NBS MONOGRAPH 25–SECTION 18

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

Standard X-ray Diffraction Powder Patterns

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Standard X-ray Diffraction Powder Patterns
Section 18 — Data for 58 Substances

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JCPDS®

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 accompnaying 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.

NBS Publication	Number	NBS Publication	Number
Circular 539, Volume 1	PB 178 902	Monograph 25, Section 1	PB 178 429
Volume 2	PB 178 903	Section 2	PB 178 430
Volume 3	PB 178 904	Section 3	PB 178 431
Volume 4	PB 178 905	Section 4	
Volume 5	PB 178 906	Section 5	
Volume 6	PB 178 907	Section 6	
Volume 7	PB 178 908	Section 7	
Volume 8	PB 178 909	Section 8	PB 194 872
Volume 9	PB 178 910	Section 9	COM 72-50002
Volume 10	PB 178 911	Section 10	COM 72-51079
		Section 11	COM 74-50183
		Section 12	COM 75-50162
		Section 13	PB 254 073
		Section 14	PB 272 372
		Section 15	PB 287 182

Also, until the present supply is exhausted, the following issues are for sale from the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402. Order by given catalog number, and add 25% to the price for other than U.S. mailing.

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ERRATA

Monograph 25

Section 9, pp. 73,74: Much of the data is incorrect. See a corrected pattern in this issue.
Section 15, p. 136: The correct year should be 1970 for the reference to Fletcher et al.
Section 17, p. 41: The color should be light grayish yellowish brown.
p. 62: Under "Structure," the date should be 1967 for reference to Katz and Megaw.
p. 64: Under "References," after J. Appl. Crystallogr., add 2, 89.
p. 70: Under "Synonym," at line 1, delete hydrate.
p. 70: Under "Lattice constants," the value for c should be 5.567.
pp. 103,104: The text is out of order. Page 104 should precede page 103.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 18 --- Data for 58 Substances

by

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and

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Standard x-ray powder diffraction patterns are presented for 58 substances. These experimental patterns, useful for identification, were obtained by diffractometer methods. The lattice constants were refined by least-squares methods, and reflections were assigned Miller indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

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

INTRODUCTION

The Powder Diffraction File (PDF) is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the JCPDS--International Centre for Diffraction Data,[1] the PDF 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 or improved data to the PDF. Our work also aids in the development of diffraction techniques. This report presents information for 58 experimental patterns, and is the twenty-eighth of the series of Standard X-ray Diffraction Powder Patterns.[2]

EXPERIMENTAL POWDER PATTERNS

Names. The nonmenclature follows the current practice of the PDF.

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

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 are selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. All spacing determinations were made using an internal standard mixed with the sample, packed in a shallow holder. 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. 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.

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 10^5 [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 patterns were recorded at 25 ± 1 °C on a diffractometer equipped with a focusing graphite or

[1] 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 Francaise de Minéralogie et de Cristallographie.

[2] See previous page for other published volumes.

lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All data were collected using copper radiation: $\lambda(CuK\alpha_1$, peak) = 1.540598Å [Deslattes and Henins, 1973].

Table 1

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

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

The readings of 2θ were taken at positions about 20% of the way down from the top, and in the center of the peak width. This avoided errors associated with aberrations at the very top of the peaks. The $K\alpha_2$ peaks were occasionally read to assist in establishing a $K\alpha_1$ peak position, but $K\alpha_2$ peaks are 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. In general, if the internal standard correction varied along the length of the pattern, linear interpolations were used.

Structure, lattice constants. The space group symbols are given the short Hermann-Mauguin notation. Also given are the space group numbers listed in the International Tables for X-ray Crystallography, Vol. I [1965].

Orthorhombic cell dimensions are arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants are transformed if necessary in order to follow the convention of Crystal Data [1973]. The lattice constant ratios, a/b, c/b, and c/a, also follow the conventions used for the determinative ratios in Crystal Data [1973].

In most cases, preliminary lattice constants were available in the literature, and were used for the initial indexing and refinement. In cases where such data were not available, other methods were tried. If suitable single crystals were available, the lattice constants were obtained by use of a four-circle diffractometer. Axial ratios and densities from Groth [1908] were sometimes useful. Cell constants were also found in some instances by use of the Visser computer program [1969].

A least squares program [Evans et al., 1963] assigned hkℓ's and refined 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 used. Cell refinement was based only upon $2\theta_{obs}$ values which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{obs}-\theta_{calc})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants published in this series prior to 1973. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

For each d-value, the number of significant figures was derived from the average error in $|2\theta_{obs} - 2\theta_{calc}|$ and the equation $\Delta d/d = -(\cot\theta)\Delta\theta$. With these conditions, the rounded value of d agrees with its appropriate 2θ within the average error in 2θ. The value of Δθ varies with the symmetry and crystallinity of each sample.

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and 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_{20} [de Wolff, 1968] is a criterion for the reliability of the unit cell and indexing. A value of $M_{20} > 10$ will guarantee the essential correctness of the indexing provided there are not more than 2 spurious lines ($X_{20} \leq 2$) [de Wolff, 1968]. In general, patterns reported in this publication had $M_{20} > 20$ and X = 0. M_{20} is reported if a cell was derived only through computer indexing from powder data, without further confirmation.

The accuracy and completeness of measured interplanar spacings is conveniently reported as F_N [Smith and Snyder, 1979]. The format used in this publication is F_N = overall value ($|\overline{\Delta 2\theta}|$, N_{poss}), 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" is the figure of merit, F_N, as defined by Smith and Snyder [1979], and $|\overline{\Delta 2\theta}|^N$ is the average absolute magnitude of discrepancy between observed and calculated 2θ values for each reported $hk\ell$. N_{poss} is the number of diffraction lines allowed in the space group, up to the N^{th} observed and indexed line. Co-positional lines such as the cubic 221 and 300 are counted as one possible line.

Intensity measurements. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentage of the strongest line. It has been found that samples which give satisfactory intensity patterns usually have an average particle size smaller than 10 μm, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (see Figure 2). As a general practice, approximately 50 volume percent of finely ground silica-gel was added as a diluent. Occasionally, a rotating sample holder was used.

As a check on reproducibility, each sample was mounted at least 3 times. The intensity values were determined for each of the mountings. The reported I^{rel} value for each observed spacing is the average of 3 or more observations and is rounded to the nearest integer. Theta-compensating (variable divergence) slits were sometimes used to gather the intensity data. In that case, the average I(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 estimated standard deviation, σ, in the relative intensity values was calculated from the values of the five strongest lines, excluding the line with $I^{rel}=100$.

$$\sigma_i^2 = \frac{1}{n-1} \sum_{k=1}^{n} \left(I_i^{rel}(k) - \langle I \rangle_i\right)^2$$

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.

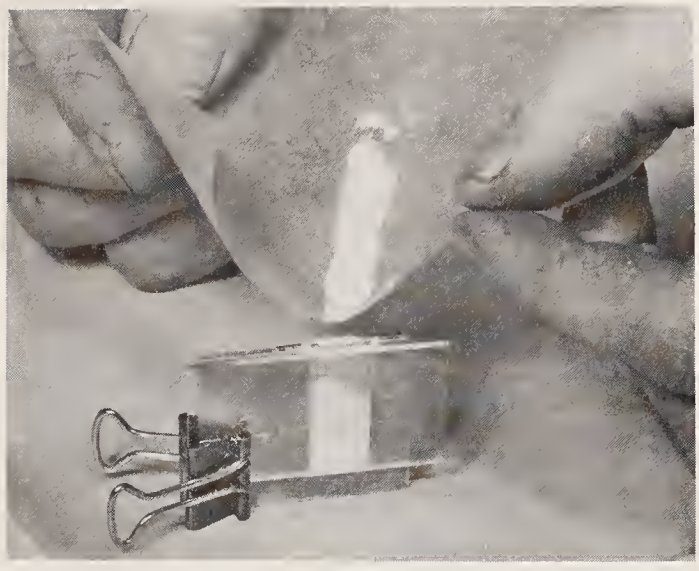

Figure 1.

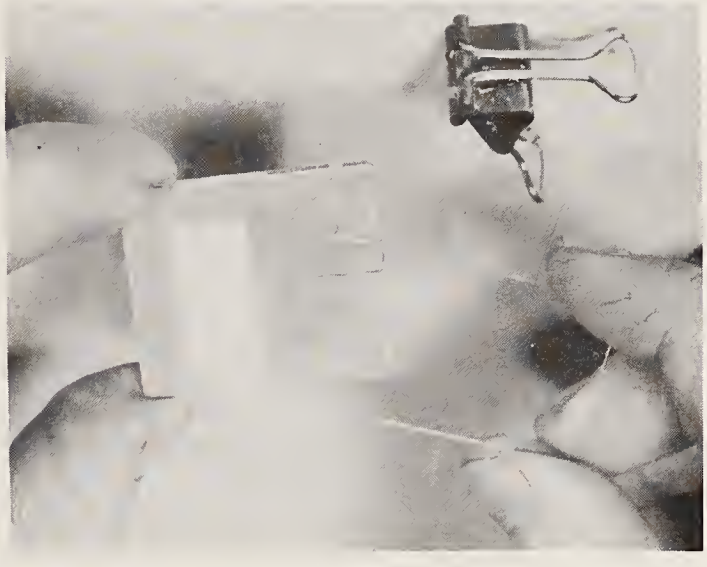

Figure 2.

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

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

Reference intensity ratio, $I/I_{corundum}$

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 113 (hexagonal) reflection of corundum (α-Al_2O_3) [Visser and de Wolff, 1964]. In this publication the ratios I/I_c are tabulated for copper $K\alpha_1$ radiation, for a 1:1 mixture by weight of the sample and corundum. I/I_c was determined only for very common phases.

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 2θ, to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{I(h_o)}{I_c(113)} = \frac{X_c}{X_s} \cdot \frac{I_c^{rel}(\underline{k})}{I^{rel}(\underline{h})} \cdot \frac{I(\underline{h})}{I_c(\underline{k})}$$

where (h_o) indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection (h_o) 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 yielded, the tabulated average $\langle I/I_c \rangle$. From these data, the standard deviation, σ, was obtained from

$$\sigma^2 = \frac{\sum_{i=1}^{n} \left((I/I_c)_i - \langle I/I_c \rangle \right)^2}{n(n-1)}$$

where $\underline{n}$ was the number of measurements of the reference intensity ratio. The standard deviation in the least significant figures is given in parentheses.

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

UNITS

In this publication the Ångström unit (1Å = 100 pm) was selected for presentation of the d-spacings and lattice parameters. This maintained consistency with (a) the earlier publications of Standard X-ray Diffraction Powder Patterns (Circular 539 and Monograph 25), (b) the publications of the International Union of Crystallography, and (c) the continuing publication of cards and search manuals of the PDF (now consisting of over 35,000 entries). The PDF search manuals are based on the d-spacings in Å of the 3 strongest lines. Consistent with the choice of the Å unit for length, the volume of the unit cell is expressed in $Å^3$ ($1Å^3 = 1 \times 10^{-30}$ m^3). Densities are reported in g/cm^3 ($1\ gm/cm^3 = 10^3\ kg/m^3$).

ACKNOWLEDGMENTS

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Aluminum Iron, AlFe

Synonym
Iron aluminum

CAS registry no.
12042-17-0

Sample
The sample was obtained from the Metallurgy Section of the National Bureau of Standards. It had been heated to 800 °C for 5 days and cooled to room temperature in 4 days.

Color
Dark gray

Structure
Cubic, Pm3m (221), Z = 1. The structure was determined by Bradley and Jay [1932].

Lattice constant of this sample
$a = 2.8954(2)$ Å

Volume
24.274 Å^3

Density
(calculated) 5.666 g/cm^3

Figure of merit
$F_{10} = 52.9(0.017,11)$

Additional pattern
PDF card 1-1257 [Hanawalt et al. 1938]

References
Bradley, A. J. and Jay, A. H. (1932). Proc. Roy. Soc. Ser. A, 136, 210.

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

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
2.899	8	1 0 0	30.82
2.048	100	1 1 0	44.18
1.6722	3	1 1 1	54.86
1.4472	13	2 0 0	64.32
1.2949	2	2 1 0	73.01
1.1820	24	2 1 1	81.34
1.0238	8	2 2 0	97.59
.9650	1	3 0 0	105.92
.9157	9	3 1 0	114.54
.8358	4	2 2 2	134.33

Ammonium Cerium Nitrate, $(NH_4)_2Ce(NO_3)_6$

Synonym
Diammonium hexanitratocerate

CAS registry no.
16774-21-3

Sample
The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ. The material is a strong oxidant, deliquescent, and unstable, causing some inconsistency in intensity measurements.

Color
Unground, vivid orange
Ground, vivid yellow

Structure
Monoclinic, $P2_1/n$ (14), Z = 2. The structure was determined by Beineke and Delgaudio [1968].

Lattice constants of this sample
a = 13.069(3) Å
b = 6.8461(12)
c = 8.1732(16)
β = 91.36(2)°

a/b = 1.9090
c/b = 1.1938

Volume
731.06 Å^3

Density
(calculated) 2.490 g/cm^3

Figure of merit
F_{30} = 42.9(0.016,43)

Reference
Beineke, T. A. and Delgaudio, J. (1968). Inorg. Chem. 7, 715.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±6	hkℓ	2θ(°)
7.00	100	-1 0 1	12.63
6.87	75	1 0 1	12.88
6.54	58	2 0 0	13.53
6.07	78	1 1 0	14.59
5.248	72	0 1 1	16.88
4.902	6	-1 1 1	18.08
4.849	5	1 1 1	18.28
4.731	3	2 1 0	18.74
4.122	38	-2 1 1	21.54
4.064	46	2 1 1	21.85
3.879	6	-3 0 1	22.91
3.807	5	3 0 1	23.35
3.676	27	3 1 0	24.19
3.511	9	0 1 2	25.35
3.408	26	-1 1 2	26.13
3.375M	23	-3 1 1	26.39
3.375M		1 1 2	26.39
3.328	6	3 1 1	26.77
3.269	3	4 0 0	27.26
3.160	1L	0 2 1	28.22
3.116	23	-2 1 2	28.62
3.068	28	2 1 2	29.08
3.032	9	2 2 0	29.44
2.946	15	4 1 0	30.31
2.852	1	-2 2 1	31.34
2.791	9	-4 1 1	32.04
2.757M	6	-3 1 2	32.45
2.757M		4 1 1	32.45
2.703	11	3 1 2	33.11
2.654	11	1 0 3	33.75
2.623	8	0 2 2	34.16
2.579M	13	-4 0 2	34.76
2.579M		-1 2 2	34.76
2.566M	17	-3 2 1	34.94
2.566M		1 2 2	34.94
2.545	11	3 2 1	35.24
2.471	11	5 0 1	36.33
2.447	23	-2 2 2	36.69
2.441	21	5 1 0	36.79
2.421	23	2 2 2	37.10
2.377	22	-2 1 3	37.81
2.364	23	4 2 0	38.04
2.343	15	2 1 3	38.39
2.335	11	-3 0 3	38.53
2.285	8	3 0 3	39.40
2.279	6	-4 2 1	39.51
2.260	6	4 2 1	39.86
2.248	15	1 3 0	40.08
2.197	6	0 3 1	41.04
2.177	7	6 0 0	41.44
2.132	3	0 2 3	42.37
2.110	15	-1 2 3	42.83
2.098	10	1 2 3	43.09
2.077M	10	2 3 1	43.53
2.077M		5 2 0	43.53
2.060	7	-4 2 2	43.92
2.031	12	4 2 2	44.57
2.021+	33	-5 2 1	44.80
2.021+		3 3 0	44.80
2.000	11	6 1 1	45.30

d(Å)	I^{rel} $\sigma = \pm 6$	hkℓ	2θ(°)
1.978	8	4 1 3	45.83
1.965M	10	-3 3 1	46.15
1.965M		1 3 2	46.15
1.941M	5	-1 1 4	46.76
1.941M		-6 0 2	46.76
1.929M	10	1 1 4	47.07
1.929M		-3 2 3	47.07
1.901M	8	3 2 3	47.82
1.901M		2 3 2	47.82
1.864M	4	5 0 3	48.83
1.864M		2 1 4	48.83
1.836	6	6 2 0	49.61
1.829M	8	-7 0 1	49.83
1.829M		-4 3 1	49.83
1.818	10	4 3 1	50.14
1.800+	10	-4 2 3	50.68
1.800+		-6 2 1	50.68
1.770M	8	3 1 4	51.59
1.770M		4 2 3	51.59
1.7484	6	0 3 3	52.28
1.7135	4	4 0 4	53.43
1.7096	3	-4 3 2	53.56
1.7026	2	-2 2 4	53.80
1.6835	4	2 3 3	54.46
1.6671	5	-5 2 3	55.04
1.6615+	9	4 1 4	55.24
1.6615+		-7 1 2	55.24
1.6557	5	2 4 0	55.45

Ammonium Tin Fluoride, NH_4SnF_3

Synonyms
Ammonium fluorostannite
Ammonium tin trifluoride
Ammonium trifluorostannate

Sample
The sample was obtained from ICN Pharmaceuticals, Inc., Plainview, NY.

Color
Pale yellow green

Optical data
Uniaxial (+) $N_\varepsilon = 1.564$, $N_o = 1.536$

Structure
Hexagonal, R*, Z = 6. The cell was measured on a single crystal diffractometer by V. Himes at NBS. The value of Z was assumed from the reported density. Donaldson and O'Donoghue [1964] reported this phase as being orthorhombic.

Lattice constants of this sample
a = 6.8426(9) Å
c = 15.925(3)

c/a = 2.3273

Volume
645.73 Å^3

Density
(calculated) 2.989 g/cm^3

Figure of merit
$F_{30} = 61.2(0.013,38)$

Additional pattern
PDF card 16-747 [Donaldson and O'Donoghue, 1964]

Reference
Donaldson, J. D. and O'Donoghue, J. D. (1964). J. Chem. Soc. 1964, 271.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±5	hkℓ	2θ(°)
5.559	49	1 0 1	15.93
5.311	100	0 0 3	16.68
4.759	17	0 1 2	18.63
3.422	84	1 1 0	26.02
3.305	70	1 0 4	26.96
2.913	20	0 2 1	30.67
2.877	54	1 1 3	31.06
2.655	1L	0 0 6	33.73
2.377	50	0 2 4	37.81
2.217	16	2 1 1	40.66
2.170	5	2 0 5	41.59
2.154	1	1 2 2	41.90
2.124	17	1 0 7	42.53
2.097	14	1 1 6	43.10
1.975	17	3 0 0	45.92
1.951	39	2 1 4	46.50
1.8865	17	0 1 8	48.20
1.8515	16	3 0 3	49.17
1.8326	3	1 2 5	49.71
1.8045	15	0 2 7	50.54
1.7102	9	2 2 0	53.54
1.6530	8	2 0 8	55.55
1.6357	7	1 3 1	56.19
1.6288	8	2 2 3	56.45
1.5959	17	2 1 7	57.72
1.5854	3	3 0 6	58.14
1.5376	3	1 0 10	60.13
1.5188	9	1 3 4	60.95
1.4878	6	1 2 8	62.36
1.4376	2	2 2 6	64.80
1.4064	6	0 1 11	66.42

Arsenic Bromide, $AsBr_3$

Synonym
Arsenic tribromide

CAS registry no.
7784-33-0

Sample
The sample was obtained from the Alfa Products, Thiokol/Ventron Division, Danvers, MA. The compound decomposed rapidly in the atmosphere. Therefore, both experimental and calculated intensities are reported. Both gave the same 6 strongest lines, but their order was different. The calculated intensities are based on Trotter's structure.

Color
Colorless

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure was determined by Trotter [1965] and Singh and Swaminathan [1967].

Lattice constants of this sample
a = 10.240(3) Å
b = 12.182(2)
c = 4.3226(9)

a/b = 0.8406
c/b = 0.3551

Volume
539.22 $Å^3$

Density
(calculated) 3.896 g/cm^3

Figure of merit
F_{30} = 42.8(0.016,44)

References
Singh, A. K. and Swaminathan, S. (1967). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 124, 375.

Trotter, J. (1965). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 122, 230.

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

d_{obs}	I_{obs}	I_{calc} peaks	hkℓ	$2\theta_{obs}$
7.85	1L	5	1 1 0	11.26
6.09	30	34	0 2 0	14.53
5.242	6	3	1 2 0	16.90
5.128	14	19	2 0 0	17.28
4.719	8	12	2 1 0	18.79
4.077	12	18	0 1 1	21.78
3.980	10	16	1 0 1	22.32
3.917	10	11	2 2 0	22.68
3.783	65	100	1 1 1	23.50
3.527	25	25	0 2 1	25.23
3.335	14	12	1 2 1	26.71
3.290	18	20	3 1 0	27.08
3.185M	35	53	2 1 1	27.99
3.185M			2 3 0	27.99
3.043	100	48	0 4 0	29.33
2.974	70	76	3 2 0	30.02
2.960	40	-	0 3 1	30.17
2.904	65	78	2 2 1	30.76
2.843	55	50	1 3 1	31.44
2.680	10	10	3 0 1	33.41
2.616M	12	9	3 1 1	34.25
2.616M			3 3 0	34.25
2.562M	25	22	2 3 1	35.00
2.562M			4 0 0	35.00
2.504	10	9	4 1 0	35.83
2.419	20	14	1 4 1	37.14
2.370	12	6	1 5 0	37.93
2.273	4	3	3 4 0	39.62
2.237	8	7	3 3 1	40.29
2.202M	6	4	4 0 1	40.96
2.202M			2 5 0	40.96
2.167M	18	17	4 1 1	41.64
2.167M			4 3 0	41.64
2.162	18	16	0 0 2	41.75
2.122	5	2	0 5 1	42.56
2.078	25	13	1 5 1	43.52
2.037	6	3	0 2 2	44.44
2.011	12	8	3 4 1	45.05
1.991M	10	4	1 6 0	45.52
1.991M			2 0 2	45.52
1.983	15	10	3 5 0	45.72
1.961M	20	12	2 5 1	46.27
1.961M			4 4 0	46.27
1.941	8	-	5 2 0	46.76
1.936	12	9	4 3 1	46.90
1.892	8	6	2 2 2	48.05
1.888	8	-	2 6 0	48.15
1.875	6	3	1 3 2	48.51
1.849	14	13	5 0 1	49.23
1.838	8	3	0 6 1	49.55
1.826	6	3	3 0 2	49.89
1.808	16	9	1 6 1	50.42
1.805	14	-	3 1 2	50.51
1.785	6	4	4 4 1	51.12
1.763	35	27	0 4 2	51.82
1.7453	65	47	3 6 0	52.38
1.7294	25	12	2 6 1	52.90
1.7159	8	3	1 7 0	53.35

- Calc. peak unresolved

Barium Aluminum Titanium Oxide, $Ba_{1.23}Al_{2.46}Ti_{5.54}O_{16}$

Sample
The requisite materials were ground up in the ratio of 1m BaO, 1m Al_2O_3 and 4.5m TiO_2, heated at 800 °C for 26 hrs at 1000 °C for 5 days and at 1200 °C for 7 days with periodic grindings.

