	8m	77
Rubidium chlorate, $RbClO_4$ .....	2m	30	Samarium vanadium oxide, $SmVO_4$ ....	5m	47
Rubidium chloride, $RbCl$ .....	4	41	Scandium arsenate, $ScAsO_4$ .....	4m	35
Rubidium chromium oxide, $Rb_2CrO_4$ ..	3m	46	Scandium arsenide, $ScAs$ .....	4m	68
Rubidium chromium oxide, $Rb_2Cr_2O_7$	15m	60	Scandium boride, $ScB_2$ .....	17m	66
Rubidium chromium sulfate hydrate, $RbCr(SO_4)_2 \cdot 12H_2O$ .....	6	47			
Rubidium cobalt(II) chloride, $RbCoCl_3$ .....	6m	57			
Rubidium cobalt fluoride, $RbCoF_3$ ..	8m	58			
Rubidium cobalt sulfate, $Rb_2Co_2(SO_4)_3$ .....	8m	59			
Rubidium copper chloride hydrate, $Rb_2CuCl_4 \cdot 2H_2O$ .....	10m	47			



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Scandium phosphate, $\text{ScPO}_4$ .....	8	50	Sodium borate, $\text{Na}_2\text{B}_4\text{O}_7$ .....	16m	64
Scandium silicate (thortveitite), $\text{Sc}_2\text{Si}_2\text{O}_7$ .....	7m	58	Sodium borate, $\text{Na}_2\text{B}_2\text{O}_3$ .....	7m	160
Selenium, Se .....	5	54	Sodium borate hydroxide hydrate (borax), $\text{Na}_2\text{B}_4\text{O}_5(\text{OH})_4 \cdot 8\text{H}_2\text{O}$ .....	16m	66
Selenium oxide (selenolite), $\text{SeO}_2$	7m	60	Sodium boron hydride, $\text{NaBH}_4$ .....	9	51
Silicon, Si .....	13m	35	Sodium bromate, $\text{NaBrO}_3$ .....	5	65
Silicon, Si (reference standard) ..	12m	2	Sodium bromide, $\text{NaBr}$ .....	3	47
Silicon nitride, $\beta\text{-Si}_3\text{N}_4$ .....	14m	116	Sodium bromide chloride, $\text{NaBr}_{.33}\text{Cl}_{.67}$ .....	11m	49
Silicon oxide ( $\alpha$ or low cristobalite), $\text{SiO}_2$ (tetragonal)	10	48	Sodium bromide chloride, $\text{NaBr}_{.67}\text{Cl}_{.33}$ .....	11m	50
Silicon oxide ( $\alpha$ or low cristobalite), $\text{SiO}_2$ (tetragonal) (calculated pattern) .....	15m	180	Sodium calcium aluminum fluoride hydrate, thomsenolite, $\text{NaCaAlF}_6 \cdot \text{H}_2\text{O}$ .....	8m	132
Silicon oxide ( $\alpha$ or low quartz), $\text{SiO}_2$ (hexagonal) .....	3	24	Sodium calcium carbonate hydrate, pirssonite, $\text{Na}_2\text{Ca}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$ .....	9m	106
Silicon oxide ( $\beta$ or high cristobalite), $\text{SiO}_2$ (cubic) .....	1	42	Sodium calcium phosphate, $\beta\text{-NaCaPO}_4$	15m	69
Silver, Ag .....	1	23	Sodium calcium silicate, $\text{Na}_2\text{CaSiO}_4$	10m	48
Silver, Ag (reference standard) ...	8m	2	Sodium calcium sulfate (glauberite), $\text{Na}_2\text{Ca}(\text{SO}_4)_2$ .....	6m	59
Silver arsenate, $\text{Ag}_3\text{AsO}_4$ .....	5	56	Sodium carbonate hydrate (thermo- natrite), $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O}$ .....	8	54
Silver arsenic sulfide, xanthoconite, $\text{Ag}_3\text{AsS}_3$ .....	8m	126	Sodium carbonate sulfate, $\text{Na}_4\text{CO}_3\text{SO}_4$	11m	51
Silver bromate, $\text{AgBrO}_3$ .....	5	57	Sodium carbonate sulfate (burkeite), $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$ .....	11m	52
Silver bromide (bromargyrite), $\text{AgBr}$	4	46	Sodium carbonate sulfate, $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$ .....	11m	53
Silver carbonate, $\text{Ag}_2\text{CO}_3$ .....	13m	36	Sodium carbonate sulfate, $\text{Na}_6(\text{CO}_3)_2\text{SO}_4$ .....	11m	54
Silver chlorate, $\text{AgClO}_3$ .....	7	44	Sodium chlorate, $\text{NaClO}_3$ .....	3	51
Silver chloride (chlorargyrite), AgCl .....	4	44	Sodium chlorate, $\text{NaClO}_4$ (orthorhombic) .....	7	49
Silver chromium oxide, $\text{Ag}_2\text{CrO}_4$ ....	12m	30	Sodium chlorate hydrate, $\text{NaClO}_4 \cdot \text{H}_2\text{O}$ .....	17m	68
Silver cyanide, $\text{AgCN}$ .....	9m	48	Sodium chloride (halite), $\text{NaCl}$ ....	2	41
Silver fluoride, $\text{Ag}_2\text{F}$ .....	5m	53	Sodium chromium oxide, $\text{Na}_2\text{CrO}_4$ ....	9m	48
Silver iodate, $\text{AgIO}_4$ .....	9	49	Sodium chromium oxide hydrate, $\text{Na}_2\text{CrO}_4 \cdot 4\text{H}_2\text{O}$ .....	9m	50
Silver iodide (iodargyrite), AgI (hexagonal) .....	8	51	Sodium chromium oxide hydrate, $\text{Na}_2\text{Cr}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$ .....	7m	62