Color
Grayish white

Structure
Tetragonal, I4/m (87), Z = 1. The compound is of the hollandite structure type. Its unit cell was determined by Roth [1981] on the basis of a related hollandite type phase, whose structure was determined by Sinclair et al. [1980].

Lattice constants of this sample
a = 9.9619(5) Å
c = 2.9242(3)

c/a = 0.2935

Volume
290.20 $Å^3$

Density
(calculated) 4.330 g/cm^3

Figure of merit
F_{30} = 76.8(0.011,35)

References
Roth, R. S. (1981) private communication.

Sinclair, W., McLaughlin, G. M., and Ringwood, A. E. (1980). Acta Crystallogr. B 36, 2913.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
4.973	3	2 0 0	17.82
3.524	21	2 2 0	25.25
3.153	100	3 1 0	28.28
2.805	7	1 0 1	31.88
2.490	3	4 0 0	36.04
2.445	34	2 1 1	36.73
2.228	24	4 2 0	40.45
2.194	39	3 0 1	41.10
2.0082	8	3 2 1	45.11
1.9542	9	5 1 0	46.43
1.8629	25	4 1 1	48.85
1.7603	5	4 4 0	51.90
1.7084	5	5 3 0	53.60
1.6602	20	6 0 0	55.29
1.6462	2	4 3 1	55.80
1.5748	3	6 2 0	58.57
1.5631	30	5 2 1	59.05
1.4618	7	0 0 2	63.60
1.4317	3	1 1 2	65.10
1.4288	6	6 1 1	65.25
1.4087	2	5 5 0	66.30
1.4030	3	2 0 2	66.60
1.3736	21	5 4 1	68.22
1.3260	6	3 1 2	71.03
1.3239	5	6 3 1	71.16
1.3085	8	7 3 0	72.13
1.2798	1L	7 0 1	74.01
1.2609	3	4 0 2	75.31
1.2413	2	3 3 2	76.71
1.2396	2	7 2 1	76.84
1.2224	1	4 2 2	78.12
1.2082	1	8 2 0	79.22
1.1740	4	6 6 0	82.01
1.1707	3	5 1 2	82.29
1.1581	2	7 5 0	83.39
1.1383	2	7 4 1	85.17
1.1136	2	8 4 0	87.53
1.0999	4	9 1 0	88.91
1.0972	6	6 0 2	89.18
1.0830	2	8 3 1	90.67
1.0715	1L	6 2 2	91.93
1.0352	1L	9 0 1	96.16
1.0135	5	9 2 1	98.93

Barium Manganese Oxide, $BaMnO_4$

Synonym
Barium manganate

CAS registry no.
7787-35-1

Sample
The sample was prepared at NBS using the procedure given by Schlesinger and Siems [1924] and Jellinek [1960].

Color
Blackish purple

Structure
Orthorhombic, Pbnm (62), Z = 4, isostructural with $BaSO_4$. The structure was studied by Jellinek [1960].

Lattice constants of this sample
a = 7.3360(9) Å
b = 9.1101(12)
c = 5.4982(9)

a/b = 0.8053
c/b = 0.6035

Volume
367.45 Å^3

Density
(calculated) 4.633 g/cm^3

Figure of merit
F_{30} = 78.6(0.011,36)

Additional pattern
PDF card 1-569 [Hanawalt et al., 1938]

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

Jellinek, F. (1960). J. Inorg. Nucl. Chem. 13, 329.

Schlesinger, H. I. and Siems, H. B. (1924). J. Am. Chem. Soc. 46, 1965.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
5.716	2	1 1 0	15.49
4.560	6	0 2 0	19.45
4.403	13	1 0 1	20.15
3.962	37	1 1 1	22.42
3.870	6	1 2 0	22.96
3.670	35	2 0 0	24.23
3.507	100	0 2 1	25.38
3.402	70	2 1 0	26.17
3.164	100	1 2 1	28.18
2.892	66	2 1 1	30.89
2.858	3	2 2 0	31.27
2.807	13	1 3 0	31.86
2.750	45	0 0 2	32.53
2.535	13	2 2 1	35.38
2.499	3	1 3 1	35.91
2.478	2	1 1 2	36.22
2.361	9	3 1 0	38.09
2.353	11	0 2 2	38.22
2.340	5	2 3 0	38.44
2.277	2	0 4 0	39.55
2.240	20	1 2 2	40.23
2.200	4	2 0 2	41.00
2.174	76	1 4 0	41.51
2.170	75	3 1 1	41.59
2.151	53	2 3 1	41.96
2.138	46	2 1 2	42.23
2.104	13	0 4 1	42.95
1.9642	7	1 3 2	46.18
1.9051	24	3 3 0	47.70
1.8340	6	4 0 0	49.67
1.7982	13	4 1 0	50.73
1.7683	3	1 5 0	51.65
1.7444	3	1 1 3	52.41
1.7058	28	1 4 2	53.69
1.7011M	26	4 2 0	53.85
1.7011M		0 2 3	53.85
1.6838	4	1 5 1	54.45
1.6566	10	1 2 3	55.42
1.6251	4	4 2 1	56.59
1.6136	7	2 1 3	57.03
1.5648M	22	3 3 2	58.98
1.5648M		2 5 1	58.98
1.5422	1	2 2 3	59.93
1.5261	2	4 0 2	60.63
1.5090	5	4 3 1	61.39
1.5050	5	4 1 2	61.57
1.4874M	3	1 5 2	62.38
1.4874M		1 6 0	62.38
1.4616	8	3 5 0	63.61
1.4470	8	4 2 2	64.33
1.4431	9	2 3 3	64.52
1.4350	10	1 6 1	64.93
1.4289	3	4 4 0	65.24
1.4174	4	5 0 1	65.84
1.4119	8	3 5 1	66.13
1.3965M	3	5 2 0	66.95
1.3965M		3 2 3	66.95
1.3823	5	4 4 1	67.73
1.3596	2	2 6 1	69.02
1.3535	5	5 2 1	69.38

Barium Neodymium Titanium Oxide, $BaNd_2Ti_3O_{10}$

Synonym
Barium neodymium titanate

Sample
Stoichiometric amounts of BaO, Nd_2O_3, and TiO_2 were ground together and heated at 1200 °C for one day, then at 1425 °C for 6 days and finally at 1500 °C for 7 days with intermittent grindings.

Color
Very pale violet

Structure
Orthorhombic Amam (63) Z = 4 [Kolar et al., 1981]. The structure is pseudo-orthorhombic, but the true symmetry is monoclinic with a double "c" [Olsen et al., 1981].

Lattice constants of this sample
a = 7.624(1) Å
b = 28.164(3)
c = 3.8654(6)

a/b = 0.2707
c/a = 0.1372

Volume
829.99 $Å^3$

Density
(calculated) 5.838 g/cm^3

Figure of merit
F_{30} = 58.7(0.012,43)

Additional pattern
Kolar et al. [1981]

Reference
Olsen, A., Goodman, P., and Roth, R. S. (1981). Int. Union Crystallogr. Meeting, Ottawa.

Kolar, D., Gaberšček, S., Volavšek, B., Parker, H. S., and Roth, R. S. (1981). J. Solid State Chem. 38, (2), 158.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±5	hkℓ	2θ(°)
14.02	1L	0 2 0	6.30
5.172	1L	1 4 0	17.13
4.687	64	0 6 0	18.92
3.994	9	1 6 0	22.24
3.829	18	0 1 1	23.21
3.811	1L	2 0 0	23.32
3.573	1	0 3 1	24.90
3.520	1L	0 8 0	25.28
3.420	14	1 1 1	26.03
3.239	13	1 3 1	27.52
3.195	23	1 8 0	27.90
3.186	24	0 5 1	27.98
2.958	100	2 6 0	30.19
2.814	13	0 10 0	31.77
2.785	60	0 7 1	32.11
2.701	45	2 1 1	33.14
2.641	8	1 10 0	33.91
2.616	7	1 7 1	34.25
2.587	9	2 8 0	34.65
2.444	5	2 5 1	36.74
2.346	43	0 12 0	38.33
2.318	8	1 9 1	38.82
2.250	41	2 7 1	40.04
2.134	3	0 11 1	42.31
2.118	6	3 1 1	42.65
2.070	8	3 3 1	43.69
2.055	10	1 11 1	44.02
2.051	10	2 9 1	44.12
2.012	51	0 14 0	45.03
1.998	22	2 12 0	45.35
1.9330	18	0 0 2	46.97
1.9069	21	4 0 0	47.65
1.8898M	12	0 13 1	48.11
1.8898M		4 2 0	48.11
1.8351	1L	1 13 1	49.64
1.7873	7	0 6 2	51.06
1.7660	8	4 6 0	51.72
1.7600	6	0 16 0	51.91
1.7572	5	3 9 1	52.00
1.7234M	5	3 12 0	53.10
1.7234M		2 0 2	53.10
1.7153	5	1 16 0	53.37
1.6935M	49	0 8 2	54.11
1.6935M		2 13 1	54.11
1.6352M	7	4 5 1	56.21
1.6352M		3 11 1	56.21
1.6182	24	2 6 2	56.85
1.5979	3	2 16 0	57.64
1.5941	3	0 10 2	57.79
1.5735	20	4 7 1	58.62

d(Å)	I^{rel} $\sigma = \pm 5$	hkℓ	2θ(°)
1.5650	7	0 18 0	58.97
1.5330	4	1 18 0	60.33
1.5231	3	0 17 1	60.76
1.4926M	7	1 17 1	62.14
1.4926M		0 12 2	62.14
1.4797	7	4 12 0	62.74
1.4476M	7	2 18 0	64.30
1.4476M		3 16 0	64.30
1.4079	3	0 20 0	66.34
1.3938	8	0 14 2	67.10
1.3892	10	2 12 2	67.35
1.3841M	22	0 19 1	67.63
1.3841M		4 14 0	67.63
1.3569	8	4 0 2	69.18
1.3421	4	4 13 1	70.05
1.3327M	3	4 4 2	70.62
1.3327M		3 18 0	70.62
1.3213	12	2 20 0	71.32
1.3036	8	4 6 2	72.44
1.3011	10	2 19 1	72.60

Benzidine Hydrochloride, $C_{12}H_{12}N_2 \cdot 2HCl$

Synonym
(1-1-Biphenyl)-4,4-diamine dihydrochloride

CAS registry no.
531-85-1

Sample
The sample was obtained from Mallinckrodt Chemical Co., St. Louis, MO. Only one intensity pattern was made because the compound is carcinogenic.

Color
Colorless

Structure
Triclinic, $P\bar{1}$ (2), Z = 1. The structure was determined by Koo et al. [1942].

Lattice constants of this sample
a = 5.760(2) Å
b = 12.585(3)
c = 4.3533(11)
α = 95.55(3)°
β = 98.67(3)
γ = 101.55(3)

a/b = 0.4577
c/b = 0.3459

Volume
302.86 Å^3

Density
(calculated) 1.409 g/cm^3

Figure of merit
F_{30} = 50.8(0.013,33)

Additional pattern
PDF card 7-744 [Polytechnic Inst. of Brooklyn, Brooklyn, NY, 1955]

Reference
Koo, C. H., Kim, H. S., and Shin, H. S. (1972). Daehan Hwahak Hwoejee (J. Korean Chem. Soc.) 16, 18.

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

d(Å)	I^{rel}	hkℓ	2θ(°)
12.18	10	0 1 0	7.25
5.545	80	1 0 0	15.97
4.689	8	1 1 0	18.91
4.648	16	-1 2 0	19.08
4.263	10	0 0 1	20.82
4.201	30	0 -1 1	21.13
3.870	6	0 1 1	22.96
3.734	100	0 -2 1	23.81
3.583	18	-1 1 1	24.83
3.520	6	-1 -1 1	25.28
3.301	6	0 2 1	26.99
3.208	45	1 -1 1	27.79
3.160	25	0 -3 1	28.22
3.128M	30	1 0 1	28.51
3.128M		-1 -2 1	28.51
3.072	50	1 -2 1	29.04
2.987	14	1 3 0	29.89
2.963	8	-1 4 0	30.14
2.882	10	1 1 1	31.00
2.848	12	-2 1 0	31.38
2.774	25	0 3 1	32.25
2.703	10	-1 -3 1	33.11
2.655	2	0 -4 1	33.73
2.590	6	2 1 0	34.60
2.567	8	1 2 1	34.92
2.538	10	-2 0 1	35.33
2.474	4	1 -4 1	36.28
2.461	8	1 4 0	36.48
2.453	8	-2 2 1	36.61
2.444M	10	0 5 0	36.75
2.444M		-1 5 0	36.75
2.429	4	-2 -1 1	36.98
2.342M	12	2 2 0	38.41
2.342M		0 4 1	38.41
2.249	6	-2 -2 1	40.06
2.172	4	1 -5 1	41.54
2.150	4	0 -1 2	41.99
2.129	8	2 -3 1	42.43
2.120	10	-1 0 2	42.61
2.104	8	-1 -1 2	42.96
2.076	6	1 5 0	43.56
2.056	6	0 1 2	44.00
2.046	10	-2 -3 1	44.24
2.037	10	0 6 0	44.43
2.012M	2	-1 -5 1	45.03
2.012M		0 5 1	45.03
2.003	2	2 -4 1	45.24
1.939	2	0 -6 1	46.82
1.9179M	2	1 -1 2	47.36
1.9179M		-1 -3 2	47.36
1.9103	2	1 -6 1	47.56
1.8850	2	1 0 2	48.24
1.8795	2	-2 5 1	48.39
1.8636	4	2 4 0	48.83
1.8473M	6	-2 6 0	49.29
1.8473M		-2 -4 1	49.29
1.8431M	6	-2 1 2	49.41
1.8431M		-3 1 1	49.41

Beryllium Nitride, Be_3N_2

CAS registry no.
1304-54-7

Sample
The sample was obtained from Brush Beryllium Co., Cleveland, OH. The lattice constant reported here was obtained from a thin sample on a slide smeared with high vacuum grease. The peak positions from a thick sample are shifted to lower angles resulting from the penetration of the beam owing to the unusually low absorption of the sample. For a thick sample an apparent lattice parameter of 8.150 Å would be expected for lines below 100° 2θ.

Color
Light gray

Structure
Cubic, Ia3 (206), Z = 16. The structure was determined by von Stackelberg and Paulus (1933).

Lattic constant of this sample
a = 8.1482(2)Å

Volume
540.98 $Å^3$

Density
(calculated) 2.704 g/cm^3

Polymorphism
There is a hexagonal β-form, prepared by heating the cubic form above 1400 °C.

Figure of merit
F_{30} = 56.3(0.013,41)

Additional pattern
PDF card 4-786 [von Stackelberg and Paulus, 1933]

References
Eckerlin, P. and Rabenau, A. (1960). Z. Anorg. Allgem. Chem. 304, 218.

Stackelberg, von, M. and Paulus, R. (1933). Z. Phys. Chem. Leipzig B22, 305.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
4.072	1L	2 0 0	21.81
3.328	17	2 1 1	26.77
2.351	100	2 2 2	38.25
2.178	5	3 2 1	41.43
2.037	5	4 0 0	44.43
1.9210	1	4 1 1	47.28
1.8223	1L	4 2 0	50.01
1.7367	9	3 3 2	52.66
1.5974	3	4 3 1	57.66
1.4883	1L	5 2 1	62.34
1.4404	36	4 4 0	64.66
1.3973	1L	4 3 3	66.91
1.3216	2	6 1 1	71.30
1.2571	2	5 4 1	75.58
1.2281	10	6 2 2	77.69
1.2015	3	6 3 1	79.75
1.1088	3	7 2 1	88.01
1.0348	2	6 5 1	96.21
1.0186	4	8 0 0	98.26
1.0031	1L	7 4 1	100.34
.9741	1L	6 5 3	104.52
.9604	1L	6 6 0	106.65
.9472	1L	7 4 3	108.82
.9347	5	6 6 2	110.99
.9228	1L	7 5 2	113.18
.8998	1L	8 3 3	117.76
.8890	1L	8 4 2	120.11
.8787	1L	7 6 1	122.49
.8589	1L	7 5 4	127.48
.8404	4	9 3 2	132.87
.8316	12	8 4 4	135.71
.8231	1L	9 4 1	138.75
.8148	1L	8 6 0	141.95
.8068	1	10 1 1	145.42
.7990	1L	10 2 0	149.21

Bismuth Selenide (Paraguanajuatite), Bi_2Se_3

CAS registry no.
12068-69-8

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA.

Color
Unground, gray metallic
Ground, dark gray

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with tetradymite, Bi_2Te_2S. The structure of Bi_2Se_3 was refined by Nakajima [1963], following earlier work by Semiletov and Pinsker [1955].

Lattice constants of this sample
a = 4.1396(4)Å
c = 28.636(4)

c/a = 6.9176

Volume
424.97 Å^3

Density
(calculated) 7.676 g/cm^3

Figure of merit
F_{30} = 54.4(0.012,44)

Additional patterns
PDF card 12-732 [Thompson, R. M., Univ. British Columbia, Vancouver, Canada]

Gobrecht et al. [1964]

Godovikov [1962]

References

Gobrecht, H., Boeters, K.-E., and Pantzer, G. (1964). Z. Phys. 177, 68.

Godovikov, A. A. (1962). Zh. Strukt. Khim. 3, 44.

Nakajima, S. (1963). J. Phys. Chem. Solids 24, 479.

Semiletov, S. A. and Pinsker, Z. G. (1966). Dokl. Akad. Nauk SSSR 100, 1079.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
9.56	7	0 0 3	9.24
4.777	19	0 0 6	18.56
3.559	16	1 0 1	25.00
3.478	3	0 1 2	25.59
3.205	7	1 0 4	27.81
3.183	4	0 0 9	28.01
3.040	100	0 1 5	29.36
2.698	1L	1 0 7	33.18
2.534	2	0 1 8	35.39
2.386	1L	0 0 12	37.67
2.238	26	1 0 10	40.27
2.106	9	0 1 11	42.92
2.070	26	1 1 0	43.70
1.9085	8	0 0 15	47.61
1.8998	8	1 1 6	47.84
1.8780	2	1 0 13	48.43
1.7893	2	0 2 1	51.00
1.7782	1L	2 0 2	51.34
1.7392	2	0 2 4	52.58
1.7349	2	1 1 9	52.72
1.7102	10	2 0 5	53.54
1.6007	3	1 0 16	57.53
1.5909	1	0 0 18	57.92
1.5191	7	0 2 10	60.94
1.4770	1	2 0 11	62.87
1.4029	7	1 1 15	66.61
1.3636	1L	0 0 21	68.79
1.3296	4	0 1 20	70.81
1.3186	7	1 2 5	71.49
1.2667	2	0 2 16	74.91
1.2245	4	2 1 10	77.96
1.2019	3	1 2 11	79.72
1.1950	3	3 0 0	80.27
1.1763	1L	0 1 23	81.82

Calcium Borate, CaB_2O_4

Synonym
Calcium metaborate

CAS registry no.
13701-64-9

Sample
The sample was prepared by fusion of B_2O_3 and $CaCO_3$ using a small excess of fused B_2O_3. The sample was quenched. Later, it was annealed in a sealed platinum tube and held at 945 °C for 31 days, then quenched again.

Color
Colorless

Structure
Orthorhombic, Pnca (60), Z = 4. The structure was determined by Marezio et al. [1963].

Lattice constants of this sample
a = 6.2156(5) Å
b = 11.607(13)
c = 4.2828(6)

a/b = 0.5355
c/b = 0.3690

Volume
308.98 $Å^3$

Density
(calculated) 2.702 g/cm^3

Polymorphism
Calcium borate crystallizes in 4 forms, depending on the pressures used in its synthesis. Form I, described here, exists up to pressures of 12 kbars. Form II occurs at pressures of 12-15 kbars, form III at 15-25 kbars, and form IV at 25-40 kbars [Marezio et al., 1969].

Figure of merit
F_{30} = 55.5(0.013,42)

Reference intensity
$I/I_{corundum}$ = 1.11(2)

Additional patterns
PDF card 18-281 [Stojanovic,Inst. for Refractories, Kraljevo, Yugoslavia]

PDF card 23-407 [Fletcher et al., 1970]

Morris et al. [1978]

References

Fletcher, B. L., Stevenson, J. R., and Whitaker, A. (1970). J. Amer. Ceram. Soc. 53, 95.

Marezio, M., Plettinger, H. A., and Zachariasen, W. H. (1963). Acta Crystallogr. 16, 390.

Marezio, M., Remeika, J. P., and Dernier, P. D. (1969). Acta Crystallogr. 25B, 965.

Morris, M. C., McMurdie, H. F., Evans, E. H., Paretzkin, B., de Groot, J. H., Weeks, B., and Newberry, R. J. (1978). Natl. Bur. Stand. U.S. Monogr. 25, Sec. 15, 136.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
5.809	15	0 2 0	15.24
3.372	38	1 1 1	26.41
3.109	18	2 0 0	28.69
3.002	100	2 1 0	29.74
2.902	16	0 4 0	30.79
2.872	12	0 3 1	31.12
2.739	12	2 2 0	32.67
2.607	27	1 3 1	34.37
2.308	1	2 2 1	38.99
2.241	10	1 4 1	40.21
2.140	25	0 0 2	42.20
2.120	20	2 4 0	42.62
2.040	3	0 5 1	44.38
2.009	8	0 2 2	45.08
1.938	36	1 5 1	46.83
1.9107	6	1 2 2	47.55
1.9009	6	2 4 1	47.81
1.8604	3	2 5 0	48.92
1.8420	26	3 1 1	49.44
1.7641	3	2 0 2	51.78
1.7438	4	2 1 2	52.43
1.7234	3	0 4 2	53.10
1.6959	2	1 6 1	54.03
1.6872	5	2 2 2	54.33
1.6804	6	3 3 1	54.57
1.6424	6	2 6 0	55.94
1.6048	1	2 3 2	57.37
1.5689	1L	3 4 1	58.81
1.5533	1	4 0 0	59.46
1.5465	1	0 7 1	59.75
1.5339	1	2 6 1	60.29
1.5066	8	2 4 2	61.50
1.5006M	11	4 2 0	61.77
1.5006M		1 7 1	61.77
1.4770	1L	3 1 2	62.87

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.4538	1	3 5 1	63.99
1.4418M	1	3 2 2	64.59
1.4418M		4 3 0	64.59
1.3701	1L	4 4 0	68.42
1.3393	1	0 3 3	70.22
1.3143	1	2 8 0	71.76
1.3091	3	1 3 3	72.09
1.3036	5	2 6 2	72.44
1.2392	1	3 7 1	76.87
1.2365	1	4 5 1	77.07
1.2292	2	4 2 2	77.61
1.2114M	4	4 6 0	78.97
1.2114M		1 9 1	78.97
1.1912	5	2 9 0	80.58
1.1874	3	5 1 1	80.89
1.1694M	2	3 1 3	82.40
1.1694M		5 2 1	82.40
1.1608	2	0 10 0	83.15
1.1539	2	4 4 2	83.76
1.1409	1	5 3 1	84.93
1.0877M	1	1 9 2	90.18
1.0877M		2 10 0	90.18
1.0607M	4	3 9 1	93.14
1.0607M		4 8 0	93.14
1.0359M	1	6 0 0	96.08
1.0359M		5 3 2	96.08
1.0318	1L	6 1 0	96.58
1.0197	3	6 2 0	98.12

Calcium Cyanamide, $CaCN_2$

CAS registry no.
27668-50-4

Sample
The sample was from Alfa Products, Thiokol/ Ventron Division, Danvers, MA. The sample contained some graphite and the intensities may be somewhat in error.

Color
Black

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3. The structure of $CaCN_2$ was discussed by Bredig [1942] and Dehlinger [1942]. It was determined by Vannerberg [1962].

Lattice constants of this sample
a = 3.6961(6) Å
c = 14.743(3)

c/a = 3.9888

Volume
174.42 $Å^3$

Density
(calculated) 2.288 g/cm^3

Figure of merit
F_{20} = 43.2(0.018,26)

Additional patterns
PDF card 16-685 [Vannerberg, 1962]

References

Bredig, M. A. (1942). J. Am. Chem. Soc. 64, 1730.

Dehlinger, U. (1942). Z. Kristallogr. Kristallgeometric Kristallphys. Kristallchem. 65, 286.

Vannerberg, N-G. (1962). Acta Chem. Scand. 16, 2263.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
4.916	20	0 0 3	18.03
2.936	100	0 1 2	30.42
2.457	4	0 0 6	36.54
2.416	23	1 0 4	37.19
2.170	21	0 1 5	41.58
1.848	28	1 1 0	49.26
1.759	7	1 0 7	51.94
1.730	6	1 1 3	52.87
1.6389	1	0 0 9	56.07
1.5964	3	0 1 8	57.70
1.5648	7	2 0 2	58.98
1.4764	2	1 1 6	62.90
1.4686	2	0 2 4	63.27
1.4060	3	2 0 5	66.44
1.3390	3	1 0 10	70.24
1.2742	1	0 2 7	74.39
1.2288	1	0 0 12	77.64
1.1942	4	1 2 2	80.34
1.1491	1	2 1 4	84.19
1.1192	1	1 2 5	86.98

Calcium Iron Oxide, $CaFe_2O_4$

Synonym
Calcium ferrate

CAS registry no.
12013-33-1

Sample
The sample was prepared from stoichiometric amounts of $CaCO_3$ and α-Fe_2O_3, blended by grinding in an agate mortar. Initial heat treatments at 600°, 800°, and 900 °C for periods of 20 hrs. were used to drive off CO_2 from the mixture. Successively higher heat treatments at 1050 °C for 6½ days and 1200 °C for 13 days, with periodic grinding were performed to ensure complete reaction.

Color
Unground, dark grayish red
Ground, medium brown

Structure
Orthorhombic, Pnam (62), Z = 4, isomorphous with β-calcium chromite. Structure determinations were made by Hill et al. [1956] and by Decker and Kasper [1957].

Lattice constants of this sample
a = 9.2281(13) Å
b = 10.7052(12)
c = 3.0185(5)

a/b = 0.8620
c/b = 0.2820

Volume
298.19 Å^3

Density
(calculated) 4.806 g/cm^3

Figure of merit
F_{30} = 48.9(0.015,41)

Additional patterns
PDF card 8-100 [Hadfields, Ltd., Sheffield, England]

PDF card 19-219 [Hughes et al., 1967]

Burdese [1952]

Decker and Kasper [1957]

References

Burdese, A. (1952). Ric. Sci. 22, 259.

Decker, B. F. and Kasper, J. S. (1957). Acta Crystallogr. 10, 332.

Hill, P. M., Peiser, H. S., and Rait, J. R. (1956). Acta Crystallogr. 9, 981.

Hughes, H., Roos, P., and Goldring, D. C. (1967). Mineral. Mag. 36, 280.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
5.349	2	0 2 0	16.56
4.612	20	2 0 0	19.23
3.492	9	2 2 0	25.49
3.329	2	1 3 0	26.76
2.956	4	3 1 0	30.21
2.905	6	0 1 1	30.75
2.826	2	2 3 0	31.64
2.770	4	1 1 1	32.29
2.675	85	0 4 0	33.47
2.668	100	3 2 0	33.56
2.572	4	1 4 0	34.85
2.527M	70	1 2 1	35.49
2.527M		2 0 1	35.49
2.331	2	3 3 0	38.59
2.314	2	2 4 0	38.88
2.305M	4	4 0 0	39.05
2.305M		0 3 1	39.05
2.254	4	4 1 0	39.97
2.236	24	1 3 1	40.31
2.118	16	4 2 0	42.66
2.113	20	3 1 1	42.77
2.086	3	1 5 0	43.35
2.061	2	2 3 1	43.90
1.999	2	3 2 1	45.34
1.957	9	1 4 1	46.35
1.942	1	2 5 0	46.73
1.845	12	3 3 1	49.35
1.837	37	2 4 1	49.59
1.832	40	4 0 1	49.72
1.807	10	4 1 1	50.47
1.7581	2	3 5 0	51.97
1.7528	3	1 6 0	52.14
1.7463M	6	4 4 0	52.35
1.7463M		0 5 1	52.35
1.7349	2	4 2 1	52.72
1.6640	10	2 6 0	55.15
1.6325	2	2 5 1	56.31
1.6301	2	4 3 1	56.40
1.5432	12	3 6 0	59.89
1.5376	13	6 0 0	60.13
1.5231	2	6 1 0	60.76
1.5186M	12	5 4 0	60.96
1.5186M		3 5 1	60.96
1.5150	27	1 6 1	61.12
1.5086M	38	0 0 2	61.41

Calcium Iron Oxide, $CaFe_2O_4$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.5086M		1 7 0	61.41
1.4569	5	2 6 1	63.84
1.4410	1L	5 3 1	64.63
1.4352M	1	1 2 2	64.92
1.4352M		2 0 2	64.92
1.4115	1	4 6 0	66.15
1.3860	1L	2 2 2	67.53
1.3747M	2	1 3 2	68.16
1.3747M		3 6 1	68.16
1.3708	1	6 0 1	68.38
1.3499	2	1 7 1	69.59
1.3381	2	0 8 0	70.29
1.3335	5	6 4 0	70.57
1.3276	3	6 2 1	70.93
1.3242	3	1 8 0	71.14
1.3137	14	3 2 2	71.80
1.3015	1L	1 4 2	72.58
1.2850	1L	2 8 0	73.66
1.2795M	2	7 2 0	74.03
1.2795M		6 3 1	74.03
1.2785	2	4 6 1	74.10
1.2642	1L	2 4 2	75.08
1.2487	1	6 5 0	76.18
1.2289	1	4 2 2	77.63
1.2197	1L	6 4 1	78.33
1.2127	1L	1 8 1	78.87

Calcium Sulfate Hydrate (Bassanite), $CaSO_4 \cdot 0.5H_2O$

Synonym
Plaster of Paris

CAS registry no.
10034-76-1

Sample
The sample was prepared at NBS by adding H_2SO_4 to an aqueous solution of $Ca(NO_3)_2$ to form $CaSO_4 \cdot 2H_2O$. The wet fresh material was mixed with concentrated HNO_3, heated at 80 °C, and held there for several days. Extremely fine crystals developed and were bottled while still moist. Just before measurements were taken, the crystals were dried in air at room temperature. The material was somewhat unstable, slowly changing to $CaSO_4 \cdot 2H_2O$ under conditions of high atmospheric humidity.

Consistent intensity data were difficult to obtain. The data here were measured on samples which had been side-drifted into holders, with no further packing or smoothing. Other measurements on packed samples showed different intensities; in particular, the reflection at d=2.807 showed values as low as 19, and at d=1.847, the packed samples had values as low as 29.

Color
Colorless

Structure
Pseudo-orthorhombic, I***, Z = 12. The literature on $CaSO_4 \cdot 0.5H_2O$ is extensive and confusing as noted by Gay [1965] and Clifton [1972]. The cell below was modified from one given by Gay [1965] who stated that the true symmetry was monoclinic, with $\beta \cong 90°$. This NBS cell was also consistent with one found by use of the Visser program and associated refinement procedures. Bushuev [1980] reported a similar monoclinic cell for $CaSO_4 \cdot 0.67H_2O$ with a=12.028, b=38.022, c=6.927, γ=90.21°, space group I2. There was no evidence to require the monoclinic cell for NBS data.

Lattice constants of this sample
a = 12.031(4) Å
b = 12.695(6)
c = 6.934(2)

a/b = 0.9477
c/b = 0.5462

Volume
1059.1 Å^3

Density
(calculated) 2.731 g/cm^3

Polymorphism
Two forms, α and β have been described by several authors, as noted by Clifton [1972]. He concluded that although slight differences have been observed between the properties of the two forms, it could not be conclusively determined whether the differences were sufficiently significant to consider the supposed α and β forms as separate entities.

Figures of merit
F_{30} = 17.6(0.017,99)
M_{20} = 17.6

Additional patterns
PDF card 24-1067 [Rowe and Bigelow, 1972, The University of Michigan]

PDF card 24-1068. The data is attributed to Weiser et al. [1936] but differs from the journal reference quoted.

Powell [1962]

References

Bushuev, N. N. (1980). Dokl. Akad. Nauk. SSSR 225 (No. 5), 1104.

Clifton, J. R. (1972). J. Res. Natl. Bur. Stand. Sect. A 76A, 41.

Gay, P. (1965). Mineral. Mag. 35, 354.

Powell, D. A. (1962). Aust. J. Chem. 15, 868.

Weiser, H. B., Milligan, W. O., and Ekholm, W. C. (1936). J. Amer. Chem. Soc. 58, 1261.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
6.00	70	1 0 1	14.76
4.360M	4	2 2 0	20.35
4.360M		1 2 1	20.35
4.283	2	2 1 1	20.72
3.989	1	1 3 0	22.27
3.826	1	3 1 0	23.23
3.613	1	0 3 1	24.62
3.469M	54	3 0 1	25.66
3.469M		0 0 2	25.66
3.225	1	1 1 2	27.64
3.042	15	0 2 2	29.34
3.006M	100	4 0 0	29.70
3.006M		2 0 2	29.70
2.807M	86	2 4 0	31.86
2.807M		1 4 1	31.86

d(Å)	I^{rel} $\sigma = \pm 4$	hkℓ			2θ(°)
2.717M	8	4	2	0	32.94
2.717M		2	2	2	32.94
2.617	1L	1	3	2	34.24
2.570	1L	3	1	2	34.88
2.343M	6	3	4	1	38.39
2.343M		0	4	2	38.39
2.273+	5	5	0	1	39.62
2.273+		4	0	2	39.62
2.228	2	3	3	2	40.46
2.184M	4	4	4	0	41.31
2.184M		2	4	2	41.31
2.139+	22	5	2	1	42.21
2.139+		4	2	2	42.21
2.117	8	0	6	0	42.68
2.028	1L	0	3	3	44.64
2.004	2	6	0	0	45.20
1.954	1	5	1	2	46.44
1.909	8	3	2	3	47.59
1.847M	56	4	4	2	49.31
1.847M		1	4	3	49.31
1.736	6	6	0	2	52.69
1.6947M	14	6	4	0	54.07
1.6947M		3	4	3	54.07
1.6674M	9	7	0	1	55.03
1.6674M		5	0	3	55.03
1.6123M	1	5	2	3	57.08
1.6123M		2	2	4	57.08
1.5789	1L	3	1	4	58.40
1.5495	1	5	6	1	59.62
1.5348+	1	6	5	1	60.25
1.5348+		2	8	0	60.25
1.5213	1	0	4	4	60.84
1.5035M	1L	6	1	3	61.64
1.5035M		8	0	0	61.64
1.4753M	3	5	4	3	62.95
1.4753M		2	4	4	62.95
1.4618	1L	4	2	4	63.60

Carbamazepine, β-$C_{15}H_{12}N_2O$

Synonyms
5H-Dibenz(b,f)azepine-5-carboxamide
Carbamazepen
Carbazepine
Tegretal

CAS registry no.
298-46-4

Sample
The sample was the U.S. Pharmacopoeia Reference Standard recrystallized from benzene.

Color
Colorless

Optical data
Biaxial. $N_\alpha = 1.600$, $N_\beta \cong 1.675$, $N_\gamma = 1.745$. 2V is very large.

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure was determined by Himes et al. [1981].

Lattice constants of this sample
a = 13.918(7) Å
b = 11.159(5)
c = 7.543(4)
β = 92.84(5)°

a/b = 1.2472
c/b = 0.6760

Volume
1170.1 $Å^3$

Density
(calculated) 1.341 g/cm^3

Polymorphism
This β-phase transforms above 180 °C to give an α-phase [De Camp, Brannon, and Maienthal, 1981].

Figure of merit
F_{30} = 47.0(0.013,49)

Intensities
The crystals were long needles which oriented strongly, and the quantity was limited. Two sets of intensities are presented here. The first set was measured from only one experimental pattern and may be distorted by orientation. The 2nd set of I's was calculated from the structure data of Himes et al. [1981]. At 2θ = 24.37, a calculated peak of intensity 3 was not observed on the experimental pattern.

References
De Camp, W. H., Brannon, W. L., and Maienthal, M. M. (1981). Manuscript in preparation.

Himes, V., Mighell, A., and De Camp, W. H. (1981). To be published in Acta Crystallogr. B37.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d_{obs}	I_{obs}	I_{calc} peaks	hkℓ			$2\theta_{obs}$
8.71	5	6	1	1	0	10.15
6.94	37	11	2	0	0	12.74
6.77	89	93	-1	0	1	13.07
6.49	16	15	1	0	1	13.63
6.24	24	27	0	1	1	14.18
5.90	90	40	2	1	0	15.01
5.786	100	100	-1	1	1	15.30
5.604	54	13*	1	1	1	15.80
5.576	57	59	0	2	0	15.88
5.181	15	20	1	2	0	17.10
4.741	35	39	-2	1	1	18.70
4.549	63	41	2	1	1	19.50
4.485	12	12	0	2	1	19.78
4.346	38	30	2	2	0	20.42
4.302	18	20	-1	2	1	20.63
4.039	5	7	-3	0	1	21.99
3.799	29	26	-3	1	1	23.40
3.719	36	40	2	2	1	23.91
3.593	53	30	1	3	0	24.76
3.565M	61	53	0	1	2	24.96
3.565M			3	2	0	24.96
3.381	10	8	-2	0	2	26.34
3.337	39	38	0	3	1	26.69
3.277	75	43	2	3	0	27.19
3.259	75	47	-1	3	1	27.34
3.234	73	58	-2	1	2	27.56
3.122	1L	2	0	2	2	28.57
3.077	8	6	-1	2	2	29.00
3.035	6	8	-2	3	1	29.41
2.988	2	5	4	1	1	29.88
2.953	1L	-	4	2	0	30.24
2.900	5	-	3	3	0	30.81
2.893M	6	6	-3	1	2	30.88
2.893M			-2	2	2	30.88
2.807	9	6	2	2	2	31.86
2.790M	16	15	0	4	0	32.06
2.790M			-4	2	1	32.06
2.736M	2	3	-3	3	1	32.70
2.736M			1	4	0	32.70
2.651	3	1L	-5	0	1	33.79
2.641	5	4	-3	2	2	33.92
2.621	3	4	-4	0	2	34.18
2.566M	7	7	5	0	1	34.94
2.566M			1	4	1	34.94
2.503M	1	1	-2	3	2	35.85
2.503M			5	1	1	35.85
2.394M	3	3	-5	2	1	37.54
2.394M			1	1	3	37.54

*This intensity is reported as integrated rather than peak height, which lacked resolution.

Cerium Niobium Oxide, $CeNbO_4$

Synonym
Cerium niobate

CAS registry no.
12014-72-1

Sample
The sample was prepared at NBS by heating CeO_2 and Nb_2O_5 at 1000 °C for 21 hours, at 1500 °C for 21 hours, and at 800 °C for 4 days under a high vacuum.

Color
Medium bright green

Structure
Monoclinic, I2/a (15), Z = 4. The structure of $CeNbO_4$ has been determined using neutron powder diffraction by Santoro et al. [1980]. This phase had earlier been reported to be in space group Ia(5) by Komkov [1959]. $CeNbO_4$ is isostructural with other rare earth niobates and tantalates [Roth et al., 1977]. The structure is a distorted scheelite type called beta-fergusonite-(Ce) or brocenite [Kuo et al., 1975].

Lattice constants of this sample
$a = 5.5403(7)$ Å
$b = 11.4087(14)$
$c = 5.1631(7)$
$\beta = 94.602(13)°$

$a/b = 0.4856$
$c/b = 0.4526$

Volume
325.30 $Å^3$

Density
(calculated) 6.065 g/cm^3

Polymorphism
When heated to about 580 °C, $CeNbO_4$ undergoes a readily reversible phase change to a tetragonal structure of the fergusonite type, very similar to scheelite, $CaWO_4$ [Gingerich and Bair, 1963].

Figure of merit
$F_{30} = 75.8(0.010,40)$

Additional patterns
PDF card 23-1047 [McCarthy, G., Pennsylvania State University, University Park, PA]

PDF card 29-402 [Kuo et al., 1973]

References
Gingerich, K. A. and Bair, H. E. (1963). Advan. X-Ray Anal. 7, 22.

Komkov, A. I. (1959). Sov. Phys. Crystallogr. 4, 796.

Kuo, C., Wang, I., Wang, H., Wang, C., and Hou, H. (1973). Ti Chiu Hua Hsueh (Geochimica Peking) 2, 86.

Roth, R. S., Negas, T., Parker, H. S., Minor, D. B., and Jones, C. (1977). Mat. Res. Bull. 12, 1173.

Santoro, A., Marezio, M., Roth, R. S., and Minor, D. (1980). J. Solid State Chem. 35, 167.

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

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
5.705	3	0 2 0	15.52
4.973	1	1 1 0	17.82
4.697	7	0 1 1	18.88
3.233	100	-1 2 1	27.57
3.133	7	1 3 0	28.47
3.059M	97	0 3 1	29.17
3.059M		1 2 1	29.17
2.852	31	0 4 0	31.34
2.761	18	2 0 0	32.40
2.574	15	0 0 2	34.83
2.462	1L	-2 1 1	36.47
2.357	5	-1 1 2	38.15
2.346	4	0 2 2	38.34
2.308M	5	-1 4 1	38.99
2.308M		2 1 1	38.99
2.242	6	1 4 1	40.19
2.0861	8	0 5 1	43.34
2.0343	14	-1 3 2	44.50
2.0019	1L	2 3 1	45.26
1.9841	27	2 4 0	45.69
1.9622	17	-2 0 2	46.23
1.9455	3	1 3 2	46.65
1.9111	20	0 4 2	47.54
1.9017	3	0 6 0	47.79
1.8557	1	-2 2 2	49.05
1.8112	12	2 0 2	50.34
1.7264	1	2 2 2	53.00
1.7114	16	-1 6 1	53.50
1.6982	17	-3 2 1	53.95
1.6840	11	1 6 1	54.44
1.6568M	1	3 3 0	55.41
1.6568M		-1 5 2	55.41
1.6392	2	2 5 1	56.06
1.6214	15	3 2 1	56.73
1.6169	16	-2 4 2	56.90
1.6087	11	-1 2 3	57.22
1.5633M	5	0 3 3	59.04
1.5633M		1 7 0	59.04
1.5429M	9	-3 1 2	59.90
1.5429M		1 2 3	59.90

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.5291M	9	0 6 2	60.50
1.5291M		2 4 2	60.50
1.5090	1	-3 4 1	61.39
1.4995	1L	-2 1 3	61.82
1.4452	1	-1 4 3	64.42
1.4416	1L	-3 3 2	64.60
1.4321	6	3 1 2	65.08
1.4259	3	0 8 0	65.40
1.3806	3	4 0 0	67.83
1.3708	1	0 5 3	68.38
1.3494M	2	-1 7 2	69.62
1.3494M		3 3 2	69.62
1.3406M	2	-1 8 1	70.14
1.3406M		2 7 1	70.14
1.3228	1	1 7 2	71.23
1.2992M	3	-3 6 1	72.73
1.2992M		4 1 1	72.73
1.2870	4	0 0 4	73.53
1.2669	5	2 8 0	74.89
1.2635	5	3 6 1	75.13

Cerium Tantalum Oxide, $CeTaO_4$

Synonym
Cerium tantalate

CAS registry no.
12343-76-9

Sample
A 2:1 mixture of CeO_2 and Ta_2O_5 was heated at 1000 °C for 21½ hours, next at 1400 °C for 2 hours, then at 1500 °C for 17 hours. It was cooled and sealed in an evacuated glass tube. It was heated again at 800 °C for 6 days at a total pressure equal to or less than $2x10^{-6}$ Torr.

Color
Light olive

Structure
Monoclinic, $P2_1/a$ (14), Z = 4, with $LaTaO_4$-type structure. The structure was refined by Santoro et al. [1980]. Neutron powder diffraction techniques were used.

Lattice constants of this sample
a = 7.7654(5)Å
b = 5.5294(4)
c = 7.6230(6)
β = 100.865(7)°

a/b = 1.4044
c/b = 1.3786

Volume
321.45Å^3

Density
(calculated) 7.957 g/cm^3

Polymorphism
A monoclinic to orthorhombic phase transition was observed at 820 °C in vacuum [Cava et al., 1978].