Silver iodide, $\gamma\text{-AgI}$ (cubic) .....	9	48	Sodium chromium oxide sulfate, $\text{Na}_4(\text{CrO}_4)(\text{SO}_4)$ .....	11m	55
Silver manganese oxide, $\text{AgMnO}_4$ ....	7m	155	Sodium cobalt nitrite, $\text{Na}_3\text{Co}(\text{NO}_2)_6$	15m	70
Silver mercury iodide, $\beta\text{-Ag}_2\text{HgI}_4$ ..	17m	67	Sodium cobalt(II) sulfate hydrate, $\text{Na}_2\text{Co}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ .....	6m	61
Silver molybdenum oxide, $\text{Ag}_2\text{MoO}_4$ ..	7	45	Sodium cyanate, $\text{NaCNO}$ .....	2m	33
Silver nitrate, $\text{AgNO}_3$ .....	5	59	Sodium cyanide, $\text{NaCN}$ (cubic) .....	1	78
Silver nitrite, $\text{AgNO}_2$ .....	5	60	Sodium cyanide, $\text{NaCN}$ (orthorhombic) at 6 °C .....	1	79
Silver oxide, $\text{Ag}_2\text{O}$ .....	1m	45	Sodium fluoride (villiaumite), $\text{NaF}$	1	63
Silver(II) oxide nitrate, $\text{Ag}_7\text{O}_8\text{NO}_3$	4	61	Sodium hydrogen carbonate hydrate, trona, $\text{Na}_3\text{H}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$ .....	15m	71
Silver phosphate, $\text{Ag}_3\text{PO}_4$ .....	5	62	Sodium hydrogen fluoride, $\text{NaHF}_2$ ...	5	63
Silver rhenium oxide, $\text{AgReO}_4$ .....	8	53	Sodium hydrogen phosphate, $\text{Na}_3\text{H}(\text{PO}_3)_4$ .....	10m	130
Silver selenate, $\text{Ag}_2\text{SeO}_4$ .....	2m	32	Sodium hydrogen silicate hydrate, $\text{Na}_2\text{H}_2\text{SiO}_4 \cdot 4\text{H}_2\text{O}$ .....	7m	163
Silver sodium chloride, $\text{Ag}_{0.5}\text{Na}_{0.5}\text{Cl}$ .....	8m	79	Sodium hydrogen sulfate hydrate, $\text{NaHSO}_4 \cdot \text{H}_2\text{O}$ .....	9m	52
Silver sulfate, $\text{Ag}_2\text{SO}_4$ .....	13m	37	Sodium hydroxide, $\text{NaOH}$ at 300 °C ..	4m	69
Silver sulfide (acanthite), $\text{Ag}_2\text{S}$ ..	10	51	Sodium iodate, $\text{NaIO}_3$ .....	7	47
Silver terbium, $\text{AgTb}$ .....	5m	74	Sodium iodate, $\text{NaIO}_4$ .....	7	48
Silver thiocyanate, $\text{AgCNS}$ .....	16m	62	Sodium iodate hydrate, $\text{NaIO}_3 \cdot \text{H}_2\text{O}$ ..	17m	73
Silver thulium, $\text{AgTm}$ .....	5m	74	Sodium iodide, $\text{NaI}$ .....	4	31
Silver yttrium, $\text{AgY}$ .....	5m	75			
Sodium, Na .....	9m	105			
Sodium aluminum chloride silicate, sodalite, $\text{Na}_8\text{Al}_6\text{Cl}_2(\text{SiO}_4)_6$ .....	7m	158			
Sodium aluminum fluoride (chiolite), $\text{Na}_5\text{Al}_3\text{F}_{14}$ .....	16m	63			
Sodium aluminum sulfate hydrate (soda alum), $\text{NaAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ ....	15m	68			
Sodium azide, $\alpha\text{-NaN}_3$ , at -90 to -100 °C .....	8m	129			
Sodium azide, $\beta\text{-NaN}_3$ .....	8m	130			
Sodium beryllium calcium aluminum fluoride oxide silicate, meliphanite, $(\text{Na}_{0.63}\text{Ca}_{1.37})\text{Be}(\text{Al}_{0.13}\text{Si}_{1.87})$ $(\text{F}_{0.75}\text{O}_{6.25})$ .....	8m	135			

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Sodium iron fluoride, $\text{Na}_3\text{FeF}_6$ .....	9m	54	Strontium aluminum oxide, $\text{Sr}_3\text{Al}_2\text{O}_6$	10m	52
Sodium lanthanum fluoride silicate, $(\text{Na}_2\text{La}_8)\text{F}_2(\text{SiO}_4)_6$ .....	7m	64	Strontium arsenate, $\text{Sr}_3(\text{AsO}_4)_2$ .....	2m	36
Sodium lanthanum molybdenum oxide, $\text{NaLa}(\text{MoO}_4)_2$ .....	10m	49	Strontium azide, $\text{Sr}(\text{N}_3)_2$ .....	8m	146
Sodium magnesium aluminum boron hydroxide silicate, dravite, $\text{NaMg}_3\text{Al}_6\text{B}_3(\text{OH})_4\text{Si}_6\text{O}_{27}$ .....	3m	47	Strontium borate, $\text{SrB}_2\text{O}_4$ .....	3m	53
Sodium magnesium carbonate (eitelite), $\text{Na}_2\text{Mg}(\text{CO}_3)_2$ .....	11m	56	Strontium borate, $\text{SrB}_4\text{O}_7$ .....	4m	36
Sodium magnesium sulfate (vanthoffite), $\text{Na}_6\text{Mg}(\text{SO}_4)_4$ .....	15m	72	Strontium bromate hydrate, $\text{Sr}(\text{BrO}_3)_2 \cdot \text{H}_2\text{O}$ .....	17m	76
Sodium magnesium sulfate hydrate, bloedite, $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ .....	6m	63	Strontium bromide fluoride, $\text{SrBrF}$	10m	54
Sodium magnesium sulfate hydrate (loewite), $\text{Na}_{12}\text{Mg}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$	14m	35	Strontium bromide hydrate, $\text{SrBr}_2 \cdot 6\text{H}_2\text{O}$ .....	4	60
Sodium manganese(II) fluoride, $\text{NaMnF}_3$ .....	6m	65	Strontium carbonate (strontianite), $\text{SrCO}_3$ .....	3	56
Sodium manganese sulfate hydrate, $\text{Na}_{12}\text{Mn}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$ .....	14m	37	Strontium chloride, $\text{SrCl}_2$ .....	4	40
Sodium mercury(II) chloride hydrate, $\text{NaHgCl}_3 \cdot 2\text{H}_2\text{O}$ .....	6m	66	Strontium chloride fluoride, $\text{SrClF}$	10m	55
Sodium molybdenum oxide, $\text{Na}_2\text{MoO}_4$ ..	1m	46	Strontium chloride hydrate, $\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$ .....	11m	58
Sodium molybdenum oxide, $\text{Na}_2\text{Mo}_2\text{O}_7$	9m	110	Strontium chloride hydrate, $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ .....	4	58
Sodium neodymium fluoride silicate, $(\text{Na}_2\text{Nd}_8)\text{F}_2(\text{SiO}_4)_6$ .....	7m	66	Strontium chloride hydroxide phosphate, $\text{Sr}_5\text{Cl}_{.65}(\text{OH})_{.35}(\text{PO}_4)_3$	11m	60
Sodium nickel(II) sulfate hydrate, $\text{Na}_2\text{Ni}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ .....	6m	68	Strontium chromium oxide, $\text{SrCr}_2\text{O}_7$ .....	17m	77
Sodium nitrate (soda niter), $\text{NaNO}_3$	6	50	Strontium chromium oxide, $\text{Sr}_2\text{CrO}_4$	16m	71
Sodium nitrite, $\text{NaNO}_2$ .....	4	62	Strontium chromium oxide hydrate, $\text{SrCr}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$ .....	17m	79
Sodium oxide, $\text{Na}_2\text{O}$ .....	10m	134	Strontium fluoride, $\text{SrF}_2$ .....	5	67
Sodium phosphate, $\text{Na}_3\text{P}_3\text{O}_9$ .....	3m	49	Strontium hydroxide, $\text{Sr}(\text{OH})_2$ .....	13m	41
Sodium phosphate hydrate, $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$ .....	3m	50	Strontium hydroxide hydrate, $\text{Sr}(\text{OH})_2 \cdot \text{H}_2\text{O}$ .....	13m	42
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Sodium phosphate hydrate, $\text{Na}_6\text{P}_6\text{O}_{18} \cdot 6\text{H}_2\text{O}$ .....	5m	54	Strontium iodide hydrate, $\text{SrI}_2 \cdot 6\text{H}_2\text{O}$ .....	8	58
Sodium praseodymium fluoride silicate, $(\text{Na}_2\text{Pr}_8)\text{F}_2(\text{SiO}_4)_6$ .....	7m	68	Strontium manganese oxide, $\text{SrMnO}_3$ (cubic) .....	10m	56
Sodium selenate, $\text{Na}_2\text{SeO}_4$ .....	9m	55	Strontium manganese oxide, $\text{SrMnO}_3$ (hexagonal) .....	10m	58
Sodium selenide, $\text{Na}_2\text{Se}$ .....	10m	135	Strontium molybdenum oxide, $\text{SrMoO}_4$	7	50
Sodium silicate, $\alpha$ (III), $\text{Na}_2\text{Si}_2\text{O}_5$	8m	141	Strontium nitrate, $\text{Sr}(\text{NO}_3)_2$ .....	12m	31
Sodium silicate, $\beta\text{-Na}_2\text{Si}_2\text{O}_5$ .....	10m	136	Strontium oxide, $\text{SrO}$ .....	5	68
Sodium silicon fluoride (malladrite), $\text{Na}_2\text{SiF}_6$ .....	16m	68	Strontium oxide, $\text{SrO}_2$ .....	6	52
Sodium sulfate, $\text{Na}_2\text{SO}_4$ .....	11m	57	Strontium oxide hydrate, $\text{SrO}_2 \cdot 8\text{H}_2\text{O}$	11m	61
Sodium sulfate (thenardite), $\text{Na}_2\text{SO}_4$	2	59	Strontium phosphate, $\alpha\text{-Sr}_2\text{P}_2\text{O}_7$ .....	11m	62
Sodium sulfate hydrate, $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ .....	17m	74	Strontium phosphate, $\alpha\text{-Sr}_3(\text{PO}_4)_2$	11m	64
Sodium sulfide, $\text{Na}_2\text{S}$ .....	10m	140	Strontium scandium oxide hydrate, $\text{Sr}_3\text{Sc}_2\text{O}_6 \cdot 6\text{H}_2\text{O}$ .....	6m	78
Sodium sulfite, $\text{Na}_2\text{SO}_3$ .....	3	60	Strontium silicate, $\text{Sr}_3\text{SiO}_5$ .....	13m	44
Sodium telluride, $\text{Na}_2\text{Te}$ .....	10m	141	Strontium sulfate (celestite), $\text{SrSO}_4$ .....	2	61