Figure of merit
F_{30} = 82.4(0.007,53)

Additional pattern
PDF card 23-148 [Bodiot, 1968]

References

Bodiot, D. (1968). Rev. Chim. Miner. 5, 569.

Cava, R. J., Negas, T., Roth, R. S., Parker, H. S., Minor, D. B., and Olson, C. D. (1978). In The Rare Earths in Modern Science and Technology (Plenum Publishing Corp. New York, NY), p. 181.

Santoro, A., Marezio, M., Roth, R. S., and Minor, D. (1980). J. Solid State Chem. 35, 167.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
7.500	1L	0 0 1	11.79
4.478	5	1 1 0	19.81
4.447	8	0 1 1	19.95
3.813	13	2 0 0	23.31
3.742	20	0 0 2	23.76
3.690	10	-2 0 1	24.10
3.138	81	2 1 0	28.42
3.100	100	0 1 2	28.78
3.070	42	-2 1 1	29.06
2.966	10	-2 0 2	30.11
2.764	35	0 2 0	32.36
2.747	15	2 1 1	32.57
2.613	19	-2 1 2	34.29
2.4513	12	2 0 2	36.63
2.3219	3	-3 1 1	38.75
2.2957	8	-2 0 3	39.21
2.2746	1	0 1 3	39.59
2.2388M	4	2 1 2	40.25
2.2388M		2 2 0	40.25
2.2240	9	0 2 2	40.53
2.2130	3	-2 2 1	40.74
2.2026	1L	-1 2 2	40.94
2.0815	7	2 2 1	43.44
2.0223	12	-2 2 2	44.78
1.9368	21	-4 0 1	46.87
1.9279	5	2 0 3	47.10
1.9073	2	4 0 0	47.64
1.8715M	7	0 0 4	48.61
1.8715M		3 2 0	48.61
1.8525	2	0 2 3	49.14
1.8459	2	-4 0 2	49.33
1.8337	20	2 2 2	49.68
1.8213M	8	-2 0 4	50.04
1.8213M		2 1 3	50.04
1.8025	4	4 1 0	50.60
1.7912	2	1 3 0	50.94
1.7724	18	0 1 4	51.52
1.7679M	17	4 0 1	51.66
1.7679M		-2 2 3	51.66
1.7303	1L	-2 1 4	52.87
1.6852	11	4 1 1	54.40
1.6755	3	-4 0 3	54.74
1.6593	11	2 3 0	55.32
1.6541	16	0 3 2	55.51
1.6495	11	-2 3 1	55.68

d(Å)	I^{rel} $\sigma = \pm 4$	hkℓ	2θ(°)
1.6443	5	-1 3 2	55.87
1.6028	14	-4 1 3	57.45
1.5926	13	2 3 1	57.85
1.5861	9	-4 2 1	58.11
1.5824M	8	4 0 2	58.26
1.5824M		2 2 3	58.26
1.5655	9	-2 3 2	58.95
1.5500	3	0 2 4	59.60
1.5346	2	-4 2 2	60.26
1.5211M	7	4 1 2	60.85
1.5211M		-2 2 4	60.85
1.5077	6	2 1 4	61.45
1.4919M	2	-2 0 5	62.17
1.4919M		3 3 0	62.17
1.4902	3	4 2 1	62.25
1.4414M	3	-2 1 5	64.61
1.4414M		-3 3 2	64.61
1.4331M	2	3 3 1	65.03
1.4331M		-4 2 3	65.03
1.4066	1L	3 2 3	66.41
1.3936	1	4 0 3	67.11
1.3822	3	0 4 0	67.74
1.3734	1	4 2 2	68.23
1.3631	2	2 2 4	68.82
1.3601	2	1 4 0	68.99
1.3511	4	4 1 3	69.52
1.3250	1L	4 3 0	71.09
1.3134M	5	-2 2 5	71.82
1.3134M		0 3 4	71.82
1.3027	2	-4 0 5	72.50
1.2996	2	2 4 0	72.70
1.2967	2	0 4 2	72.89
1.2947	2	-2 4 1	73.02
1.2764M	4	2 1 5	74.24
1.2764M		4 3 1	74.24
1.2677M	4	-4 1 5	74.84
1.2677M		-5 2 3	74.84
1.2599	5	-6 1 1	75.38
1.2530	1	-2 4 2	75.87
1.2477	4	0 0 6	76.25
1.2447	4	4 2 3	76.47
1.2394	4	-4 3 3	76.85
1.2301	1L	-6 0 3	77.54
1.2267	3	-2 1 6	77.80
1.2160M	1	-3 4 1	78.61
1.2160M		6 0 1	78.61
1.2039	2	2 4 2	79.56
1.2009M	3	-6 1 3	79.80
1.2009M		4 3 2	79.80
1.1942	1	2 3 4	80.34

Cesium Magnesium Titanium Oxide, $Cs_{1.45}Mg_{0.724}Ti_{7.27}O_{16}$

Synonym
Cesium magnesium titanate .

Sample
The sample was prepared at NBS by mixing stoichiometric proportions of cesium, magnesium, and titanium oxides. The mixture was heated at 750 °C for 18 hours, then re-heated with periodic grindings at 1200 °C for 5 hours. Finally, it was heated at 1200 °C in a sealed platinum tube for 5 days.

Color
Pale yellow

Structure
Tetragonal, I4/m (87), Z = 1. Roth [1981] determined by analogy that this compound is of the hollandite type structure. The structure of the related hollandite type phases was determined by Sinclair et al. [1980].

Lattice constants of this sample
a = 10.2818(4) Å
c = 2.9717(3)

c/a = 0.2890

Volume
314.15 $Å^3$

Density
(calculated) 4.305 g/cm^3

Figure of merit
F_{30} = 84.4(0.010,35)
M_{20} = 128.4

References
Roth, R. S. (1981) private communication.

Sinclair, W., McLaughlin, G. M., and Ringwood, A. E. (1980). Acta Crystallogr. B36, 2913.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
7.27	1	1 1 0	12.17
5.148	2	2 0 0	17.21
3.636	27	2 2 0	24.46
3.254	100	3 1 0	27.39
2.856	3	1 0 1	31.30
2.570	2	4 0 0	34.88
2.497	18	2 1 1	35.94
2.299	25	4 2 0	39.15
2.246	19	3 0 1	40.12
2.0567	5	3 2 1	43.99
2.0163	11	5 1 0	44.92
1.9107	15	4 1 1	47.55
1.8179	6	4 4 0	50.14
1.7635	7	5 3 0	51.80
1.7135	22	6 0 0	53.43
1.6912	2	4 3 1	54.19
1.6261	2	6 2 0	56.55
1.6061	21	5 2 1	57.32
1.4857	2	0 0 2	62.46
1.4692	4	6 1 1	63.24
1.4559	2	1 1 2	63.89
1.4540	3	5 5 0	63.98
1.4270	2	2 0 2	65.34
1.4124	16	5 4 1	66.10
1.3624	2	6 3 1	68.86
1.3502	12	7 3 0	69.57
1.3172	1	7 0 1	71.58
1.2865	2	4 0 2	73.56
1.2754	2	7 2 1	74.31
1.2667	1	3 3 2	74.91
1.2467	2	8 2 0	76.32
1.2115	6	6 6 0	78.96
1.2038	1L	6 5 1	79.57
1.1963	1L	5 1 2	80.17
1.1950	3	7 5 0	80.27
1.1719	3	7 4 1	82.19
1.1495	2	8 4 0	84.15
1.1353	7	9 1 0	85.45
1.1226	3	6 0 2	86.66
1.1155	1	8 3 1	87.35
1.0969	1	6 2 2	89.22
1.0837	1	9 3 0	90.60
1.0664	1	9 0 1	92.50
1.0440	4	7 6 1	95.09
1.0392	1	5 5 2	95.68
1.0289	2	6 4 2	96.95
1.0283	2	8 6 0	97.02

Chromium Boride, Cr_5B_3

CAS registry no.
12007-38-4

Sample
The sample was obtained from Cerac, Inc., Menomonee Falls, WI. It contained about 15% CrB as a second phase which did not interfere with the measurements.

Color
Dark gray

Structure
Tetragonal, I4/mcm (140), Z = 4. The structure was determined by Bertaut and Blum [1953].

Lattice constants of this sample
a = 5.4735(5) Å
c = 10.1156(15)

c/a = 1.8481

Volume
303.06 Å^3

Density
(calculated) 6.409 g/cm^3

Figure of merit
F_{25} = 53.5(0.012,38)

Additional pattern
Kuz'ma et al. [1969]

References
Bertaut, F. and Blum, P. (1953). C. R. Acad. Sci. 236, 1055.

Kuz'ma, Yu. B., Telegus, V. S., and Kovalyk, D. A. (1969). Porosh Met. 5, 79.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å			
d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
3.073	21	1 1 2	29.03
2.739	9	2 0 0	32.67
2.528	14	0 0 4	35.48
2.409	29	2 0 2	37.30
2.380	55	2 1 1	37.76
2.117	23	1 1 4	42.68
1.9808	100	2 1 3	45.77
1.9341	15	2 2 0	46.94
1.8572	39	2 0 4	49.01
1.8085	1	2 2 2	50.42
1.7306	30	3 1 0	52.86
1.6858	10	0 0 6	54.38
1.6378	3	3 1 2	56.11
1.5597	2	2 1 5	59.19
1.4352	1	2 0 6	64.92
1.3162	11	4 1 1	71.64
1.2901	4	3 3 0	73.32
1.2714	3	2 2 6	74.58
1.2643	2	0 0 8	75.07
1.2498	3	3 3 2	76.10
1.2445	13	2 1 7	76.48
1.2354	12	4 1 3	77.15
1.2237	3	4 2 0	78.02
1.2078	10	3 1 6	79.25
1.1491	11	3 3 4	84.19

Cobalt Fluoride, CoF_2

Synonym
Cobalt difluoride

CAS registry no.
10026-17-2

Sample
The sample obtained from the Apache Chemical Co., Seward, IL was heated at 180 °C.

Color
Strong pink

Structure
Tetragonal, $P4_2/mnm$ (136), Z = 2, isostructural with TiO_2, rutile. The structure was determined by Stout and Reed [1954] and refined by Baur [1958].

Lattice constants of this sample
a = 4.7106(3) Å
c = 3.1691(5)

c/a = 0.6728

Volume
70.322 $Å^3$

Density
(calculated) 4.578 g/cm^3

Figure of merit
F_{19} = 84.6(0.010,22)

Additional pattern
PDF card 3-409 [The Dow Chemical Co.]

PDF card 24-329 [Swanson et al., 1972]

References

Baur, W. H. (1958). Acta Crystallogr. 11, 488.

Stout, J. W. and Reed, A. (1954). J. Am. Chem. Soc. 76, 5279.

Swanson, H. E., McMurdie, H. F., Morris, M. C., Evans, E. H., and Paretzkin, B. (1972). Natl. Bur. Stand. U.S. Monogr. 25, Sec. 10, 85.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
3.332	100	1 1 0	26.73
2.631	50	1 0 1	34.05
2.355	7	2 0 0	38.18
2.297	24	1 1 1	39.19
2.1069	6	2 1 0	42.89
1.7547	56	2 1 1	52.08
1.6654	17	2 2 0	55.10
1.5844	9	0 0 2	58.18
1.4894	6	3 1 0	62.29
1.4307	14	1 1 2	65.15
1.4070	16	3 0 1	66.39
1.3484	1	3 1 1	69.68
1.3148	2	2 0 2	71.73
1.2662	1	2 1 2	74.94
1.2082	4	3 2 1	79.22
1.1776	1L	4 0 0	81.71
1.1481	7	2 2 2	84.28
1.1101	3	3 3 0	87.88
1.0852	3	3 1 2	90.44

Cobalt Phosphide, Co_2P

CAS registry no.
12134-02-0

Sample
The sample was obtained from ICN-K&K Laboratories, Plainview, NY. It contained a few percent of $Co_3(PO_4)_2$ which did not interfere with measurements.

Color
Black

Structure
Orthorhombic, Pnam (62), Z = 4, isostructural with Co_2Si. The structure was determined by Nowotny [1947]. It was refined by Rundqvist [1960] who stated that there is an extended homogeneity range at elevated temperatures; the widening of the range is apparently connected with random vacancies in the metal atom sites.

Lattice constants of this sample
a = 5.6465(8) Å
b = 6.6099(10)
c = 3.5130(7)

a/b = 0.8542
c/b = 0.5315

Volume
131.11 $Å^3$

Density
(calculated) 7.540 g/cm^3

Figure of merit
F_{30} = 48.8(0.013,46)

Additional pattern
PDF card 6-0595 [Nowotny, 1947]

References
Nowotny, H. (1947). Z. Anorg. Allg. Chem. 254, 31.

Rundqvist, S. (1960). Acta Chem. Scand. 14, 1961.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
3.309	3	0 2 0	26.92
2.854	5	1 2 0	31.32
2.826	4	2 0 0	31.64
2.719	6	1 1 1	32.92
2.214	100	1 2 1	40.73
2.201	69	2 0 1	40.97
2.147	11	2 2 0	42.06
2.088	71	2 1 1	43.30
2.053	33	1 3 0	44.08
1.8675	26	0 3 1	48.72
1.8326	8	2 2 1	49.71
1.8102	23	3 1 0	50.37
1.7715	19	1 3 1	51.55
1.7562	29	0 0 2	52.03
1.7370	11	2 3 0	52.65
1.6524	8	0 4 0	55.57
1.6354	17	3 2 0	56.20
1.6094	4	3 1 1	57.19
1.5856	2	1 4 0	58.13
1.5573	6	2 3 1	59.29
1.4309	2	3 3 0	65.14
1.3802	1	4 1 0	67.85
1.3596	1	2 2 2	69.02
1.3342	7	1 3 2	70.53
1.2981	4	4 2 0	72.80
1.2867	2	1 5 0	73.55
1.2844	3	4 1 1	73.70
1.2605	6	3 1 2	75.34
1.2371	5	0 5 1	77.02
1.2350	7	2 3 2	77.18
1.2181	1L	4 2 1	78.45
1.1969M	9	2 5 0	80.12
1.1969M		3 2 2	80.12
1.1708	6	3 4 1	82.28
1.1336	1	2 5 1	85.61
1.0833	4	1 2 3	90.64
1.0816+	6	3 5 0	90.83
1.0816+		2 0 3	90.83
1.0611	7	5 1 1	93.09
1.0339M	6	0 3 3	96.33
1.0339M		3 5 1	96.33

Copper Chloride Hydrate (Eriochalcite), $CuCl_2 \cdot 2H_2O$

Synonym
Cupric chloride dihydrate

CAS registry no.
13933-17-0

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

Color
Brilliant bluish green

Structure
Orthorhombic, Pbmn (53), Z = 2. The structure was determined by Harker [1936] and refined by Engberg [1970].

Lattice constants of this sample
a = 7.4164(6) Å
b = 8.0926(6)
c = 3.7494(4)

a/b = 0.9164
c/b = 0.4633

Volume
225.03 Å^3

Density
(calculated) 2.516 g/cm^3

Figure of merit
F_{30} = 87.6(0.009,37)

Additional pattern
PDF card 13-145 [Inst. of Physics, Univ. College, Cardiff, Wales]

References
Engberg, A. (1970). Acta Chem. Scand., 24, 3510.

Harker, D. (1936). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. A93, 136.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
5.467	100	1 1 0	16.20
4.050	56	0 2 0	21.93
3.750	11	0 0 1	23.71
3.708	6	2 0 0	23.98
3.346	21	1 0 1	26.62
3.093	40	1 1 1	28.84
2.734	14	2 2 0	32.73
2.638	82	2 0 1	33.96
2.578	18	1 2 1	34.77
2.534	17	1 3 0	35.39
2.365	9	3 1 0	38.02
2.2088	29	2 2 1	40.82
2.1004	13	1 3 1	43.03
2.0639	5	3 0 1	43.83
2.0240	22	0 4 0	44.74
2.0007	17	3 1 1	45.29
1.8744	5	0 0 2	48.53
1.8543	14	4 0 0	49.09
1.8389	5	3 2 1	49.53
1.8220	6	3 3 0	50.02
1.7808	4	0 4 1	51.26
1.7740	9	1 1 2	51.47
1.7312	5	1 4 1	52.84
1.7005	2	0 2 2	53.87
1.6860	9	4 2 0	54.37
1.6730	5	2 0 2	54.83
1.6624	3	4 0 1	55.21
1.6579	6	1 2 2	55.37
1.6389M	6	3 3 1	56.07
1.6389M		2 1 2	56.07
1.6048	23	2 4 1	57.37
1.5817	5	1 5 0	58.29
1.5070	3	1 3 2	61.48
1.4939	3	3 0 2	62.08
1.4686	3	3 1 2	63.27
1.4587	8	5 1 0	63.75
1.4569	4	1 5 1	63.84
1.4452	5	3 4 1	64.42
1.4015	6	3 2 2	66.68
1.3671	7	4 4 0	68.59
1.3600	3	5 1 1	69.00
1.3538	2	3 5 0	69.36

Iodoform, CHI_3

Synonym
Triiodomethane

CAS registry no.
75-47-8

Sample
The sample was obtained from Merck and Co., Inc., Rahway, NJ.

Color
Brilliant yellow

Structure
Hexagonal, $P6_3$ (173), Z = 2. The structure was determined by Huggins and Noble [1931].

Lattice constants of this sample
a = 6.8195(5) Å
c = 7.565(1)

c/a = 1.1093

Volume
304.68 $Å^3$

Density
(calculated) 4.292 g/cm^3

Figure of merit
F_{30} = 62.4(0.011,44)

Additional pattern
PDF card 2-329 [Crystallographic Laboratory, Cambridge, England]

Reference
Huggins, M. L. and Noble, B. A. (1931). Am. Mineral. 16, 519.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å			
d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
4.650	11	1 0 1	19.07
3.781	39	0 0 2	23.51
3.409	18	1 1 0	26.12
3.107	100	1 1 1	28.71
2.751	7	2 0 1	32.52
2.531	16	1 1 2	35.44
2.320	1	1 0 3	38.78
2.230	6	2 1 0	40.41
2.0270	22	1 1 3	44.67
1.9674	11	3 0 0	46.10
1.9222	7	2 1 2	47.25
1.8913	3	0 0 4	48.07
1.7456	12	3 0 2	52.37
1.7049	1	2 2 0	53.72
1.6629	9	2 2 1	55.19
1.6535	3	1 1 4	55.53
1.6381	2	3 1 0	56.10
1.6010	3	3 1 1	57.52
1.5540	2	2 2 2	59.43
1.5033	3	3 1 2	61.65
1.4492	2	4 0 1	64.22
1.4431	2	2 1 4	64.52
1.4122	2	2 2 3	66.11
1.3831	3	1 1 5	67.69
1.3734	2	3 1 3	68.23
1.3636	3	3 0 4	68.79
1.3550	1	3 2 0	69.29
1.3467	1L	2 0 5	69.78
1.3338	2	3 2 1	70.55
1.2888	1L	4 1 0	73.41
1.2755	1	3 2 2	74.30
1.2744	1	4 0 3	74.38
1.2707	3	4 1 1	74.63
1.2606	1L	0 0 6	75.33
1.2382	1L	3 1 4	76.94
1.2201	1	4 1 2	78.30

CAS registry no.
12006-84-7

Sample
The sample was obtained from Cooper Metallurgical Associates, Cleveland, OH.

Color
Unground, shiny metallic gray in chunks
Ground, olive gray

Structure
Orthorhombic, Pbnm (62), Z = 4. The structure was determined by Bjurström and Arnfelt [1929].

Lattice constants of this sample
a = 4.0587(3)Å
b = 5.5032(5)
c = 2.9474(3)

a/b = 0.7375
c/b = 0.5336

Volume
65.833 Å^3

Density
(calculated) 6.725 g/cm^3

Figure of merit
F_{29} = 79.0(0.009,39)

Intensities
Owing to the difficulty of getting reproducible intensities, a comparison between experimental intensities and those calculated on the basis of the structure given in Pearson [1967] was made. In the calculated pattern, the four strongest lines were: 2.188(100), 1.904(67), 2.384(65), 2.011(65).

Additional pattern
PDF card 3-957 [Bjurström]

References
Bjurström, T. (1933). Ark. Kemi Mineral. Geol. 11A.

Bjurström, T. and Arnfelt, H. (1929). Z. Phys. Chem. B4, 869.

Pearson, W. B. (1967). A Handbook of Lattice Spacings and Structures of Metals and Alloys, Vol. 2, (Pergamon Press Ltd., Oxford, England) p. 409.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
3.269	16	1 1 0	27.26
2.752	32	0 2 0	32.51
2.384	50	1 0 1	37.71
2.2768	33	1 2 0	39.55
2.1888	72	1 1 1	41.21
2.0116	100	0 2 1	45.03
1.9043	67	2 1 0	47.72
1.8018	28	1 2 1	50.62
1.6716	33	1 3 0	54.88
1.6335	5	2 2 0	56.27
1.5995	27	2 1 1	57.58
1.4736	22	0 0 2	63.03
1.4542	3	1 3 1	63.97
1.3435	3	1 1 2	69.97
1.3030	10	1 4 0	72.48
1.2993	6	0 2 2	72.72
1.2466	17	0 4 1	76.33
1.2374	16	1 2 2	77.00
1.2354	25	2 3 1	77.15
1.2297	8	3 0 1	77.57
1.2141	5	3 2 0	78.76
1.1999	12	3 1 1	79.88
1.1917	4	1 4 1	80.54
1.1653	22	2 1 2	82.76
1.1224	9	3 2 1	86.68
1.1054	9	1 3 2	88.35
1.0889	7	3 3 0	90.05
1.0621M	4	1 5 0	92.98
1.0621M		2 4 1	92.98
1.0147	6	4 0 0	98.78

Iron Fluoride, FeF_3

Synonym
Ferric fluoride

CAS registry no.
7783-50-8

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA. It was dried at 140° for 2-3 hours.

Color
Pale yellow green

Structure
Hexagonal, $R\bar{3}c$ (167), Z = 6. The structure was determined by Hepworth et al. [1957].

Lattice constants of this sample
a = 5.200(1) Å
c = 13.323(2)

c/a = 2.5621

Volume
311.94 $Å^3$

Density
(calculated) 3.604 g/cm^3

Figure of merit
F_{21} = 65.3(0.013,25)

Additional pattern
PDF card 2-0327 [Ebert, 1931]

References
Ebert, F. (1931). Z. Anorg. Chem. 186, 398.