Sodium tin fluoride, $\text{NaSn}_2\text{F}_5$ .....	7m	166	Strontium sulfide, $\text{SrS}$ .....	7	52
Sodium titanium oxide, $\text{Na}_2\text{Ti}_3\text{O}_7$ ..	16m	69	Strontium telluride, $\text{SrTe}$ .....	4m	69
Sodium tungsten oxide, $\text{Na}_2\text{WO}_4$ .....	1m	47	Strontium tin oxide, $\text{SrSnO}_3$ .....	8m	80
Sodium tungsten(VI) oxide hydrate, $\text{Na}_2\text{WO}_4 \cdot 2\text{H}_2\text{O}$ .....	2m	33	Strontium titanium oxide, $\text{SrTiO}_3$ ..	3	44
Sodium zinc fluoride, $\text{NaZnF}_3$ .....	6m	74	Strontium tungsten oxide, $\text{SrWO}_4$ ..	7	53
Sodium zinc sulfate hydrate, $\text{Na}_2\text{Zn}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ .....	6m	72	Strontium tungsten oxide, $\text{Sr}_2\text{WO}_5$ ..	12m	32
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Thallium(I) sulfate, Tl <sub>2</sub> SO <sub>4</sub> .....	6	59	Ytterbium telluride, YbTe .....	5m	79
Thallium(I) thiocyanate, TlCNS ....	8	63	Ytterbium(III) vanadium oxide, YbVO <sub>4</sub> .....	5m	58
Thallium tin chloride, Tl <sub>2</sub> SnCl <sub>6</sub> ...	6	54	Yttrium arsenate, YAsO <sub>4</sub> .....	2m	39
Thallium(I) tungsten oxide, Tl <sub>2</sub> WO <sub>4</sub>	1m	48	Yttrium arsenide, YAs .....	4m	74
Thallium zinc sulfate hydrate, Tl <sub>2</sub> Zn(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	7m	80	Yttrium chloride oxide, YClO .....	1m	51
Thorium arsenide, ThAs .....	4m	70	Yttrium oxide, Y <sub>2</sub> O <sub>3</sub> .....	3	28
Thorium oxide (thorianite), ThO <sub>2</sub> ..	1	57	Yttrium phosphate (xenotime), YPO <sub>4</sub>	8	67
			Yttrium sulfide, YS .....	5m	80
			Yttrium telluride, YTe .....	4m	75
			Yttrium titanium oxide, Y <sub>2</sub> TiO <sub>5</sub> ....	11m	113
			Yttrium vanadium oxide, YVO <sub>4</sub> .....	5m	59
			Zinc, Zn .....	1	16
			Zinc aluminum oxide (gahnite), ZnAl <sub>2</sub> O <sub>4</sub> .....	2	38
			Zinc ammine bromide, Zn(NH <sub>3</sub> ) <sub>2</sub> Br <sub>2</sub>	11m	68
			Zinc ammine chloride, Zn(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	10m	59
			Zinc antimony oxide, ZnSb <sub>2</sub> O <sub>4</sub> .....	4m	39
			Zinc borate, Zn <sub>4</sub> B <sub>6</sub> O <sub>13</sub> .....	13m	48
			Zinc carbonate, smithsonite, ZnCO <sub>3</sub>	8	69
			Zinc chlorate hydrate, Zn(ClO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O .....	16m	79
			Zinc chromium oxide, ZnCr <sub>2</sub> O <sub>4</sub> .....	9m	59
			Zinc cobalt oxide, ZnCo <sub>2</sub> O <sub>4</sub> .....	10m	60

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Zinc cyanide, $Zn(CN)_2$ .....	5	73
Zinc fluoride, $ZnF_2$ .....	6	60
Zinc fluoride hydrate, $ZnF_2 \cdot 4H_2O$ ..	11m	69
Zinc germanium oxide, $Zn_2GeO_4$ .....	10	56
Zinc hydroxide silicate hydrate, hemimorphite, $Zn_4(OH)_2Si_2O_7 \cdot H_2O$ ..	2	62
Zinc iodide, $ZnI_2$ .....	9	60
Zinc iron oxide (franklinite), $ZnFe_2O_4$ .....	9m	60
Zinc manganese oxide (hetaerolite), $ZnMn_2O_4$ .....	10m	61
Zinc molybdenum oxide, $Zn_2Mo_3O_8$ ...	7m	173
Zinc nitrate hydrate, $\alpha$ - $Zn(NO_3)_2 \cdot 6H_2O$ .....	12m	36
Zinc oxide (zincite), $ZnO$ .....	2	25
Zinc phosphate, $\alpha$ - $Zn_3(PO_4)_2$ .....	16m	80
Zinc phosphate, $\beta$ - $Zn_3(PO_4)_2$ .....	16m	81
Zinc phosphate, $\gamma$ - $Zn_3(PO_4)_2$ .....	16m	83
Zinc phosphate hydrate (hopeite), $Zn_3(PO_4)_2 \cdot 4H_2O$ .....	16m	85
Zinc selenide, $ZnSe$ .....	3	23
Zinc silicate (willemite), $Zn_2SiO_4$	7	62
Zinc silicon fluoride hydrate, $ZnSiF_6 \cdot 6H_2O$ .....	8	70
Zinc sulfate (zinkosite), $ZnSO_4$ ...	7	64
Zinc sulfate hydrate (goslarite), $ZnSO_4 \cdot 7H_2O$ .....	8	71
Zinc sulfide (wurtzite), $\alpha$ - $ZnS$ (hexagonal) .....	2	14
Zinc sulfide (sphaelerite), $\beta$ - $ZnS$ (cubic) .....	2	16
Zinc telluride, $ZnTe$ .....	3m	58
Zinc tin oxide, $Zn_2SnO_4$ .....	10m	62
Zinc titanium oxide, $ZnTiO_3$ .....	13m	49
Zinc titanium oxide, $Zn_2TiO_4$ .....	12m	37
Zinc tungsten oxide (sanmartinite), $ZnWO_4$ .....	2m	40
Zirconium, $\alpha$ -Zr .....	2	11