Hepworth, M. A., Jack, K. H., Peacock, R. D., and Westland, G. J. (1957). Acta Crystallogr. 10, 63.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
3.731	100	0 1 2	23.83
2.678	15	1 0 4	33.43
2.602	7	1 1 0	34.44
2.244	14	1 1 3	40.15
2.133	2	2 0 2	42.34
1.8664	21	0 2 4	48.75
1.6889M	21	1 1 6	54.27
1.6889M		2 1 1	54.27
1.6486	10	1 2 2	55.71
1.5619	3	0 1 8	59.10
1.5157	6	2 1 4	61.09
1.5011	5	3 0 0	61.75
1.4346	1	1 2 5	64.95
1.3386	5	2 0 8	70.26
1.2996	2	2 2 0	72.70
1.2861	1	1 1 9	73.59
1.2777	3	1 0 10	74.15
1.2690	1	2 1 7	74.75
1.2434M	2	3 0 6	76.56
1.2434M		1 3 1	76.56
1.2276	5	3 1 2	77.73
1.1902	2	1 2 8	80.66
1.1692	1	1 3 4	82.42

Iron Oxide (Hematite), α-Fe_2O_3

Synonyms
Iron sesquioxide
Diiron trioxide
Ferric oxide

CAS registry no.
1309-37-1

Sample
The sample was obtained from Pfizer, Inc., New York, NY. It was heated at 800 °C for 3 days.

Color
Dark reddish brown

Structure
Hexagonal, $R\bar{3}c$ (167), Z = 6. The structure was determined by Pauling and Hendricks (1925) and refined by Blake et al. (1966). It is isostructural with α-Al_2O_3, corundum.

Lattice constants of this sample
a = 5.0356(1) Å
c = 13.7489(7)

c/a = 2.7303

Volume
301.93 Å^3

Density
(calculated) 5.270 g/cm^3

Figure of merit
F_{30} = 67.6(0.011,40)

Polymorphism
Three other forms of this compound have been reported. Delta-Fe_2O_3 crystallizes in a hexagonal form. Maghemite, γ-Fe_2O_3 has been reported in both a cubic and a tetragonal form.

Reference intensity
$I/I_{corundum}$ = 2.60(1)

Additional patterns
PDF card 13-534 [Aravindaksman and Ali, Council of Sci. and Indust. Res., Central Fuel Res. Inst., Binat, India]

PDF card 24-72 [Smith et al., Penn. State U., University Park, PA]

References
Blake, R. L., Hessevick, R. E., Zoltai, T., and Finger, L. W. [1966]. Am. Mineral. 51, 123.

Pauling, L. and Hendricks, S. B. [1925]. J. Amer. Chem. Soc. 47, 781.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
3.684	30	0 1 2	24.14
2.700	100	1 0 4	33.15
2.519	71	1 1 0	35.61
2.292	3	0 0 6	39.28
2.207	22	1 1 3	40.86
2.0779	3	2 0 2	43.52
1.8406	39	0 2 4	49.48
1.6941	47	1 1 6	54.09
1.6367	1	2 1 1	56.15
1.6033	5	1 2 2	57.43
1.5992	10	0 1 8	57.59
1.4859	30	2 1 4	62.45
1.4538	30	3 0 0	63.99
1.3497	3	2 0 8	69.60
1.3115	10	1 0 10	71.94
1.3064	6	1 1 9	72.26
1.2592	8	2 2 0	75.43
1.2276	4	3 0 6	77.73
1.2141	2	2 2 3	78.76
1.1896	5	1 2 8	80.71
1.1632	5	0 2 10	82.94
1.1411	7	1 3 4	84.92
1.1035	7	2 2 6	88.54
1.0768	2	0 4 2	91.35
1.0557	7	2 1 10	93.71
1.0428	1L	1 1 12	95.24
1.0393	3	4 0 4	95.66
.9892	4	3 1 8	102.29
.9715	1L	2 2 9	104.92
.9606	5	3 2 4	106.63
.9581	4	0 1 14	107.03
.9516	5	4 1 0	108.09
.9318	2	4 1 3	111.51
.9206	2	0 4 8	113.60
.9081	5	1 3 10	116.04
.8998	1	3 0 12	117.75
.8954	3	2 0 14	118.69
.8789	6	4 1 6	122.44
.8648	1	2 3 8	125.94
.8543	3	4 0 10	128.77
.8436	5	1 2 14	131.87
.8392	3	3 3 0	133.24
.8089	4	3 2 10	144.44
.8014	4	2 4 4	147.96

Iron Yttrium Oxide, $Fe_5Y_3O_{12}$

Synonyms
YIG, Yttrium iron garnet, $Y_3Fe_2(FeO_4)_3$
Diiron triyttrium trisferrate, $Fe_2Y_3(FeO_4)_3$

CAS registry no.
12063-56-8

Sample
The sample was obtained from Trans-Tech, Inc., Gaithersburg, MD.

Color
Medium olive

Structure
Cubic, Ia3d (230), Z = 8, garnet structure. The structure was refined by Euler and Bruce [1965] following earlier determinations [Geller and Gilleo, 1957; Batt and Post, 1962].

Lattice constant of this sample
a = 12.3774(2) Å

Volume
1896.22 Å^3

Density
(calculated) 5.170 g/cm^3

Polymorphism
Shimada et al. [1968] reported the existence of a dense allotropic form.

Figure of merit
F_{30} = 88.4(0.010,35)

Reference intensity
$I/I_{corundum}$ = 4.12(13)

Additional pattern
PDF card 27-977 [B. Greenberg (1966). Polytechnic Institute of New York, Brooklyn, NY]

References

Batt, A. and Post, B. (1962). Acta Crystallogr. 15, 1268.

Euler, F. and Bruce, J. A. (1965). Acta Crystallogr. 19, 971.

Geller, S. and Gilleo, J. (1957). J. Phys. Chem. Solids 3, 30.

Shimada, M., Kume, S., and Koizumi, M. (1968). J. Amer. Ceram. Soc. 51, 713.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
5.055	6	2 1 1	17.53
4.377	1	2 2 0	20.27
3.307	3	3 2 1	26.94
3.093	32	4 0 0	28.84
2.768	100	4 2 0	32.32
2.639	2	3 3 2	33.94
2.527	44	4 2 2	35.50
2.428	4	4 3 1	37.00
2.259	10	5 2 1	39.87
2.188	2	4 4 0	41.23
2.0082	9	6 1 1	45.11
1.8261	1L	6 3 1	49.90
1.7870	14	4 4 4	51.07
1.7171	36	6 4 0	53.31
1.6840	3	7 2 1	54.44
1.6544	42	6 4 2	55.50
1.5718	1	7 3 2	58.69
1.5469	14	8 0 0	59.73
1.5236	1L	7 4 1	60.74
1.5013	1L	8 2 0	61.74
1.4791	1L	6 5 3	62.77
1.4589	1L	8 2 2	63.74
1.4382	1L	8 3 1	64.77
1.3840	8	8 4 0	67.64
1.3506	19	8 4 2	69.55
1.3345	1	9 2 1	70.51
1.3194	6	6 6 4	71.44
1.3047	1L	8 5 1	72.37
1.2764	2	9 3 2	74.24
1.2503	1	9 4 1	76.06
1.2255	1L	10 1 1	77.89
1.2138	2	10 2 0	78.78
1.1801	2	10 3 1	81.50
1.1492	22	10 4 0	84.18
1.1395	1L	10 3 3	85.06
1.1300	12	10 4 2	85.95
1.1026	2	11 2 1	88.63
1.0940	10	8 8 0	89.52
1.0691	1L	11 3 2	92.19
1.0612	1L	10 6 0	93.08
1.0387	1L	9 6 5	95.74
1.0314	5	12 0 0	96.64
1.0242	1L	11 4 3	97.55
1.0173	5	12 2 0	98.43
1.0107	2	11 5 2	99.31
1.0039	10	12 2 2	100.22
.9845	1L	11 6 1	102.96
.9608	2	11 6 3	106.59
.9383	1L	13 2 1	110.36
.9330	5	12 4 4	111.31

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
.9277	1L	12 5 3	112.26
.9225	13	12 6 0	113.23
.9175	6	13 3 2	114.19
.9125	5	12 6 2	115.17
.8933	5	8 8 8	119.15
.8624	2	14 3 1	126.56
.8582	3	12 8 0	127.67
.8501	12	14 4 0	129.95
.8422	11	14 4 2	132.31

Lithium Iodide Hydrate, $LiI \cdot 3H_2O$

Synonym
Lithium iodide trihydrate

CAS registry no.
7790-22-9

Sample
The sample was from ICN Pharmaceuticals Inc., Plainview, NY. It was marked "Lithium Iodide Anhydrous." The material was hygroscopic and the intensities may be somewhat in error.

Color
Light brown

Structure
Hexagonal, $P6_3mc$ (186), Z = 2. The structure of $LiI \cdot 3H_2O$ was studied by Hendricks [1928] and discussed by West [1934].

Lattice constants of this sample
a = 7.4907(11) Å
c = 5.4859(11)

c/a = 0.7323

Volume
266.58 $Å^3$

Density
(calculated) 2.341 g/cm^3

Figure of merit
F_{27} = 59.9(0.015,30)

Additional pattern
PDF card 1-0411 [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. (1928). Am. J. Sci. 15, 403.

West, C. D. (1934). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 88, 198.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å			
d(Å)	I^{rel} σ = ±5	hkℓ	2θ(°)
6.50	7	1 0 0	13.62
4.186	100	1 0 1	21.21
3.743	57	1 1 0	23.75
3.242	19	2 0 0	27.49
2.793	92	2 0 1	32.02
2.741	23	0 0 2	32.64
2.527	6	1 0 2	35.49
2.452	17	2 1 0	36.62
2.238	39	2 1 1	40.27
2.211	30	1 1 2	40.78
2.164	14	3 0 0	41.71
2.093	17	2 0 2	43.18
2.012	3	3 0 1	45.02
1.872	13	2 2 0	48.61
1.827	15	2 1 2	49.86
1.7992	4	3 1 0	50.70
1.7603	9	1 0 3	51.90
1.7102	28	3 1 1	53.54
1.6985	9	3 0 2	53.94
1.5931	10	2 0 3	57.83
1.5552	10	4 0 1	59.38
1.5474	9	2 2 2	59.71
1.5044	5	3 1 2	61.60
1.4661	7	2 1 3	63.39
1.4362	15	3 2 1	64.87
1.4157	8	4 1 0	65.93
1.3956	3	4 0 2	67.00

Magnesium Phosphate, α-$Mg_2P_2O_7$

Synonym
Magnesium pyrophosphate

Sample
The sample was prepared at NBS. The composition of a commercially available sample of magnesium phosphate (mixed phases) was adjusted with additions of $(NH_4)H_2PO_4$. The mixture was fused and resolidified to yield single phase α-$Mg_2P_2O_7$. After being ground, the sample was annealed at 140 °C for 5 hours and slowly cooled to room temperature.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure was determined by Calvo [1967].

Lattice constants of this sample
a = 8.9124(16) Å
b = 8.290(2)
c = 6.9492(15)
β = 111.70(1)°

a/b = 1.0751
c/b = 0.8383

Volume
477.05 Å^3

Density
(calculated) 3.099 g/cm^3

Polymorphism
A high-temperature β-form exists and is also monoclinic, with a and c roughly half as large as in the α-phase. The phase transformation was found to be reversible, and both phases coexist from 59 to 63 °C [Calvo et al., 1967].

Figure of merit
F_{30} = 27.6(0.016,70)

Reference intensity
$I/I_{corundum}$ = 1.72(3)

Additional pattern
PDF card 22-1152 [Swanson et al., 1971]. This pattern on the card and in the reference both have substantial errors.

References

Calvo, C. (1967). Acta Crystallogr. 23, 289.

Calvo, C., Datars, W. R., and Leung, J. S. (1967). J. Chem. Phys. 46, 796.

Swanson, H. E., McMurdie, H. F., Morris, M. C., Evans, E. H., and Paretzkin, B. (1971). Natl. Bur. Stand. U.S. Monogr. 25, Sec. 9, 73.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
6.37	2	-1 0 1	13.90
5.104	3	0 1 1	17.36
4.373	3	1 0 1	20.29
4.149	23	0 2 0	21.40
3.860	1	1 1 1	23.02
3.805	3	-2 1 1	23.36
3.710M	1	1 2 0	23.97
3.710M		2 1 0	23.97
3.492	3	0 2 1	25.49
3.181	6	-2 0 2	28.03
3.008M	100	0 1 2	29.68
3.008M		1 2 1	29.68
2.965M	44	-2 1 2	30.12
2.965M		-3 0 1	30.12
2.929	3	2 2 0	30.50
2.834	3	2 1 1	31.54
2.795	1L	-3 1 1	32.00
2.664	1	-1 2 2	33.62
2.620M	4	1 3 0	34.19
2.620M		3 1 0	34.19
2.534	7	-1 3 1	35.40
2.523	12	-2 2 2	35.55
2.411	6	-3 2 1	37.26
2.299M	1	2 3 0	39.16
2.299M		3 2 0	39.16
2.257	1L	1 2 2	39.91
2.149	4	-4 1 1	42.01
2.121	1L	-3 0 3	42.60
2.099	13	0 3 2	43.06
2.071+	6	-4 1 2	43.67
2.071+		4 0 0	43.67
2.053	3	-3 1 3	44.07
2.011M	4	-1 2 3	45.04
2.011M		1 4 0	45.04
1.980	1L	3 2 1	45.80
1.973	1L	0 4 1	45.97
1.953	1L	3 3 0	46.46
1.932	1L	2 2 2	46.99
1.928	1L	1 3 2	47.11
1.910	1L	0 2 3	47.57
1.907	1L	-3 3 2	47.65
1.886	1L	-3 2 3	48.21
1.873	6	1 4 1	48.57
1.869	6	1 1 3	48.68
1.851	8	4 2 0	49.17

Magnesium Phosphate, α-$Mg_2P_2O_7$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ			2θ(°)
1.780	1L	-1	4	2	51.30
1.770	2	-5	0	1	51.61
1.7466	1	3	3	1	52.34
1.7364M	1	-2	0	4	52.67
1.7364M		-2	4	2	52.67
1.7333	1L	-4	3	1	52.77
1.7111	4	-4	2	3	53.51
1.6991M	6	-2	1	4	53.92
1.6991M		-3	4	1	53.92
1.6812	1	-3	3	3	54.54
1.6579M	1L	-3	1	4	55.37
1.6579M		3	4	0	55.37
1.6410+	2	1	4	2	55.99
1.6410+		2	1	3	55.99
1.6373	1	-5	0	3	56.13
1.6245	5	5	1	0	56.61
1.6214	4	-5	2	2	56.73
1.6138	5	0	0	4	57.02
1.6056M	4	-5	1	3	57.34
1.6056M		0	5	1	57.34
1.5889	2	-4	0	4	58.00
1.5752	11	1	3	3	58.55
1.5519	1L	2	2	3	59.52
1.5254	1	3	4	1	60.66
1.5222	2	-5	2	3	60.80
1.5035M	1	0	2	4	61.64
1.5035M		2	4	2	61.64
1.4825+	2	-6	0	2	62.61
1.4825+		-3	4	3	62.61
1.4751	2	0	5	2	62.96
1.4697M	4	-2	3	4	63.22
1.4697M		-2	5	2	63.22
1.4645	4	4	4	0	63.47
1.4546	1L	5	1	1	63.95
1.4333M	1L	3	1	3	65.02
1.4333M		-5	1	4	65.02

CAS registry no.
7439-96-5

Sample
A sample of α-Mn from Fisher Scientific Co., Fair Lawn, NJ, was heated to 1065 °C in vacuum and annealed for 3 hours. It contained a small amount of MnO.

Color
Olive gray

Structure
Cubic, $P4_{1,3}32$ (212 or 213), Z = 20. The structure was determined by Westgren and Phragmén [1925].

Lattice constant of this sample
a = 6.3116(3) Å

Volume
251.43 Å^3

Density
(calculated) 7.270 g/cm^3

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

Figure of merit
F_{26} = 71.2(0.011,33)

Additional pattern
PDF card 1-1234 [Hanawalt, Rinn, and Frevel, 1938]

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
4.458	3	1 1 0	19.90
2.823	5	2 1 0	31.67
2.577	5	2 1 1	34.79
2.231	7	2 2 0	40.39
2.104	100	2 2 1	42.95
1.9965	62	3 1 0	45.39
1.9039	27	3 1 1	47.73
1.7509	2	3 2 0	52.20
1.6872	9	3 2 1	54.33
1.5307	1L	4 1 0	60.43
1.4874	6	3 3 0	62.38
1.4478	1L	3 3 1	64.29
1.4115	5	4 2 0	66.15
1.3775	1	4 2 1	68.00
1.3457	3	3 3 2	69.84
1.2880	3	4 2 2	73.46
1.2625	2	4 3 0	75.20
1.2377	26	5 1 0	76.98
1.2146	5	5 1 1	78.72
1.1721	19	5 2 0	82.17
1.1526	5	5 2 1	83.87
1.0824	2	5 3 0	90.74
1.0668	5	5 3 1	92.45
1.0518	8	4 4 2	94.17
1.0377	4	6 1 0	95.86
1.0237	3	6 1 1	97.61

References
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.

Westgren, A. and Phragmén, G. (1925). Z. Phys. 33, 777.

Molybdenum Oxide, MoO_2

Synonym
Molybdenum dioxide

CAS registry no.
18868-43-4

Sample
The sample was made at NBS by H. S. Parker by heating MoO_3 in a Mo boat for 20 hours at 372 °C in an atmosphere of 95% N_2 and 5% H_2 gases. This was followed by heating at 590 °C for 90 hours under the same conditions.

Color
Black

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. Distorted rutile structure. The structure of MoO_2 was studied by Magnéli et al. [1952] and by Magnéli and Andersson [1955]. The structure was refined by Brandt and Skapski [1967]. The latter gave the structure using the $P2_1/c$ form of the space group.

Lattice constants of this sample
a = 5.6068(7) Å
b = 4.8595(9)
c = 5.5373(9)
β = 119.37°

a/b = 1.1538
c/b = 1.1395

Volume
131.48 $Å^3$

Density
(calculated) 6.463 g/cm^3

Figure of merit
F_{30} = 25.5(0.017,68)

Additional patterns
PDF card 5-452 [Magnéli et al., Univ. of Uppasla, Sweden]

Magnéli et al. [1952]

Brandt and Skapski [1967]

References

Brandt, B. G. and Skapski, A. C. (1967). Acta Chem. Scand. 21, 661.

Magnéli, A. and Andersson, G. (1955). Acta Chem. Scand. 9, 1378.

Magnéli, A., Andersson, G., Blomberg, B., and Kihlborg, L. (1952). Anal. Chem., 24, 1998.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±6	hkℓ	2θ(°)
4.805	2	-1 0 1	18.45
3.420M	100	0 1 1	26.03
3.420M		-1 1 1	26.03
2.813	4	1 0 1	31.78
2.442	28	2 0 0	36.78
2.437	32	1 1 1	36.86
2.426	69	-2 1 1	37.03
2.403	34	-2 0 2	37.40
2.181	6	2 1 0	41.36
2.171M	2	0 2 1	41.57
2.171M		-1 2 1	41.57
2.156	5	-2 1 2	41.87
1.841	11	-3 0 1	49.48
1.725	28	2 1 1	53.04
1.723	34	2 2 0	53.11
1.711	41	-3 1 2	53.52
1.709	33	-2 2 2	53.58
1.6976	22	-2 1 3	53.97
1.6033	1	-3 0 3	57.43
1.5443	7	3 1 0	59.84
1.5360M	13	0 3 1	60.20
1.5360M		-1 3 1	60.20
1.5272	9	0 1 3	60.58
1.4676	4	-3 2 1	63.32
1.4057	4	2 0 2	66.46
1.4019M	21	-2 3 1	66.66
1.4019M		-4 0 2	66.66
1.3845	5	-2 0 4	67.61
1.3548	2	3 0 1	69.30
1.3448M	1	0 3 2	69.89
1.3448M		1 0 3	69.89
1.3381	1	-3 2 3	70.29
1.3033	5	-4 1 1	72.46
1.2912	5	-4 1 3	73.25
1.2829	1L	-3 1 4	73.80
1.2219	7	4 0 0	78.16
1.2175M	10	2 3 1	78.50
1.2175M		2 2 2	78.50
1.2146M	6	0 4 0	78.72
1.2146M		1 3 2	78.72
1.2076	7	-2 3 3	79.27
1.2028M	4	-2 2 4	79.65
1.2028M		-4 0 4	79.65
1.1837	2	3 2 1	81.20
1.1764	1	1 2 3	81.81

d(Å)	I^{rel} $\sigma = \pm 6$	hkℓ	2θ(°)
1.1485	2	3 3 0	84.24
1.1414	4	0 3 3	84.89
1.1155	1L	1 4 1	87.35
1.1113	2	-5 0 3	87.76
1.0911	6	4 2 0	89.82
1.0879M	10	2 4 0	90.16
1.0879M		-5 1 2	90.16
1.0849	8	0 4 2	90.47
1.0807	4	0 2 4	90.92
1.0780	8	-4 2 4	91.22

Neodymium Tantalum Oxide, $NdTaO_4$

Synonym
Neodymium tantalate

CAS registry no.
12344-26-4

Sample
The sample was prepared at NBS by heating Nd_2O_3 and Ta_2O_5 overnight at 1000 °C, grinding and reheating at 1600 °C for a period of 16-20 hours, and quenched.

Color
Very pale violet

Structure
Monoclinic, I2/a (15), Z = 4. The structure of $NdTaO_4$ has been determined using neutron powder diffraction by Santoro et al. [1980]. This phase was earlier reported to be in space group Ia(5) by Komkov [1959]. $NdTaO_4$ is isostructural with other rare earth niobates and tantalates [Roth et al., 1977]. The structure type is a distorted scheelite called beta-fergusonite (Ce) or brocenite. [Kuo et al., 1975].

Lattice constants of this sample
a = 5.5136(7)Å
b = 11.2356(8)
c = 5.1151(5)
β = 95.717(11)°

a/b = 0.4907
c/a = 0.4553

Volume
315.30 Å^3

Density
(calculated) 8.199 g/cm^3

Polymorphism
When heated to about 1320 °C $NdTaO_4$ undergoes a readily reversible phase change to a tetragonal structure of the fergusonite type, very similar to scheelite, $CaWO_4$ [Stubican, 1964].

Figure of Merit
F_{30} = 101.2(0.007,41)

Additional pattern
PDF card 16-745 [Stubican, 1964]

References
Komkov, A. I. (1959). Sov. Phys. Crystallogr. 4, 796.