Zirconium hydride, $ZrH_2$ .....	5m	60
Zirconium iodate, $Zr(IO_3)_4$ .....	1m	51
Zirconium nitride, $ZrN$ .....	5m	80
Zirconium oxide, $ZrO$ .....	5m	81
Zirconium phosphide, $ZrP$ .....	4m	75
Zirconium silicate, zircon, $ZrSiO_4$	4	68
Zirconium silicide, $ZrSi_2$ .....	17m	86
Zirconium sulfate hydrate (zircosulfate), $Zr(SO_4)_2 \cdot 4H_2O$ ....	7	66

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C <sub>7</sub> H <sub>5</sub> ClO <sub>2</sub>	m-Chlorobenzoic acid	16m	30
C <sub>7</sub> H <sub>5</sub> FO <sub>2</sub>	p-Fluorobenzoic acid	16m	36
C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub> S	Methyl sulfonanilide	9m	78
C <sub>7</sub> H <sub>12</sub> O <sub>4</sub>	Pimelic acid	7m	153
C <sub>8</sub> H <sub>4</sub> Hg <sub>2</sub> O <sub>4</sub>	Mercury o-phthalate	10m	113
C <sub>8</sub> H <sub>5</sub> KO <sub>4</sub>	Potassium hydrogen o-phthalate	4m	30
C <sub>8</sub> H <sub>5</sub> O <sub>4</sub> Tl	Thallium hydrogen phthalate	16m	75
C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>7</sub>	2,4,6-Trinitrophenetole	8m	152
C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	p-Anisic acid	16m	11
C <sub>8</sub> H <sub>9</sub> NO	Acetanilide (calc. pattern)	14m	38
C <sub>8</sub> H <sub>9</sub> NO	Acetanilide	16m	7
C <sub>8</sub> H <sub>11</sub> N <sub>2</sub> NaO <sub>3</sub>	Sodium barbital	16m	157
C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	Barbital, form I	15m	126
C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	Barbital, form II	15m	128
C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	Barbital, form IV	15m	130
C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	Metharbital	15m	177
C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	Allobarbital	14m	41
C <sub>10</sub> H <sub>16</sub> ClNO	(-)-Ephedrine hydrochloride	16m	124
C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	Vinbarbital, form I	16m	162
C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	Amobarbital, form I	15m	114
C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	Amobarbital, form II	15m	117
C <sub>12</sub> H <sub>10</sub> N <sub>2</sub>	Azobenzene	7m	86
C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	Phenobarbital, form III	16m	144
C <sub>12</sub> H <sub>16</sub> Cl <sub>2</sub> CuN <sub>8</sub>	Copper tetrapyrazole chloride	8m	31
C <sub>12</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>8</sub> Ni	Nickel tetrapyrazole chloride	8m	44
C <sub>12</sub> H <sub>16</sub> CuN <sub>10</sub> O <sub>6</sub>	Copper tetraimidazole nitrate	13m	24
C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>	(N,N)-Dimethyltryptamine	14m	109
C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O	Bufotenine	15m	133
C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O	Psilocin	16m	152
C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	Sucrose	11m	66
C <sub>12</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>	Hexamethylenediammonium adipate	7m	121
C <sub>13</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>2</sub>	Procaine hydrochloride	16m	149
C <sub>13</sub> H <sub>21</sub> N <sub>2</sub> O <sub>4</sub> P	Psilocybin methanolate	16m	154
C <sub>14</sub> H <sub>11</sub> FO	4-Acetyl-2'-fluorodiphenyl	8m	91
C <sub>14</sub> H <sub>20</sub> ClN <sub>3</sub> S	Methapyrilene hydrochloride	14m	112
C <sub>15</sub> H <sub>12</sub> O <sub>2</sub>	Dibenzoylmethane	7m	115
C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O	Diazepam	14m	106
C <sub>16</sub> H <sub>13</sub> N	N-Phenyl-2-naphthylamine	6m	29
C <sub>17</sub> H <sub>19</sub> ClN <sub>2</sub> S	Chlorpromazine	14m	60
C <sub>17</sub> H <sub>20</sub> ClNO <sub>3</sub> ·3H <sub>2</sub> O	Morphine hydrochloride hydrate	16m	133
C <sub>17</sub> H <sub>22</sub> ClNO <sub>4</sub>	L-Cocaine hydrochloride	16m	114
C <sub>17</sub> H <sub>26</sub> ClN	Phencyclidine hydrochloride	16m	141
C <sub>18</sub> H <sub>22</sub> BrNO <sub>3</sub> ·2H <sub>2</sub> O	Codeine hydrobromide hydrate	16m	117
C <sub>18</sub> H <sub>24</sub> CdN <sub>14</sub> O <sub>6</sub>	Cadmium hexaimidazole nitrate	8m	23
C <sub>18</sub> H <sub>24</sub> N <sub>14</sub> NiO <sub>6</sub>	Nickel hexaimidazole nitrate	7m	27
C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub> S	(+)-Amphetamine sulfate	15m	119
C <sub>19</sub> H <sub>22</sub> ClNO <sub>4</sub> ·2H <sub>2</sub> O	Naloxone hydrochloride hydrate	16m	136
C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O	Cinchonine	17m	26
C <sub>19</sub> H <sub>25</sub> ClN <sub>2</sub>	Imipramine hydrochloride	16m	129
C <sub>20</sub> H <sub>26</sub> ClNO <sub>3</sub>	Benactyzine hydrochloride	16m	92
C <sub>20</sub> H <sub>34</sub>	α-Dihydrophylloladene, hartite (or bombiccite)	16m	122
C <sub>21</sub> H <sub>23</sub> ClFNO <sub>2</sub>	Haloperidol	16m	127
C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>	Cannabidiol	16m	111
C <sub>22</sub> H <sub>25</sub> ClN <sub>2</sub> OS·2H <sub>2</sub> O	Clopentixol hydrate	17m	28
C <sub>22</sub> H <sub>30</sub> O <sub>4</sub>	Δ <sup>9</sup> -Tetrahydrocannabinolic acid B	16m	160
C <sub>24</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub> Pd	Palladium bis-(N-isopropyl-3-ethylsalicylaldiminate)	7m	144
C <sub>25</sub> H <sub>15</sub> N <sub>6</sub>	N-Methylphenazinium-7,7,8,8-tetracyanoquinodimethanide	7m	146
C <sub>33</sub> H <sub>40</sub> N <sub>2</sub> O <sub>9</sub>	Reserpine	8m	123

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CH <sub>4</sub> N <sub>2</sub> O	Urea	7	61
CH <sub>4</sub> N <sub>2</sub> S	Thiourea	17m	83
CH <sub>5</sub> NO <sub>2</sub>	Ammonium formate	11m	9
CH <sub>5</sub> N <sub>3</sub> ·HCl	Guanidinium chloride	17m	35
CH <sub>5</sub> N <sub>3</sub> S	Thiosemicarbazide	17m	81
C <sub>2</sub> Ag <sub>2</sub> O <sub>4</sub>	Silver oxalate	9m	47
C <sub>2</sub> FeO <sub>4</sub> ·2H <sub>2</sub> O	Iron oxalate hydrate (humboldtine)	10m	24
C <sub>2</sub> HNaO <sub>4</sub> ·H <sub>2</sub> O	Sodium hydrogen oxalate hydrate	17m	72
C <sub>2</sub> H <sub>2</sub> CaO <sub>4</sub>	Calcium formate	8	16
C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> ·2H <sub>2</sub> O	Oxalic acid hydrate	16m	55
C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> Pb	Lead formate	8	30
C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> Sr	Strontium formate	8	55
C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> Sr·2H <sub>2</sub> O	Strontium formate hydrate (orthorhombic)	8	56
C <sub>2</sub> H <sub>3</sub> KO <sub>4</sub>	Potassium formate-formic acid complex	9m	93
C <sub>2</sub> H <sub>3</sub> NaO <sub>2</sub> ·3H <sub>2</sub> O	Sodium acetate hydrate	15m	66
C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	Glyoxime	8m	102
C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	α-Glycine	17m	34
C <sub>2</sub> H <sub>7</sub> NO <sub>2</sub>	Ammonium acetate	8m	95
C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O	Ammonium oxalate hydrate (oxammite)	7	5
C <sub>2</sub> K <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O	Potassium oxalate hydrate	9m	39
C <sub>2</sub> Li <sub>2</sub> O <sub>4</sub>	Lithium oxalate	10m	34
C <sub>2</sub> Na <sub>2</sub> O <sub>4</sub>	Sodium oxalate	6m	70
C <sub>2</sub> O <sub>4</sub> Rb <sub>2</sub> ·H <sub>2</sub> O <sub>2</sub>	Rubidium oxalate perhydrate	9m	102
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	L-Alanine	8m	93
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S	L-Cysteine	11m	86
C <sub>3</sub> H <sub>10</sub> ClN	Trimethylammonium chloride	9m	113
C <sub>4</sub> H <sub>3</sub> KO <sub>8</sub> ·2H <sub>2</sub> O	Potassium hydrogen oxalate hydrate	17m	60
C <sub>4</sub> H <sub>4</sub> CaO <sub>5</sub> ·2H <sub>2</sub> O	Calcium malate hydrate	10m	76
C <sub>4</sub> H <sub>4</sub> KNaO <sub>6</sub> ·4H <sub>2</sub> O	Potassium sodium tartrate hydrate	15m	55
C <sub>4</sub> H <sub>4</sub> NO <sub>8</sub> Y·H <sub>2</sub> O	Ammonium yttrium oxalate hydrate	8m	97
C <sub>4</sub> H <sub>4</sub> Na <sub>2</sub> O <sub>6</sub> ·2H <sub>2</sub> O	Sodium D-tartrate hydrate	11m	110