Kuo, C., Wang, I., Wang, H., Wang, C., and Hou, H. (1973). Ti Chiu Hua Hsueh (Geochemica Peking) 2, 86.

Roth, R. S., Negas, T., Parker, H. S., Minor, D. B., and Jones, C. (1977). Mat. Res. Bull. 12, 1173.

Santoro, A., Marezio, M., Roth, R. S., and Minor, D. B. (1980). J. Solid State Chem. 35, 167.

Stubican, V. S. (1964). J. Amer. Ceram. Soc. 47, 55.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
5.619	5	0 2 0	15.76
4.930	8	1 1 0	17.98
3.221	100	-1 2 1	27.67
3.093	5	1 3 0	28.84
3.006	88	1 2 1	29.70
2.810	24	0 4 0	31.82
2.745	23	2 0 0	32.60
2.5447	21	0 0 2	35.24
2.4610	1L	-2 1 1	36.48
2.3191	1L	0 2 2	38.80
2.2047	1	1 4 1	40.90
2.1827	1	1 1 2	41.33
2.0925	1	-2 3 1	43.20
2.0797	2	1 5 0	43.48
2.0554	8	0 5 1	44.02
2.0218	3	-1 3 2	44.79
1.9718	11	2 3 1	45.99
1.9630	38	2 4 0	46.21
1.9130	3	1 3 2	47.49
1.8854	30	0 4 2	48.23
1.8730	2	0 6 0	48.57
1.8557	1	-2 2 2	49.05
1.7795	11	2 0 2	51.30
1.6950	21	-3 2 1	54.06
1.6912	20	-1 6 1	54.19
1.6775M	3	-2 5 1	54.67
1.6775M		0 1 3	54.67
1.6571	9	1 6 1	55.40
1.6408	3	-1 5 2	56.00
1.6141	10	2 5 1	57.01
1.6105	6	-2 4 2	57.15
1.6000M	29	3 2 1	57.56
1.6000M		-1 2 3	57.56
1.5812	2	1 5 2	58.31
1.5462M	4	2 6 0	59.76
1.5462M		-3 1 2	59.76
1.5406	5	1 7 0	60.00
1.5307	1	0 7 1	60.43
1.5184	12	1 2 3	60.97
1.5086	3	0 6 2	61.41

d(Å)	I^{rel} $\sigma = \pm 4$	hkℓ	2θ(°)
1.5030M	8	2 4 2	61.66
1.5030M		-3 4 1	61.66
1.4342M	5	3 4 1	64.97
1.4342M		-1 4 3	64.97
1.4181	1	3 5 0	65.80
1.4042	2	0 8 0	66.54
1.4015	1	-2 3 3	66.68
1.3715	4	4 0 0	68.34
1.3545M	1	-2 7 1	69.32
1.3545M		0 5 3	69.32
1.3345	3	-1 7 2	70.51
1.3224	1	-1 8 1	71.25
1.3066	1L	1 8 1	72.25
1.3018	2	1 7 2	72.56
1.2895M	3	2 6 2	73.36
1.2895M		-3 6 1	73.36
1.2726	6	0 0 4	74.50
1.2609	6	-4 0 2	75.31

Neodymium Titanium Oxide, Nd_2TiO_5

Synonym
Neodymium titanate

CAS registry no.
12058-94-5

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA. The material was heated at 1450 °C for 5½ days, then reheated at 1550 °C for 6½ days in a platinum crucible. Material appears to be slightly rich in TiO_2.

Color
Pale blue

Structure
Orthorhombic, Pnam (62), Z = 4, isostructural with La_2TiO_5. The structure of Nd_2TiO_5 was determined by Müller-Buschbaum and Scheunemann (1973).

Lattice constants of this sample

a = 10.7251(9) Å
b = 11.3407(10)
c = 3.8457(4)

a/b = 0.9457
c/b = 0.3391

Volume
467.75 $Å^3$

Density
(calculated) 5.913 g/cm^3

Figure of merit
F_{30} = 98.8(0.008,36)

References
Müller-Buschbaum, Hk. and Scheunemann, K. [1973]. J. Inorg. Nucl. Chem. 35, 1091.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
7.78	15	1 1 0	11.36
5.669	5	0 2 0	15.62
5.359	6	2 0 0	16.53
5.010	11	1 2 0	17.69
4.847	9	2 1 0	18.29
3.895	7	2 2 0	22.81
3.642	5	0 1 1	24.42
3.566	25	1 3 0	24.95
3.449	8	1 1 1	25.81
3.409	5	3 1 0	26.12
3.126	100	2 0 1	28.53
3.089	76	2 3 0	28.88
3.051	13	1 2 1	29.25
3.023	21	3 2 0	29.52
3.014	17	2 1 1	29.62
2.836	3	0 4 0	31.52
2.743	4	1 4 0	32.62
2.736	4	2 2 1	32.70
2.695	41	0 3 1	33.21
2.683	19	4 0 0	33.37
2.616	19	1 3 1	34.25
2.609	18	4 1 0	34.34
2.598	13	3 3 0	34.50
2.550	6	3 1 1	35.16
2.4082	1	2 3 1	37.31
2.3763	10	3 2 1	37.83
2.2187	9	1 5 0	40.63
2.1588	9	4 1 1	41.81
2.1529	16	3 3 1	41.93
2.1078	4	5 1 0	42.87
2.1004	6	2 4 1	43.03
2.0510	11	4 2 1	44.12
2.0070	3	5 2 0	45.14
1.9478	5	4 4 0	46.59
1.9233+	26	3 4 1	47.22
1.9233+		0 0 2	47.22
1.9009	42	4 3 1	47.81
1.8901	6	0 6 0	48.10
1.8650	8	5 3 0	48.79
1.8607	16	1 6 0	48.91
1.8483	8	5 1 1	49.26
1.8354	1	2 5 1	49.63
1.8206	2	0 2 2	50.06
1.7955	2	1 2 2	50.81
1.7873M	3	6 0 0	51.06

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.7873M		2 1 2	51.06
1.7785	10	5 2 1	51.33
1.7657	2	6 1 0	51.73
1.7376	4	4 4 1	52.63
1.7248	2	2 2 2	53.05
1.7150	9	3 5 1	53.38
1.7105	7	5 4 0	53.53
1.7049	5	6 2 0	53.72
1.6927	6	1 3 2	54.14
1.6758M	18	1 6 1	54.73
1.6758M		3 1 2	54.73
1.6710	8	3 6 0	54.90
1.6320	23	2 3 2	56.33
1.6227	11	3 2 2	56.68
1.6164M	13	6 3 0	56.92
1.6164M		2 6 1	56.92
1.6046	8	6 1 1	57.38
1.5916	1	0 4 2	57.89
1.5787	2	4 5 1	58.41
1.5745	1	1 4 2	58.58
1.5626M	7	5 4 1	59.07
1.5626M		4 0 2	59.07
1.5588M	6	6 2 1	59.23
1.5588M		5 5 0	59.23
1.5481	6	4 1 2	59.68
1.5448M	8	3 3 2	59.82
1.5448M		4 6 0	59.82
1.5323	7	3 6 1	60.36
1.5184	5	7 1 0	60.97
1.5121	2	6 4 0	61.25
1.4932	2	0 7 1	62.11
1.4787M	4	7 2 0	62.79
1.4787M		1 7 1	62.79
1.4538	5	3 4 2	63.99
1.4445M	1	5 5 1	64.45
1.4445M		4 3 2	64.45
1.4384	3	2 7 1	64.76
1.4206M	3	5 1 2	65.67
1.4206M		7 3 0	65.67
1.4181M	3	5 6 0	65.80
1.4181M		0 8 0	65.80
1.4070	4	6 4 1	66.39
1.4042	3	6 5 0	66.54
1.3880	3	5 2 2	67.42
1.3807	3	7 2 1	67.82
1.3777	3	3 7 1	67.99
1.3685	3	4 4 2	68.51

Neodymium Titanium Oxide, $Nd_2Ti_2O_7$

Synonym
Neodymium titanate

CAS registry no.
12035-31-3

Sample
The sample was prepared at NBS by solid state reaction of stoichiometric amounts of Nd_2O_3 and TiO_2. The mixture was heated at 1200 °C for 1 day, then ground and heated at 1425 °C for 6 days.

Color
Unground, light violet
Ground, very light purplish blue

Structure
Monoclinic, $P2_1$ (4), Z = 4. [Kimura et al., 1974].

Lattice constants of this sample
a = 13.008(2)Å
b = 5.4648(7)
c = 7.679(2)
β = 98.56(2)°

a/b = 2.3803
c/b = 1.4052

Volume
539.79 Å^3

Density
(calculated) 6.107 g/cm^3

Figure of merit
F_{30} = 41.7(0.012,61)

Additional pattern
PDF card 29-923 [Smith, C. and McCarthy (1977). Pennsylvania State Univ., University Park, PA]

Reference
Kimura, M., Nanamatsu, S., Kauamura, T., and Matsushita, S. (1974). Jpn. J. Appl. Phys. 13, 1473.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
12.87	1L	1 0 0	6.86
7.03	1L	-1 0 1	12.59
6.43	9	2 0 0	13.76
6.15	1L	1 0 1	14.39
5.029	5	1 1 0	17.62
4.432	1L	0 1 1	20.02
4.314	1L	-1 1 1	20.57
4.162	46	2 1 0	21.33
4.085	1	1 1 1	21.74
3.998	1	-3 0 1	22.22
3.797M	12	-1 0 2	23.41
3.797M		0 0 2	23.41
3.511M	1L	2 1 1	25.35
3.511M		-2 0 2	25.35
3.372	9	3 1 0	26.41
3.216	50	4 0 0	27.72
3.119M	26	-1 1 2	28.60
3.119M		0 1 2	28.60
3.077M	13	-3 0 2	29.00
3.077M		2 0 2	29.00
2.950M	100	-2 1 2	30.27
2.950M		1 1 2	30.27
2.770	29	4 1 0	32.29
2.732	35	0 2 0	32.75
2.681M	50	-3 1 2	33.40
2.681M		2 1 2	33.40
2.654M	24	-4 0 2	33.74
2.654M		3 0 2	33.74
2.571M	3	5 0 0	34.87
2.571M		0 2 1	34.87
2.556M	4	-1 0 3	35.08
2.556M		-5 0 1	35.08
2.548	3	-1 2 1	35.20
2.503	1	4 1 1	35.85
2.431	1L	-2 2 1	36.95
2.387M	1L	-4 1 2	37.65
2.387M		3 1 2	37.65
2.347	2	2 2 1	38.32
2.328	6	5 1 0	38.64
2.315M	3	-1 1 3	38.87
2.315M		-5 1 1	38.87
2.293M	2	-5 0 2	39.26
2.293M		4 0 2	39.26
2.256	3	-3 2 1	39.93
2.218M	18	-1 2 2	40.64
2.218M		0 2 2	40.64
2.154M	4	-2 2 2	41.90
2.154M		1 2 2	41.90
2.144	6	6 0 0	42.12
2.114M	12	-5 1 2	42.74
2.114M		4 1 2	42.74
2.082	26	4 2 0	43.43
2.043M	14	-3 2 2	44.30
2.043M		2 2 2	44.30
1.9961M	10	5 0 2	45.40

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
1.9961M		6 1 0	45.40
1.9605	1	4 2 1	46.27
1.9558	1	-5 0 3	46.39
1.9199M	28	-1 0 4	47.31
1.9199M		3 1 3	47.31
1.9043M	18	-4 2 2	47.72
1.9043M		3 2 2	47.72
1.8748	20	5 1 2	48.52
1.8682M	10	6 1 1	48.70
1.8682M		-1 2 3	48.70
1.8593	5	4 0 3	48.95
1.8403+	1	-5 1 3	49.49
1.8403+		-3 0 4	49.49
1.8368	1	7 0 0	49.59
1.8038	1L	1 3 0	50.56
1.7756M	4	-3 2 3	51.42
1.7756M		5 2 1	51.42
1.7708M	4	0 3 1	51.57
1.7708M		-6 0 3	51.57
1.7584	8	6 0 2	51.96
1.7531+	10	-4 0 4	52.13
1.7531+		2 3 0	52.13
1.7438M	13	-3 1 4	52.43
1.7438M		1 1 4	52.43
1.7282	1	7 0 1	52.94
1.6927	2	2 3 1	54.14
1.6872	4	6 2 0	54.33
1.6744M	7	-7 1 2	54.78
1.6744M		6 1 2	54.78
1.6688M	4	-4 1 4	54.98
1.6688M		2 1 4	54.98
1.6574	3	-3 3 1	55.39
1.6481M	13	7 1 1	55.73
1.6481M		3 0 4	55.73
1.6424M	10	-1 3 2	55.94
1.6424M		0 3 2	55.94
1.6164+	12	-2 3 2	56.92
1.6164+		1 3 2	56.92
1.6125M	6	-6 2 2	57.07
1.6125M		5 2 2	57.07
1.6084M	3	5 1 3	57.23
1.6084M		8 0 0	57.23
1.5901	2	-5 2 3	57.95
1.5846	6	4 3 0	58.17
1.5782M	9	-5 1 4	58.43
1.5782M		3 1 4	58.43
1.5706	20	-1 2 4	58.74
1.5679M	24	-3 3 2	58.85
1.5679M		2 3 2	58.85
1.5597M	4	-2 2 4	59.19
1.5597M		0 2 4	59.19
1.5422	5	8 1 0	59.93
1.5387	5	-6 0 4	60.08
1.5279M	2	6 0 3	60.55
1.5279M		8 0 1	60.55
1.5050	5	7 1 2	61.57
1.4861M	2	5 3 0	62.44
1.4861M		-6 2 3	62.44
1.4791M	5	-7 2 2	62.77
1.4791M		0 3 3	62.77
1.4713M	3	6 1 3	63.14
1.4713M		8 1 1	63.14
1.4295M	3	5 0 4	65.21
1.4295M		9 0 0	65.21

Neodymium Titanium Oxide, $Nd_4Ti_9O_{24}$

Synonym
Neodymium titanate

Sample
The sample was prepared at NBS using $BaTiO_3$, TiO_2, and very low alkaline content Nd_2O_3. Stoichiometric amounts of the constituents were blended with mortar and pestle, then calcined in a platinum crucible, with periodic grindings. An initial calcine at 1250 °C for 1 day, followed by a second heating at 1350 °C for about 3 days was sufficient to yield a single phase product.

Color
Very light purplish blue

Structure
Orthorhombic, Fddd (70), determined from a single crystal, by Kolar et al. [1981]. Z = 16 is consistent with the density of 5.13, measured by Kolar et al. [1978].

Lattice constants of this sample
a = 14.475(2) Å
b = 35.304(5)
c = 13.996(2)

a/b = 0.4100
c/b = 0.3964

Volume
7152.3 Å^3

Density
(calculated) 5.171 g/cm^3
(observed) 5.13 [Kolar et al., 1978]

Figure of merit
F_{30} = 53.1(0.011,51)

Additional patterns
Kolar et al. [1981]

Kolar et al. [1978], labeled $Nd_2Ti_4O_{11}$

References
Kolar, D. Gaberšček, S., Barbulescu, A., and Volavšek, B. (1978). J. Less-Common Metals 60, 137.

Kolar, D., Gaberšček, S., Volavšek, B., Parker, H. S., and Roth, R. S. (1981). J. Solid State Chem. 38, 158.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
9.70	4	1 1 1	9.11
6.71	4	2 2 0	13.19
6.51	4	0 2 2	13.60
5.775	10	1 5 1	15.33
5.029	10	2 0 2	17.62
4.512M	5	1 7 1	19.66
4.512M		0 6 2	19.66
4.412M	11	0 8 0	20.11
4.412M		1 1 3	20.11
4.373	6	2 4 2	20.29
4.157	5	1 3 3	21.36
3.759	3	1 5 3	23.65
3.655	2	1 9 1	24.33
3.617	2	4 0 0	24.59
3.500	3	0 0 4	25.43
3.382	17	3 7 1	26.33
3.347	100	4 4 0	26.61
3.317	46	2 8 2	26.86
3.251	92	0 4 4	27.41
3.225	9	3 3 3	27.64
3.172	18	2 10 0	28.11
3.151	12	0 10 2	28.30
3.102	4	2 2 4	28.76
3.056	4	1 11 1	29.20
3.030	18	3 5 3	29.46
2.974	25	3 9 1	30.02
2.941M	22	0 12 0	30.37
2.941M		1 9 3	30.37
2.823M	14	5 1 1	31.67
2.823M		4 6 2	31.67
2.793	14	3 7 3	32.02
2.778	5	2 6 4	32.20
2.741M	5	0 8 4	32.64
2.741M		1 1 5	32.64
2.677	3	1 3 5	33.45
2.623M	19	3 11 1	34.16
2.623M		1 13 1	34.16
2.601	5	1 11 3	34.45
2.549	5	3 9 3	35.18
2.540	19	2 12 2	35.31
2.516	26	4 0 4	35.66
2.488	4	4 2 4	36.07
2.419	1	4 4 4	37.14
2.391	9	6 2 0	37.59
2.379	3	4 10 2	37.79

d(Å)	I^{rel}	hkℓ	2θ(°)
	σ = ±3		
2.351	6	2 10 4	38.25
2.334	1	3 13 1	38.55
2.313M	6	4 6 4	38.90
2.313M		0 2 6	38.90
2.298	7	5 9 1	39.17
2.283	14	4 12 0	39.43
2.251M	9	0 12 4	40.02
2.251M		1 9 5	40.02
2.231	7	6 6 0	40.39
2.220	5	2 0 6	40.61
2.207M	14	6 4 2	40.85
2.207M		0 16 0	40.85
2.186	14	4 8 4	41.27
2.168	12	0 6 6	41.62
2.153	9	2 4 6	41.92
2.111	11	3 13 3	42.81
2.091	2	3 15 1	43.23
2.087	2	1 11 5	43.33
2.081	2	1 15 3	43.46
2.0431	1	7 1 1	44.30
2.0257	3	6 8 2	44.70
2.0206	5	2 16 2	44.82
1.9833M	10	5 3 5	45.71
1.9833M		2 8 6	45.71
1.9779	8	1 1 7	45.84
1.9730	8	6 2 4	45.96
1.9682	14	2 14 4	46.08
1.9650	11	7 5 1	46.16
1.9522M	3	1 3 7	46.48
1.9522M		5 11 3	46.48
1.9466	7	0 10 6	46.62
1.9268	3	3 15 3	47.13
1.9062	2	1 5 7	47.67
1.8938	7	2 18 0	48.00
1.8887+	12	0 18 2	48.14
1.8887+		7 1 3	48.14
1.8813M	9	6 6 4	48.34
1.8813M		1 17 3	48.34
1.8672M	3	7 3 3	48.73
1.8672M		0 16 4	48.73
1.8611	1	4 6 6	48.90
1.8441M	3	3 1 7	49.38
1.8441M		1 7 7	49.38
1.8237M	5	3 3 7	49.97
1.8237M		5 13 3	49.97
1.8091	17	8 0 0	50.40
1.8028	17	6 12 2	50.59
1.7718M	20	8 4 0	51.54
1.7718M		2 12 6	51.54
1.7491	9	0 0 8	52.26

d(Å)	I^{rel}	hkℓ	2θ(°)
	σ = ±3		
1.7435M	7	6 14 0	52.44
1.7435M		8 2 2	52.44
1.7309	8	6 10 4	52.85
1.7138M	21	1 19 3	53.42
1.7138M		4 10 6	53.42
1.7032	9	7 9 3	53.78
1.6878	6	3 15 5	54.31
1.6767	8	6 0 6	54.70
1.6707M	6	3 9 7	54.91
1.6707M		2 4 8	54.91
1.6577M	5	4 16 4	55.38
1.6577M		1 21 1	55.38
1.6470+	1L	6 4 6	55.77
1.6470+		7 3 5	55.77
1.6437	1L	5 1 7	55.89
1.6338M	2	7 13 1	56.26
1.6338M		2 6 8	56.26
1.6290+	7	5 3 7	56.44
1.6290+		7 11 3	56.44
1.6251	7	3 19 3	56.59
1.6167	3	5 13 5	56.91
1.6005+	5	8 2 4	57.54
1.6005+		1 13 7	57.54
1.5864+	5	2 8 8	58.10
1.5864+		4 20 0	58.10
1.5814	12	8 4 4	58.30
1.5762M	10	3 17 5	58.51
1.5762M		0 20 4	58.51
1.5718	5	1 21 3	58.69
1.5677M	12	6 8 6	58.86
1.5677M		2 22 0	58.86
1.5641M	7	0 22 2	59.01
1.5641M		5 7 7	59.01
1.5504M	7	4 4 8	59.58
1.5504M		8 6 4	59.58
1.5481M	6	4 14 6	59.68
1.5481M		4 20 2	59.68
1.5413	2	8 12 0	59.97
1.5318M	3	2 10 8	60.38
1.5318M		7 9 5	60.38
1.5284	2	2 22 2	60.53
1.5188	1L	9 1 3	60.95

Nickel Titanium Oxide, $NiTiO_3$

Synonyms
Nickel titanate
Nickel metatitanate

CAS registry no.
12035-39-1

Sample
The sample obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA was a mixture of oxides. It was heated at 1050 °C for 4½ days in order to obtain a single phase.

Color
Medium yellow

Structure
Hexagonal, $R\bar{3}$ (148), Z = 6, isostructural with $FeTiO_3$, Taylor [1930]. The structure of $NiTiO_3$ was determined by Sullivan and Pavlovic [1962].

Lattice constants of this sample
a = 5.0302(2) Å
c = 13.7905(11)

c/a = 2.7415

Volume
302.19 $Å^3$

Density
(calculated) 5.097 g/cm^3

Figure of merit
F_{30} = 66.9(0.012,39)

Additional patterns
PDF card 17-617 [Skapski, Imperial College of Sci. and Tech., London, Eng., Thesis, priv. comm.]

Barth and Posnjak [1934]

References
Barth, T. F. W. and Posnjak, E. (1934). Z. Kristallogr. Kristallogeom. Kristallphys. Kristallchem. 88A, 271.

Sullivan, D. G. and Pavlovic, A. S. (1962). Proc. W. V. Acad. Sci. 34, 173.

Taylor, N. W. (1930). Z. Phys. Chem. Leipzig B9, 241.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
4.598	2	0 0 3	19.29
3.685	41	0 1 2	24.13
2.705	100	1 0 4	33.09
2.516	70	1 1 0	35.65
2.332	7	0 1 5	38.58
2.299	3	0 0 6	39.15
2.207	30	1 1 3	40.86
2.151	1	0 2 1	41.96
2.077	3	2 0 2	43.53
1.8417	36	0 2 4	49.45
1.7949	1	1 0 7	50.83
1.6962	53	1 1 6	54.02
1.6352	1	2 1 1	56.21
1.6025M	9	0 1 8	57.46
1.6025M		1 2 2	57.46
1.5327	1L	0 0 9	60.34
1.4859	26	2 1 4	62.45
1.4522	28	3 0 0	64.07
1.4138	1	1 2 5	66.03
1.3518	3	2 0 8	69.48
1.3146	10	1 0 10	71.74
1.3086	3	1 1 9	72.12
1.2632	1	2 1 7	75.15
1.2575	7	2 2 0	75.55
1.2275	3	3 0 6	77.74
1.2129	2	2 2 3	78.85
1.1903M	4	1 2 8	80.65
1.1903M		3 1 2	80.65
1.1650	5	0 2 10	82.78
1.1492	1	0 0 12	84.18
1.1405	6	1 3 4	84.97
1.1032	7	2 2 6	88.57
1.0757	1L	0 4 2	91.46
1.0570	7	2 1 10	93.56
1.0385	3	4 0 4	95.76
.9894	3	3 1 8	102.26
.9721	2	2 2 9	104.82
.9598	6	3 2 4	106.75
.9506	4	4 1 0	108.26
.9309	1	4 1 3	111.68
.9207	1	0 4 8	113.58
.9088	5	1 3 10	115.90

Potassium Fluoride Hydrate, $KF \cdot 2H_2O$

Synonym
Potassium fluoride dihydrate

CAS registry no.
7789-23-3

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

Color
Colorless

Structure
Orthorhombic, $Pb2_1m$ (26), Z = 2. The structure was determined by Anderson and Lingafelter [1951].

Lattice constants of this sample
a = 5.1848(7) Å
b = 8.8328(12)
c = 4.0850(6)

a/b = 0.5870
c/b = 0.4625

Volume
187.08 $Å^3$

Density
(calculated) 1.671 g/cm^3

Figure of merit
F_{30} = 110.4(0.009,32)

Additional pattern
PDF card 1-854 [Hanawalt et al., 1938]

References
Anderson, T. H. and Lingafelter, E. C. (1951). Acta Crystallogr. 4, 181.

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

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

d(Å)	$I^{rél}$ σ = ±5	hkℓ	2θ(°)
5.181	5	1 0 0	17.10
4.469	22	1 1 0	19.85
4.414	36	0 2 0	20.10
4.083	10	0 0 1	21.75
3.363	52	1 2 0	26.48
3.209	39	1 0 1	27.78
3.015	100	1 1 1	29.61
2.999	8	0 2 1	29.77
2.598	50	1 2 1	34.50
2.561	35	1 3 0	35.01
2.487	8	2 1 0	36.08
2.2356	5	2 2 0	40.31
2.2083	3	0 4 0	40.83
2.1692	25	1 3 1	41.60
2.1249	58	2 1 1	42.51
2.0426	23	0 0 2	44.31
2.0322	10	1 4 0	44.55
1.9618	9	2 2 1	46.24
1.9455	26	2 3 0	46.65
1.9427	35	0 4 1	46.72
1.9009	3	1 0 2	47.81
1.8579	7	1 1 2	48.99
1.8536	7	0 2 2	49.11
1.8193	4	1 4 1	50.10
1.7578	5	2 3 1	51.98
1.7453	8	1 2 2	52.38
1.7282	1	3 0 0	52.94
1.6962	11	3 1 0	54.02
1.6815	1L	2 4 0	54.53
1.6722	1L	1 5 0	54.86
1.6089	3	3 2 0	57.21
1.5969	8	1 3 2	57.68
1.5782	3	2 1 2	58.43
1.5662	1L	3 1 1	58.92
1.5075	1	2 2 2	61.46
1.4978	6	3 2 1	61.90
1.4599	5	2 5 0	63.69
1.4406	4	1 4 2	64.65
1.4157	1	1 6 0	65.93
1.4088	5	2 3 2	66.29
1.4001	4	3 3 1	66.76
1.3847	4	0 6 1	67.60

Potassium Iron Cyanide, $K_4Fe(CN)_6$

Synonym
Potassium ferrocyanide

CAS registry no.
13943-58-3

Sample
The sample was prepared by heating reagent $K_4Fe(CN)_6 \cdot H_2O$ at 115 °C for 3 weeks.

Color
Pale yellow

Structure
Orthorhombic, Bmmm (65), Z = 4. The cell was found by use of the Visser program [1969]. The space group was assigned by consideration of the absences in the powder pattern.

Lattice constants of this sample
a = 14.010(7) Å
b = 21.027(6)
c = 4.1751(13)

a/b = 0.6663
c/a = 0.1986

Volume
368.35 Å^3

Density
(calculated) 1.989 g/cm^3

Figures of merit
F_{30} = 24.1(0.015,83)
M_{20} = 20.7

Additional pattern
PDF card 1-0877 [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.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
10.51	5	0 2 0	8.41
6.66	7	2 1 0	13.29
5.254	10	0 4 0	16.86
4.957	12	2 3 0	17.88
4.201M	16	0 5 0	21.13
4.201M		2 4 0	21.13
3.999	6	1 0 1	22.21
3.929	13	1 1 1	22.61
3.739	11	1 2 1	23.78
3.604	89	2 5 0	24.68
3.500M	24	0 6 0	25.43
3.500M		4 0 0	25.43
3.477	22	1 3 1	25.60
3.134M	47	2 6 0	28.46
3.134M		4 3 0	28.46
3.078	39	3 1 1	28.99
2.985	100	3 2 1	29.91
2.844	65	3 3 1	31.43
2.759	22	2 7 0	32.43
2.626	2	0 8 0	34.11
2.501	7	3 5 1	35.88
2.402	10	1 7 1	37.41
2.206	22	5 3 1	40.88
2.197	35	1 8 1	41.05
2.129	32	5 4 1	42.43
2.102M	11	0 10 0	43.00
2.102M		4 8 0	43.00
2.087	20	0 0 2	43.31
2.040	21	6 5 0	44.36
2.015	8	2 10 0	44.95
2.009	8	3 8 1	45.09
1.943M	7	4 9 0	46.71
1.943M		6 6 0	46.71
1.842	7	6 7 0	49.43
1.807	16	2 5 2	50.47
1.8031	18	4 10 0	50.58
1.7453M	8	6 8 0	52.38
1.7453M		8 1 0	52.38

Potassium Vanadium Oxide, KVO_3

Synonym
Potassium vanadate

Sample
The sample was prepared at NBS by fusing K_2CO_3 and V_2O_5.

Color
Greyish pink

Structure
Orthorhombic, Pmab (57), Z = 4, isostructural with NH_4VO_3 [Evans and Block, 1954]. The structure was determined by Petrášová et al. [1958].

Lattice constants of this sample
a = 5.6955(12)Å
b = 10.7961(10)
c = 5.1796(3)

a/b = 0.5276
c/a = 0.4798

Volume
318.49 Å^3

Density
(calculated) 2.879 g/cm^3

Figure of merit
F_{30} = 107.3(0.007,41)

Additional pattern
PDF card 26-1342 [Feigelson et al., 1972]

References
Evans, H. T. Jr. and Block, S. (1954). Am. Mineral. 39, 326.

Feigelson, R. S., Martin, G. W., and Johnson, B. C. (1972). J. Cryst. Growth 13-14, 686.

Petrášová, M., Maďar, J., and Hanič, F. (1958). Chem. Zvesti 12, 410.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
5.397	9	0 2 0	16.41
5.181	18	0 0 1	17.10
4.672	1L	0 1 1	18.98
3.917	16	1 2 0	22.68
3.737	18	0 2 1	23.79
3.612	6	1 1 1	24.63
3.125	100	1 2 1	28.54
2.955	3	0 3 1	30.22
2.847	45	2 0 0	31.40
2.700	9	0 4 0	33.15
2.623	15	1 3 1	34.16
2.590	18	0 0 2	34.61
2.5185M	2	2 2 0	35.62
2.5185M		0 1 2	35.62
2.4391	18	1 4 0	36.82
2.3946	7	0 4 1	37.53
2.3353	6	0 2 2	38.52
2.3031	10	1 1 2	39.08
2.2063	2	1 4 1	40.87
2.1608	1	1 2 2	41.77
2.1018	4	0 3 2	43.00
2.0505	3	2 3 1	44.13
1.9932	3	0 5 1	45.47
1.9594	15	2 4 0	46.30
1.9164	5	2 0 2	47.40
1.8813	3	1 5 1	48.34
1.8686	3	0 4 2	48.69
1.7992	2	0 6 0	50.70
1.7753	6	1 4 2	51.43
1.7261	1	0 0 3	53.01
1.7040	9	0 1 3	53.75
1.6999	10	0 6 1	53.89
1.6915M	10	3 2 1	54.18
1.6915M		2 3 2	54.18
1.6585	1	0 5 2	55.35
1.6446	2	0 2 3	55.86
1.6328M	2	1 1 3	56.30
1.6328M		2 5 1	56.30
1.6290	2	1 6 1	56.44
1.5926	2	1 5 2	57.85
1.5799	6	1 2 3	58.36
1.5624	3	2 4 2	59.08
1.5571	3	0 3 3	59.30
1.5531	3	3 4 0	59.47
1.5206	2	2 6 0	60.87

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.5011	2	1 3 3	61.75
1.4774+	2	0 7 1	62.85
1.4774+		0 6 2	62.85
1.4591	7	2 6 1	63.73
1.4550	8	0 4 3	63.93
1.4233M	5	2 2 3	65.53
1.4233M		4 0 0	65.53
1.4090M	2	1 4 3	66.28
1.4090M		3 3 2	66.28
1.3661	2	2 3 3	68.65
1.3489M	1	0 8 0	69.65
1.3489M		0 5 3	69.65
1.3129	5	1 8 0	71.85
1.2949M	1L	2 4 3	73.01
1.2949M		0 0 4	73.01
1.2856	2	0 1 4	73.62
1.2729	2	1 8 1	74.48
1.2591M	2	4 4 0	75.44
1.2591M		0 2 4	75.44
1.2540	1	1 1 4	75.80
1.2459	3	0 6 3	76.38
1.2431	3	3 2 3	76.58
1.2296	1L	1 2 4	77.58
1.2184M	1	2 5 3	78.43
1.2184M		0 3 4	78.43

Silicon Nitride, β-Si_3N_4

Synonym
Trisilicon tetranitride

CAS registry no.
12033-89-5

Sample
The sample was prepared at NBS by J. Waring by heating Si_3N_4 obtained from GTE Products, Towanda, PA to 1785 °C for 1 hr at 15 psig. The sample was contained in a Si_3N_4 crucible within a molybdenum crucible.

Color
Greyish white

Structure
Hexagonal, $P6_3/m$ (176), Z = 2. The structure was determined by Hardie and Jack [1957] and confirmed by Borgen and Seip [1961].

Lattice constants of this sample
a = 7.6044(2)Å
c = 2.9075(1)

c/a = 0.3823

Volume
145.61 $Å^3$

Density
(calculated) 3.200 g/cm^3

Polymorphism
Turkdogan and Ignatowicz (1957) established the existence of two forms of Si_3N_4. These two forms α and β generally occur together. Ruddlesden and Popper (1958) reported the possibility of a third form having still a different stacking sequence.

Figure of merit
F_{30} = 108.2(0.009,32)

Additional patterns
PDF card 9-259 [Decker, General Elec. Co., NY, priv. comm.)

PDF card 29-1132 [Morris et al., 1977]

Hardie and Jack [1957]

Ruddlesden and Popper [1958]

Narita and Mori [1959]

References
Borgen, O. and Seip, H. M. (1961). Acta Chem. Scand. 15, 1789.

Hardie, D. and Jack, K. H. (1957). Nature London 180, 332.

Morris, M. C., McMurdie, H. F., Evans, E. H., Paritzkin, B., de Groot, J. H., Newberry, R., Hubbard, C. R., and Carmel, S. J. (1977). Natl. Bur. Stand. U.S. Monogr. 25, Sec. 14, 116.

Narita, K. and Mori, K. (1959). Bull. Chem. Soc. Jpn. 32, 417.

Ruddlesden, S. N. and Popper, P. (1958). Acta Crystallogr. 11, 465.

Turkdogan, E. T. and Ignatowicz, S. (1957). J. Iron Steel Inst. London 185, 200.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.583	34	1 0 0	13.44
3.800	35	1 1 0	23.39
3.293	100	2 0 0	27.06
2.660	99	1 0 1	33.67
2.489	93	2 1 0	36.05
2.310	9	1 1 1	38.95
2.1939	10	3 0 0	41.11
2.1797	31	2 0 1	41.39
1.9013	8	2 2 0	47.80
1.8916	5	2 1 1	48.06
1.8275	12	3 1 0	49.86
1.7525	37	3 0 1	52.15
1.5911	12	2 2 1	57.91
1.5467	6	3 1 1	59.74
1.5108	15	3 2 0	61.31
1.4534	15	0 0 2	64.01
1.4368	8	4 1 0	64.84
1.4325	5	4 0 1	65.06
1.4197	1	1 0 2	65.72
1.3579	1	1 1 2	69.12
1.3408	39	3 2 1	70.13
1.3299	6	2 0 2	70.79
1.3173	5	5 0 0	71.57
1.2883	18	4 1 1	73.44
1.2675	7	3 3 0	74.85
1.2554	16	2 1 2	75.70
1.2447	1	4 2 0	76.47
1.1998	2	5 0 1	79.89
1.1831	2	5 1 0	81.25
1.1618	1L	3 3 1	83.06
1.1551	2	2 2 2	83.65
1.1445	3	4 2 1	84.60
1.1377	3	3 1 2	85.23
1.0957	4	5 1 1	89.34
1.0828	3	4 3 0	90.70
1.0545	1L	5 2 0	93.85
1.0476	6	3 2 2	94.66
1.0269	1L	6 0 1	97.20
1.0219	4	4 1 2	97.84
1.0147	1	4 3 1	98.78

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.0043	2	6 1 0	100.17
.9914	3	5 2 1	101.97
.9761	4	5 0 2	104.21
.9589	3	1 0 3	106.90
.9554	5	3 3 2	107.46
.9492	8	6 1 1	108.49
.9455	1	4 2 2	109.12
.9408	1	5 3 0	109.93
.9298	2	2 0 3	111.89
.9175	1	5 1 2	114.19
.9132	3	6 2 0	115.02
.9034	4	4 4 1	117.00
.8950	3	5 3 1	118.78
.8866	5	3 0 3	120.65
.8722	6	7 1 0	124.06
.8712	5	6 2 1	124.29
.8682	5	4 3 2	125.05
.8634	1	2 2 3	126.29
.8561	1	3 1 3	128.27
.8537	2	5 2 2	128.93

Silicon Oxide (Quartz-low), α-SiO_2

Synonym
Silicon dioxide

CAS registry no.
7631-86-9

Sample
The sample was obtained from the Glass Section at NBS. The material was ground single crystals of optical quality.

Color
Colorless

Structure
Hexagonal, $P3_121$ (152), Z = 3, Bragg and Gibbs [1925]. Iwai et al. [1969] and Smith and Alexander [1963] refined the structure. Thermal effects have also been studied by these authors.

Lattice constants of this sample
a = 4.9133(2) Å
c = 5.4053(4)

c/a = 1.1001

Volume
113.00 Å^3

Density
(calculated) 2.649 g/cm^3

Polymorphism
Silicon oxide, SiO_2, crystallizes in many other polymorphic forms.

Figure of merit
F_{30} = 77.6(0.013,31)

Reference intensity
$I/I_{corundum}$ = 4.32(3)

Additional pattern
PDF card 5-490 [Swanson et al., 1954], pattern redone to reflect improved techniques for measuring intensities. Citation to many additional patterns is made in the above reference.

References

Bragg, W. H. and Gibbs, R. E. (1925). Proc. Roy. Soc. London A109, 405.

Iwai, et al. (1969). Yogyo Kyokai Shi (J. Ceram. Assoc. Japan) 77, 172.

Smith, G. S. and Alexander, L. (1963). Acta Crystallogr. 16, 462.

Swanson, H. S., Fuyat, R. K., and Ugrinic, G. M. (1954). Natl. Bur. Stand. U.S. Circ. 539, 3, 24.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
4.257	22	1 0 0	20.85
3.342	100	1 0 1	26.65
2.457	8	1 1 0	36.54
2.282	8	1 0 2	39.46
2.237	4	1 1 1	40.29
2.127	6	2 0 0	42.47
1.9792	4	2 0 1	45.81
1.8179	14	1 1 2	50.14
1.8021	1L	0 0 3	50.61
1.6719	4	2 0 2	54.87
1.6591	2	1 0 3	55.33
1.6082	1L	2 1 0	57.24
1.5418	9	2 1 1	59.95
1.4536	1	1 1 3	64.00
1.4189	1L	3 0 0	65.76
1.3820	6	2 1 2	67.75
1.3752	7	2 0 3	68.13
1.3718	8	3 0 1	68.32
1.2880	2	1 0 4	73.46
1.2558	2	3 0 2	75.67
1.2285	1	2 2 0	77.66
1.1999	2	2 1 3	79.88
1.1978	1	2 2 1	80.05
1.1843	3	1 1 4	81.15
1.1804	3	3 1 0	81.47
1.1532	1	3 1 1	83.82
1.1405	1L	2 0 4	84.97
1.1143	1L	3 0 3	87.46
1.0813	2	3 1 2	90.86
1.0635	1L	4 0 0	92.82
1.0476	1	1 0 5	94.66
1.0438	1L	4 0 1	95.12
1.0347	1L	2 1 4	96.22
1.0150	1	2 2 3	98.74
.9898	1	4 0 2	102.20
.9873	1	3 1 3	102.56
.9783	1L	3 0 4	103.88
.9762	1	3 2 0	104.20
.9636	1L	2 0 5	106.14
.9607	1	3 2 1	106.61
.9284	1L	4 1 0	112.13
.9181	1L	3 2 2	114.08
.9161	1	4 0 3	114.46
.9151	1L	4 1 1	114.66
.9089	1L	2 2 4	115.89

Sodium Aluminum Oxide, β-$NaAlO_2$

Synonym
Sodium aluminate

CAS registry no.
1302-42-7

Sample
The sample was obtained from ICN-K&K Laboratories, Inc., Plainview, NY. It was partially hydrated and was heated in air to 875 °C for 1 hour. It changed back readily to a hydrate.

Color
Colorless

Structure
Orthorhombic, $Pna2_1$ (33), Z = 4, isostructural with orthorhombic sodium ferrite, β-$NaFeO_2$. The unit cell and space group were determined by Théry and Briançon [1964].

Lattice constants of this sample
a = 5.3868(11) Å
b = 7.0334(15)
c = 5.2182(10)

a/b = 0.7659
c/b = 0.7419

Volume
197.70 Å^3

Density
(calculated) 2.754 g/cm^3

Polymorphism
There is a tetragonal γ-form, stable at high temperatures. The temperature of transformation $\beta \rightarrow \gamma$ is 470 °C [ibid.].

Figure of merit
F_{30} = 58.6(0.013,39)

Additional pattern
PDF card 19-1177 [ibid.]

Reference
Théry, J. and Briançon, D. (1964). Rev. Int. Hautes Temp. Refract. 1, 221.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
4.283	35	1 1 0	20.72
4.195	34	0 1 1	21.16
3.306	4	1 1 1	26.95
2.946	84	1 2 0	30.31
2.695	74	2 0 0	33.22
2.609	94	0 0 2	34.34
2.564	100	1 2 1	34.96
2.515	7	2 1 0	35.67
2.393	14	2 0 1	37.55
2.267	4	2 1 1	39.72
2.227	5	1 1 2	40.47
2.148	10	1 3 0	42.03
2.139M	12	0 3 1	42.21
2.139M		2 2 0	42.21
2.096	2	0 2 2	43.13
1.987	8	1 3 1	45.62
1.953	24	1 2 2	46.47
1.8740	16	2 0 2	48.54
1.8108	3	2 1 2	50.35
1.7695	8	2 3 0	51.61
1.7578	24	0 4 0	51.98
1.7395	4	3 1 0	52.57
1.6886	3	0 1 3	54.28
1.6741	5	2 3 1	54.79
1.6591	4	1 3 2	55.33
1.6541	5	2 2 2	55.51
1.5989	33	3 2 0	57.60
1.5286	8	3 2 1	60.52
1.4974	35	1 2 3	61.92
1.4722	15	2 4 0	63.10
1.4581	22	0 4 2	63.78
1.4170	13	2 4 1	65.86
1.3971	2	0 3 3	66.92
1.3754	3	3 3 1	68.12
1.3631	25	3 2 2	68.82
1.3039M	10	0 0 4	72.42
1.3039M		4 0 1	72.42
1.2823M	9	2 4 2	73.84
1.2823M		4 1 1	73.84
1.2475	3	1 1 4	76.26
1.2217	2	3 4 1	78.18
1.2057	2	1 4 3	79.42

Sodium Borate, $NaBO_2$

Synonym
Sodium metaborate

Sample
The sample was prepared by dehydrating $NaBO_2 \cdot 4H_2O$ obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color
Colorless

Structure
Hexagonal, $R\bar{3}c$ (167), Z = 18. The structure was redetermined by Marezio et al. [1963]. The structure had been determined earlier by Fang [1937], [1938].

Lattice constants of this sample
a = 11.9217(7) Å
c = 6.4182(5)

c/a = 0.5384

Volume
789.99 $Å^3$

Density
(calculated) 2.490 g/cm^3

Figure of merit
F_{30} = 64.8(0.012,39)

Additional patterns
PDF card 12-383 [Pistorius, Inst. Geophysics, U. Calif., Los Angeles, CA] labeled anhydrous but appears to be $4H_2O$.

PDF card 12-492 [Norment et al., 1960]

PDF card 16-267 [Bouaziz, 1962]

Coles, Scholes, and Amberg [1937]

References
Bouaziz, R. (1962). Bull. Soc. Chim. Fr. 7, 1451.

Coles, S. S., Scholes, S. R., and Amberg, C. R. (1937). J. Amer. Ceram. Soc. 20, 215.

Fang, S. M. (1937). J. Amer. Ceram. Soc. 20, 214.

Fang, S. M. (1938). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 99A, 1.

Marezio, M., Plettinger, H. A., and Zachariasen, W. H. (1963). Acta Crystallogr. 16, 594.