C <sub>4</sub> H <sub>6</sub> CoO <sub>4</sub> ·4H <sub>2</sub> O	Cobalt acetate hydrate	12m	19
C <sub>4</sub> H <sub>6</sub> Hg <sub>2</sub> O <sub>4</sub>	Mercury acetate	17m	51
C <sub>4</sub> H <sub>6</sub> NiO <sub>4</sub> ·4H <sub>2</sub> O	Nickel acetate hydrate	13m	31
C <sub>4</sub> H <sub>6</sub> O <sub>6</sub>	D-Tartaric acid	7m	168
C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O	Creatinine	15m	31
C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	α-HMX	11m	100
C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	β-HMX	11m	102
C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	Octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine, alpha-	11m	100
C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	Octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine, beta- bis-(o-Dodecacarborane)	11m 6m	102 7
C <sub>4</sub> H <sub>22</sub> B <sub>20</sub>	Uric acid, phase 1 (calc. pattern)	8m	154
C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>	Uric acid, phase 1	16m	78
C <sub>5</sub> H <sub>7</sub> CuNO <sub>4</sub> ·2H <sub>2</sub> O	Copper glutamate hydrate	7m	110
C <sub>5</sub> H <sub>7</sub> NO <sub>4</sub> Zn·2H <sub>2</sub> O	Zinc glutamate hydrate	7m	170
C <sub>5</sub> H <sub>8</sub> NNaO <sub>4</sub> ·H <sub>2</sub> O	Sodium glutamate hydrate	17m	70
C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	β-L-Glutamic acid	17m	32
C <sub>5</sub> H <sub>12</sub> O <sub>4</sub>	Pentaerythritol	17m	55
C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>7</sub>	Picric acid	16m	56
C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	Nicotinic acid	16m	54
C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	γ-Hydroquinone	8m	107
C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>4</sub> Zn	Zinc diimidazole chloride	7m	123
C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ·HCl	Phenylhydrazine hydrochloride	17m	56
C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>	L-Ascorbic acid	8m	99
C <sub>6</sub> H <sub>12</sub> N <sub>4</sub>	Hexamethylenetetramine	17m	37
C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	Dextrose	11m	28
C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	α-D-Glucose	11m	28
C <sub>6</sub> H <sub>15</sub> HoO <sub>12</sub> S <sub>3</sub> ·9H <sub>2</sub> O	Holmium ethylsulfate hydrate	1m	18
C <sub>6</sub> H <sub>15</sub> NdO <sub>12</sub> S <sub>3</sub> ·9H <sub>2</sub> O	Neodymium ethylsulfate hydrate	9	41
C <sub>7</sub> H <sub>5</sub> BrO <sub>2</sub>	o-Bromobenzoic acid	16m	22

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Acetanilide	$C_8H_9NO$ (calc. pattern)	14m	38
Acetanilide	$C_8H_9NO$	16m	7
4-Acetyl-2'-fluorodiphenyl	$C_{14}H_{11}FO$	8m	91
Alanine, L-	$CH_3CHNH_2CO_2H$	8m	93
Allobarbitol	$C_{10}H_{12}N_2O_3$	14m	41
Amobarbital, form I,	$C_{11}H_{18}N_2O_3$	15m	114
Amobarbital, form II	$C_{11}H_{18}N_2O_3$	15m	117
Ammonium acetate	$NH_4 \cdot CH_3CO_2$	8m	95
Ammonium formate	$NH_4HCO_2$	11m	9
Ammonium oxalate hydrate (oxammite)	$(NH_4)_2C_2O_4 \cdot H_2O$	7	5
Ammonium yttrium oxalate hydrate	$NH_4Y(C_2O_4)_2 \cdot H_2O$	8m	97
Amphetamine sulfate, (+)-	$C_{18}H_{28}N_2O_4S$	15m	119
p-Anisic acid	$C_8H_8O_3$	16m	11
Ascorbic acid, L-	$C_6H_8O_6$	8m	99
Azobenzene	$C_6H_5NNC_6H_5$	7m	86
Barbital, form I,	$C_8H_{12}N_2O_3$	15m	126
Barbital, form II,	$C_8H_{12}N_2O_3$	15m	128
Barbital, form IV,	$C_8H_{12}N_2O_3$	15m	130
Benactyzine hydrochloride	$C_{20}H_{26}ClNO_3$	16m	92
o-Bromobenzoic acid	$C_7H_5BrO_2$	16m	22
Bufotenine	$C_{12}H_{16}N_2O$	15m	133
Cadmium hexamidazole nitrate	$Cd(C_3H_4N_2)_6(NO_3)_2$	8m	23
Calcium formate	$Ca(HCO_2)_2$	8	16
Calcium malate hydrate,	$Ca(O_2C)_2(CH_2CHOH) \cdot 2H_2O$	10m	76
Cannabidiol	$C_{21}H_{30}O_2$	16m	111
m-Chlorobenzoic acid	$C_7H_5ClO_2$	16m	30
Chlorpromazine	$C_{17}H_{19}ClN_2S$	14m	60
Cinchonine	$C_{19}H_{22}N_2O$	17m	26
Clophenixol hydrate	$C_{22}H_{25}ClN_2OS \cdot 2H_2O$	17m	28
Cobalt acetate hydrate	$Co(C_2H_3O_2)_2 \cdot 4H_2O$	12m	19
Cocaine hydrochloride, L-	$C_{17}H_{22}ClNO_4$	16m	114
Codeine hydrobromide hydrate	$C_{18}H_{22}BrNO_3 \cdot 2H_2O$	16m	117
Copper glutamate hydrate	$Cu(O_2C)_2(H_2NCHCH_2CH_2) \cdot 2H_2O$	7m	110
Copper tetraimidazole nitrate	$Cu(C_3H_4N_2)_4(NO_3)_2$	13m	24
Copper tetrapyrazole chloride	$Cu(C_3H_4N_2)_4Cl_2$	8m	31
Creatinine	$C_4H_7N_3O$	15m	31
Cysteine, L-	$HSCH_2 \cdot CH(NH_2) \cdot COOH$	11m	86
Dextrose	$C_6H_{12}O_6$	11m	28
Diazepam	$C_{16}H_{13}ClN_2O$	14m	106
Dibenzoylmethane	$(C_6H_5CO)_2CH_2$	7m	115
$\alpha$ -Dihydrophyllocladene, hartite (or bombiccite)	$C_{20}H_{34}$	16m	122
(N,N)-Dimethyltryptamine	$C_{12}H_{16}N_2$	14m	109
bis-(o-Dodecacarborane)	$C_4B_{26}H_{22}$	6m	7
Ephedrine hydrochloride, (-)-	$C_{10}H_{16}ClNO$	16m	124
p-Fluorobenzoic acid	$C_7H_5FO_2$	16m	36
Glucose, $\alpha$ -D-	$C_6H_{12}O_6$	11m	28
Glutamic acid, $\beta$ -L-	$C_5H_9NO_4$	17m	32
$\alpha$ -Glycine	$C_2H_5NO_2$	17m	34
Glyoxime	$H_2C_2(NO_2)_2$	8m	102
Guanidinium chloride	$CH_5N_3 \cdot HCl$	17m	35
Haloperidol	$C_{21}H_{23}ClFNO_2$	16m	127
Hexamethylenediammonium adipate,	$(CH_2)_4(CO_2H_3N)_2(CH_2)_6$	7m	121
Hexamethylenetetramine	$C_6H_{12}N_4$	17m	37
$\alpha$ -HMX	$C_4H_8N_8O_8$	11m	100
$\beta$ -HMX	$C_4H_8N_8O_8$	11m	102
Holmium ethylsulfate hydrate	$Ho[(C_2H_5)SO_4]_3 \cdot 9H_2O$	1m	18
$\gamma$ -Hydroquinone	$HOC_6H_4OH$	8m	107
Imipramine hydrochloride	$C_{19}H_{25}ClN_2$	16m	129
Iron oxalate hydrate (humboldtine)	$FeC_2O_4 \cdot 2H_2O$	10m	24
Lead formate	$Pb(HCO_2)_2$	8	30
Lithium oxalate	$Li_2C_2O_4$	10m	34

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Mercury o-phthalate	$C_6H_4(CO_2Hg)_2$	10m	113
Methapyrilene hydrochloride,	$C_{14}H_{20}ClN_3S$	14m	112
Metharbital	$C_9H_{14}N_2O_3$	15m	177
Methyl sulfonanilide	$C_6H_5NHSO_2CH_3$	9m	78
N-Methylphenazinium-7,7,8,8-tetra- cyanoquinodimethanide	$C_{25}H_{15}N_6$	7m	146
Morphine hydrochloride hydrate	$C_{17}H_{20}ClNO_3 \cdot 3H_2O$	16m	133
Naloxone hydrochloride hydrate	$C_{19}H_{22}ClNO_4 \cdot 2H_2O$	16m	136
2-Naphthylamine, N-phenyl-	$C_{10}H_7NHC_6H_5$	6m	29
Neodymium ethylsulfate hydrate	$Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$	9	41
Nickel acetate hydrate	$Ni(C_2H_3O_2)_2 \cdot 4H_2O$	13m	31
Nickel hexaimidazole nitrate	$Ni(C_3H_4N_2)_6(NO_3)_2$	7m	27
Nickel tetrapyrazole chloride	$Ni(C_3H_4N_2)_4Cl_2$	8m	44
Nicotinic acid	$C_6H_5NO_2$	16m	54
Octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine ( $\alpha$ -HMX)	$C_4H_8N_8O_8$	11m	100
Octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine ( $\beta$ -HMX)	$C_4H_8N_8O_8$	11m	102
Oxalic acid hydrate	$C_2H_2O_4 \cdot 2H_2O$	16m	55
Palladium bis-(N-isopropyl-3- ethylsalicylaldiminate),	$Pd(C_{12}H_{16}NO)_2$	7m	144
Pentaerythritol	$C_5H_{12}O_4$	17m	55
Phencyclidine hydrochloride	$C_{17}H_{26}ClN$	16m	141
Phenobarbital, form III	$C_{12}H_{12}N_2O_3$	16m	144
Phenylhydrazine hydrochloride	$C_6H_8N_2 \cdot HCl$	17m	50
Picric acid	$C_6H_3N_3O_7$	16m	56
Pimelic acid	$(CH_2)_5(CO_2H)_2$	7m	153
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Potassium hydrogen oxalate hydrate	$C_4H_3KO_8 \cdot 2H_2O$	17m	60
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Potassium oxalate perhydrate	$K_2C_2O_4 \cdot H_2O_2$	9m	96
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Procaine hydrochloride	$C_{13}H_{21}ClN_2O_2$	16m	149
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Sodium glutamate hydrate	$C_5H_8NNaO_4 \cdot H_2O$	17m	70
Sodium hydrogen oxalate hydrate	$C_2HNaO_4 \cdot H_2O$	17m	72
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$\Delta^9$ -Tetrahydrocannabinolic acid B	$C_{22}H_{30}O_4$	16m	160
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Thiosemicarbazide	$CH_5N_3S$	17m	81
Thiourea	$CH_4N_2S$	17m	83
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Uric acid (phase 1)	$C_5H_4N_4O_3$	16m	78
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\* Natural mineral

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