Norment, H. G., Henderson, P. I., and South, R. L. (1960). Anal. Chem. 32, 796.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
5.953	3	1 1 0	14.87
3.441	1L	3 0 0	25.87
3.063	100	0 1 2	29.13
2.982	2	2 2 0	29.94
2.724	76	2 0 2	32.85
2.614	73	1 3 1	34.28
2.478	19	1 2 2	36.22
2.253	8	4 1 0	39.98
2.221	54	3 2 1	40.58
2.136	20	3 1 2	42.27
2.013M	49	1 1 3	45.00
2.013M		0 4 2	45.00
1.9870	43	3 3 0	45.62
1.9054	5	2 3 2	47.69
1.8672	23	2 4 1	48.73
1.7815	16	5 1 1	51.24
1.7370M	9	2 2 3	52.65
1.7370M		5 0 2	52.65
1.6674	6	4 2 2	55.03
1.6527	3	5 2 0	55.56
1.6408	6	4 3 1	56.00
1.6053	5	1 5 2	57.35
1.5854	5	1 0 4	58.14
1.5509	14L	4 1 3	59.56
1.5318	7	0 2 4	60.38
1.5002	1L	3 4 2	61.79
1.4836	1	2 1 4	62.56
1.4374	4	3 5 1	64.81
1.4136	1L	6 1 2	66.04
1.3997	2	1 3 4	66.78
1.3629	1L	4 0 4	68.83
1.3401	6	0 7 2	70.17
1.3283	1L	3 2 4	70.89
1.3074	1	2 6 2	72.20
1.2672	2	0 5 4	74.87
1.2393	2	2 4 4	76.86
1.2224M	5	4 4 3	78.12
1.2224M		4 5 2	78.12
1.2136	1	5 1 4	78.80
1.1974	2	8 0 2	80.08
1.1740	5	7 2 2	82.01
1.1713	5	3 1 5	82.24
1.1647	2	4 6 1	82.81
1.1521	3	7 1 3	83.92
1.1472	8	9 0 0	84.36
1.1311	3	1 8 2	85.85
1.1285	2	2 3 5	86.09
1.1110	2	6 4 2	87.79
1.0861	2	3 5 4	90.35
1.0725	1	4 2 5	91.82
1.0698	2	0 0 6	92.11

Sodium Niobium Oxide (Lueshite), $NaNbO_3$

Synonym
Sodium niobate

CAS registry no.
12034-09-2

Sample
The sample was obtained from Shieldalloy Corp., Newfield, NJ. It was annealed at 1275 °C for 4 days.

Color
Colorless

Structure
Orthorhombic, Pbma (57), Z = 8. It has a distorted perovskite structure which was refined by Sakowski-Cowley et al. [1969] after earlier work [Vousden, 1951; Wells and Megaw, 1958].

Lattice constants of this sample
a = 5.5687(5) Å
b = 15.523(2)
c = 5.5047(6)

a/b = 0.3587
c/b = 0.3546

Volume
475.84 Å^3

Density
(calculated) 4.575 g/cm^3

Polymorphism
$NaNbO_3$ becomes tetragonal at about 225 °C, and cubic near 435 °C [Wood, 1951]. Wood et al. [1962] described a field-induced ferroelectric polymorph which has a cell similar to the orthorhombic phase except that the c is halved. Bulakh et al. [1962] described a new mineral, natroniobite, which is principally $NaNbO_3$ and presumably monoclinic.

Figure of merit
F_{30} = 35.1(0.010,82)

Additional patterns
PDF card 14-603 [Wood, E., Bell Telephone Lab., Murray Hill, NJ]

PDF card 19-1221 [Parker et al., 1962]

References
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Sakowski-Cowley, A. C., Lukaszewicz, K., and Megaw, H. D. (1969). Acta Crystallogr. B25, 851.

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Wells, M. and Megaw, H. D. (1958). Acta Crystallogr. 11, 858.

Wood, E. (1951). Acta Crystallogr. 4, 353.

Wood, E. A., Miller, R. C., and Remeika, J. P. (1962). Acta Crystallogr. 15, 1273.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
3.912	89	1 0 1	22.71
3.882	45	0 4 0	22.89
3.797	1	1 1 1	23.41
3.122	1L	1 3 1	28.57
2.785	24	2 0 0	32.11
2.754M	100	1 4 1	32.49
2.754M		0 0 2	32.49
2.468	1	1 0 2	36.37
2.453M	1	2 1 1	36.61
2.453M		2 3 0	36.61
2.435	1	1 1 2	36.88
2.366	1	2 2 1	38.00
2.351	1	1 2 2	38.25
2.342	1	0 6 1	38.41
2.263	1	2 4 0	39.81
2.245	2	0 4 2	40.13
2.0930	1L	2 4 1	43.19
1.9574	25	2 0 2	46.35
1.9400M	16	0 8 0	46.79
1.9400M		2 5 1	46.79
1.7857M	1	0 2 3	51.11
1.7857M		1 6 2	51.11
1.7591	7	3 0 1	51.94
1.7478M	12	3 1 1	52.30
1.7478M		2 4 2	52.30
1.7432	14	1 0 3	52.45
1.7385	16	1 8 1	52.60
1.6652	1	3 3 1	55.11
1.6593	1	0 4 3	55.32
1.6018	11	3 4 1	57.49
1.5894	20	1 4 3	57.98
1.5780	1	1 9 1	58.44
1.5314M	1	2 0 3	60.40
1.5314M		3 1 2	60.40
1.5252M	1	1 8 2	60.67

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.5252M		2 1 3	60.67
1.4947	1L	0 10 1	62.04
1.3923	3	4 0 0	67.18
1.3779M	13	3 7 1	67.98
1.3779M		2 8 2	67.98
1.3745	8	2 5 3	68.17
1.3445M	1L	4 1 1	69.91
1.3445M		4 3 0	69.91
1.3362	1L	1 0 4	70.41
1.3164M	1L	1 2 4	71.63
1.3164M		2 10 1	71.63
1.3105	1	4 4 0	72.00
1.3032	4	3 8 1	72.47
1.2965M	5	0 4 4	72.90
1.2965M		1 8 3	72.90
1.2935M	3	0 12 0	73.10
1.2935M		1 3 4	73.10
1.2649	1L	3 3 3	75.03
1.2424	2	4 0 2	76.63
1.2385	3	4 1 2	76.92
1.2369	3	3 4 3	77.04
1.2336	3	2 0 4	77.28
1.2283	5	1 12 1	77.68
1.1831	1L	4 4 2	81.25
1.1757	1	2 4 4	81.87
1.1706	1	0 12 2	82.30
1.1311	1	4 8 0	85.85

Sodium Nitrosyl Iron Cyanide Hydrate, $Na_2(NO)Fe(CN)_5 \cdot 2H_2O$

Synonyms
Sodium nitroprusside dihydrate
Sodium nitroferricyanide dihydrate
Sodium nitrosylpentacyanoferrate dihydrate.

CAS registry no.
13755-38-9

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA.

Color
Unground, deep reddish brown
Ground, light yellow pink

Structure
Orthorhombic, Pnmn (58), Z = 4. [Cooke, 1946]. The structure was determined by Manoharan and Hamilton [1963].

Lattice constants of this sample
a = 11.908(4)Å
b = 15.564(4)
c = 6.2031(14)

a/b = 0.7651
c/b = 0.3986

Volume
1149.7 Å^3

Density
(calculated) 1.721 g/cm^3

Figure of merit
F_{30} = 36.6(0.012,68)

Additional pattern
PDF card 1-289 [Hanawalt et al., 1938]

References
Cooke, P. W. (1946). Nature London 157, 518.

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

Manoharan, P. T. and Hamilton, W. C. (1963). Inorg. Chem. 2, 1043.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
7.79	33	0 2 0	11.35
5.969	4	2 0 0	14.83
5.760	40	0 1 1	15.37
5.507	2	1 0 1	16.08
4.726	83	2 2 0	18.76
4.492	10	1 2 1	19.75
4.296	1	2 0 1	20.66
4.139	100	2 1 1	21.45
3.982	12	0 3 1	22.31
3.894	16	0 4 0	22.82
3.847	3	3 1 0	23.10
3.346	7	3 0 1	26.62
3.311	15	2 3 1	26.91
3.258	12	2 4 0	27.35
3.150	2	3 3 0	28.31
3.004	9	1 0 2	29.72
2.947	4	1 1 2	30.30
2.884M	95	2 4 1	30.98
2.884M		0 2 2	30.98
2.810	5	3 3 1	31.82
2.710M	19	1 5 1	33.03
2.710M		2 1 2	33.03
2.644	2	4 1 1	33.87
2.593M	22	0 6 0	34.56
2.593M		2 2 2	34.56
2.536M	31	4 2 1	35.37
2.536M		3 4 1	35.37
2.425	5	0 4 2	37.04
2.414	5	3 1 2	37.21
2.383	20	4 3 1	37.72
2.346	2	1 6 1	38.33
2.333	2	3 2 2	38.56
2.247	3	2 4 2	40.10
2.147	21	4 0 2	42.06
2.093	1	0 7 1	43.20
2.033	13	4 5 1	44.53
1.9714	7	1 2 3	46.00
1.9455	12	0 8 0	46.65
1.9384	6	2 1 3	46.83
1.9195	6	0 3 3	47.32
1.8868	8	2 6 2	48.19
1.8271	1	2 3 3	49.87
1.8045	3	1 4 3	50.54
1.7792	3	3 6 2	51.31
1.7760	4	6 3 1	51.41
1.7221	5	0 5 3	53.14
1.6988M	5	5 4 2	53.93
1.6988M		4 0 3	53.93
1.6878M	7	4 1 3	54.31
1.6878M		5 6 1	54.31

Sodium Vanadium Oxide, α-$NaVO_3$

Synonym
Alpha-sodium metavanadate

CAS registry no.
11126-25-3

Sample
The sample was contributed by Riedel-de Haën, Hannover, West Germany. It was labeled $NaVO_3 \cdot H_2O$.

Color
Colorless

Structure
Monoclinic, I2/a (15), Z = 8. [Marumo et al., 1974]. This phase has been reported to be in space group Cc (9) [Feigelson et al., 1972].

Lattice constants of this sample
a = 10.333(2) Å
b = 9.473(2)
c = 5.880(2)
β = 104.20(2)°

a/b = 1.0908
c/b = 0.6207

Volume
557.90 $Å^3$

Density
(calculated) 2.903 g/cm^3

Polymorphism
Beta $NaVO_3$ changes irreversibly to α-$NaVO_3$ at about 404 °C. [Lukacs and Strusievici, 1962].

Figure of merit
F_{30} = 43.2(0.014,48)

Additional patterns
PDF card 20-1168 [Lelong, 1966]

PDF card 27-828 [Feigelson et al., 1972]

PDF card 30-1259 [Kolta et al., 1973]

PDF card 30-1258 [Perraud, 1974]

Lukacs and Strusievici, [1962]

References

Feigelson, R. S., Martin, G. W., and Johnson, B. C. (1972). J. Cryst. Growth 13-14, 686.

Kolta, G. A., Hewaidy, I. F., Felix, N. S., and Girgis, N. N. (1973). Thermochim. Acta 6, 165.

Lelong, L. (1966). Rev. Chim. Miner. 3, 259.

Lukacs, I. and Strusievici, C. (1962). Z. Anorg. Allg. Chem. 315, 323.

Marumo, F., Isobe, M., and Iwai, S. (1974). Acta Crystallogr. B30, 1628.

Perraud, J. (1974). Rev. Chim. Miner. 11, 302.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
6.87	2	1 1 0	12.87
5.007	41	2 0 0	17.70
4.736	18	0 2 0	18.72
3.931	3	-2 1 1	22.60
3.612	62	-1 2 1	24.63
3.439	26	2 2 0	25.89
3.261	100	1 2 1	27.33
3.179	28	2 1 1	28.05
3.147	71	3 1 0	28.34
3.010	2	1 3 0	29.66
2.848	14	0 0 2	31.39
2.788	38	-2 0 2	32.08
2.764	11	0 3 1	32.37
2.680	33	-3 2 1	33.41
2.447	12	-4 1 1	36.70
2.409	3	-3 1 2	37.30
2.367	1	0 4 0	37.99
2.304	6	2 3 1	39.06
2.295	8	3 3 0	39.22
2.251	10	2 0 2	40.03
2.179	16	-1 4 1	41.40
2.150	3	-1 3 2	41.99
2.140	4	2 4 0	42.19
2.097	6	1 4 1	43.10
2.060	4	4 1 1	43.91
2.033	2	2 2 2	44.52
1.959	16	5 1 0	46.30
1.914	4	-3 4 1	47.47
1.863M	5	0 1 3	48.86
1.863M		1 5 0	48.86
1.8337	4	-5 1 2	49.68
1.8220	5	0 4 2	50.02
1.8091	21	-1 2 3	50.40
1.7550M	12	3 4 1	52.07
1.7550M		4 3 1	52.07
1.7212	2	4 4 0	53.17
1.6924M	1	-6 1 1	54.15
1.6924M		5 3 0	54.15
1.6699	2	6 0 0	54.94
1.6547	2	-2 3 3	55.49
1.6475	5	3 5 0	55.75
1.6245	2	-6 0 2	56.61
1.5792	2	0 6 0	58.39
1.5272	3	1 5 2	60.58
1.5108	13	-6 3 1	61.31
1.5086M	11	-1 4 3	61.41
1.5086M		-3 5 2	61.41
1.4602M	9	2 3 3	63.68
1.4602M		5 1 2	63.68
1.4151	4	7 1 0	65.96

Sodium Vanadium Oxide, β-$NaVO_3$

Synonym
Beta-sodium metavanadate

CAS registry no.
11126-25-3

Sample
The sample was prepared from $NaVO_3 \cdot H_2O$, which was crystallized from an aqueous solution, by heating at 300 °C for 4 days.

Color
Colorless

Structure
Orthorhombic, Z = 4. [Perraud, 1974]

Lattice constants of this sample
a = 5.3625(15) Å
b = 14.155(6)
c = 3.6499(11)

a/b = 0.3788
c/b = 0.2579

Volume
277.06 $Å^3$

Density
(calculated) 2.923) g/cm^3

Polymorphism
Beta-$NaVO_3$ changes irreversibly to α-$NaVO_3$ at about 404 °C. [Lukacs and Strusievici, 1962]

Figure of merit
F_{28} = 17.8(0.018,88)

Additional patterns
PDF card 1-246 [Hanawalt et al.], pattern mislabeled $NaVO_3 \cdot H_2O$.

PDF card 27-824 [Perraud, 1974]

PDF card 30-1260 [Feigelson et al., 1972]

Lukacs and Strusievici [1962]

References

Feigelson, R. S., Martin, G. W., and Johnson, B. C. (1972). J. Cryst. Growth 13-14, 686.

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

Lukacs, I. and Strusievici, C. (1962). Z. Anorg. Allgem. Chem. 315, 323.

Perraud, J. (1974). Rev. Chim. Miner. 11, 302.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
7.09	11	0 2 0	12.48
5.01	100	1 1 0	17.68
4.283	6	1 2 0	20.72
3.542M	24	1 3 0	25.12
3.542M		0 4 0	25.12
3.248	18	0 2 1	27.44
3.019	13	1 0 1	29.57
2.954M	35	1 4 0	30.23
2.954M		1 1 1	30.23
2.683	12	2 0 0	33.37
2.635	2	2 1 0	34.00
2.541M	7	1 3 1	35.29
2.541M		0 4 1	35.29
2.506M	5	2 2 0	35.80
2.506M		1 5 0	35.80
2.360	2	0 6 0	38.10
2.333	4	2 3 0	38.56
2.295	5	1 4 1	39.22
2.067	1	2 2 1	43.76
1.965	5	2 3 1	46.17
1.892	5	1 7 0	48.06
1.824	6	0 0 2	49.95
1.771	3	2 6 0	51.56
1.732	1	3 2 0	52.80
1.716	5	1 1 2	53.36
1.679M	2	1 7 1	54.62
1.679M		1 2 2	54.62
1.6051	4	3 0 1	57.36
1.5944M	7	3 1 1	57.78
1.5944M		2 6 1	57.78
1.5521	1	1 4 2	59.51
1.5090M	2	1 9 0	61.39
1.5090M		2 0 2	61.39
1.4745	3	1 5 2	62.99
1.3942M	2	1 9 1	67.08
1.3942M		1 6 2	67.08

Strontium Iron Oxide, $SrFe_{12}O_{19}$

Synonyms
Strontium hexaferrite
Dodecairon strontium 19-oxide

CAS registry no.
12023-91-5

Sample
The sample was prepared at NBS from a stoichiometric mixture of $SrCO_3$ and Fe_2O_3, heated at 1000 °C for 1 day, then at 1200 °C for 5 days with periodic grinding. It was then held at 1390 °C for 8 h and cooled at 2° per hour to 500 °C.

Color
Blackish blue

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 2, isostructural with magnetoplumbite, $PbFe_{12}O_{19}$, [Adelsköld 1938]. Stacking faults seemed to occur in the 00ℓ direction, without final annealing of the sample.

Lattice constants of this sample
a = 5.8868(5) Å
c = 23.037(2)

c/a = 3.9133

Volume
691.38 Å^3

Density
(calculated) 5.100 g/cm^3

Figure of merit
F_{30} = 53.2(0.011,51)

Additional pattern
PDF card 24-1207 [Smith, Allen Clark Research Centre, Plessey Co. Ltd., Towcester, Northants, U.K.]

Reference
Adelsköld, V. (1938). Ark. Kemi Mineral. Geol. 12A, #29, 9.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
11.49	1L	0 0 2	7.69
5.753	2	0 0 4	15.39
4.665	6	1 0 2	19.01
4.249	3	1 0 3	20.89
3.839	10	0 0 6	23.15
3.070	4	1 0 6	29.06
2.945	42	1 1 0	30.33
2.878	21	0 0 8	31.05
2.765	95	1 0 7	32.35
2.621	100	1 1 4	34.18
2.550	13	2 0 0	35.16
2.534	14	2 0 1	35.40
2.508	15	1 0 8	35.77
2.490	4	2 0 2	36.04
2.420	47	2 0 3	37.12
2.336	7	1 1 6	38.50
2.304	1L	0 0 10	39.06
2.232	32	2 0 5	40.38
2.124	21	2 0 6	42.52
2.0159	2	2 0 7	44.93
1.9376	5	1 0 11	46.85
1.8145	2	1 1 10	50.24
1.8061	3	2 0 9	50.49
1.7962	2	1 0 12	50.79
1.7221	2	2 1 6	53.14
1.7090	6	2 0 10	53.58
1.6993	8	3 0 0	53.91
1.6629	33	2 1 7	55.19
1.6454	10	0 0 14	55.83
1.6296	22	3 0 4	56.42
1.6182	48	2 0 11	56.85
1.6079	5	1 1 12	57.25
1.6015	10	2 1 8	57.50
1.5667	1	1 0 14	58.90
1.5538	2	3 0 6	59.44
1.5387	1L	2 1 9	60.08
1.5330	6	2 0 12	60.33
1.4715	44	2 2 0	63.13
1.4550	4	2 0 13	63.93
1.4398	2	0 0 16	64.69
1.4264	1L	2 2 4	65.37
1.4180	3	2 1 11	65.81
1.3823	12	2 0 14	67.73
1.3743	1	2 2 6	68.18
1.3598	1	2 1 12	69.01

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.3100M	6	2 2 8	72.03
1.3100M		1 0 17	72.03
1.2990	12	3 1 7	72.74
1.2935	2	1 1 16	73.10
1.2797	1L	0 0 18	74.02
1.2723M	4	4 0 1	74.52
1.2723M		3 0 12	74.52
1.2691	4	3 1 8	74.74
1.2572	4	4 0 3	75.57
1.2415	4	1 0 18	76.70
1.2095	1L	4 0 6	79.12
1.2009	1L	2 1 15	79.80
1.1966	1L	2 0 17	80.14
1.1738	4	1 1 18	82.03
1.1519	1L	0 0 20	83.94

Thorium Carbide, ThC

Synonym
Thorium monocarbide

CAS registry no.
12012-16-7

Sample
The sample was obtained from Alfa Products Thiokol/Ventron Division, Danvers, MA. It contained some semi-amorphous carbon and was somewhat unstable; therefore the intensities are subject to some error.

Color
Grey

Structure
Cubic, Fm3m (225), Z = 4. [Wilhelm and Chiotti, 1950]. ThC has a NaCl type structure.

Lattice constant of this sample
$a = 5.3313(7)$ Å

Volume
151.53 Å^3

Density
(calculated) 10.698 g/cm^3

Figure of merit
$F_{10} = 58.1(0.017, 10)$

Additional pattern
PDF card 15-36 [Kempter and Krikorian, 1962]

References
Kempter, C. P. and Krikorian, N. H. (1962). J. Less-Common Metals 4, 244.

Wilhelm, H. A., Chiotti, P. (1950). Trans. Amer. Soc. Metals 42, 1295.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; temp. 25±1 °C
Internal standard Si, $a = 5.43088$ Å

d(Å)	I^{rel} $\sigma = \pm 6$	hkℓ	2θ(°)
3.075	100	1 1 1	29.01
2.666	70	2 0 0	33.59
1.886	60	2 2 0	48.21
1.6071	70	3 1 1	57.28
1.5387	25	2 2 2	60.08
1.3322	12	4 0 0	70.65
1.2232	30	3 3 1	78.06
1.1923	30	4 2 0	80.49
1.0884	25	4 2 2	90.10
1.0260	20	5 1 1	97.32

Thorium Nitrate Hydrate, $Th(NO_3)_4 \cdot 5H_2O$

Synonym
Thorium nitrate pentahydrate

Sample
The sample was obtained from Allied Chemical, General Chemical Division, New York, NY. It was labeled $Th(NO_3)_4 \cdot 4H_2O$.

Color
Colorless

Structure
Orthorhombic, Fdd2 (43), Z = 8, [Staritsky, 1956]. The structure of $Th(NO_3)_4 \cdot 5H_2O$ was determined by Taylor et al. [1966] and Ueki et al. [1966].

Lattice constants of this sample
a = 11.201(2) Å
b = 22.896(5)
c = 10.593(2)

a/b = 0.4892
c/b = 0.4627

Volume
2716.7 $Å^3$

Density
(calculated) 2.788 g/cm^3

Figure of merit
F_{30} = 54.7(0.016,35)

Additional pattern
PDF card 9-36 [Staritsky, 1956]

References
Staritsky, E. (1956). Anal. Chem. 28, 2021.

Taylor, J. C., Miller, M. H., and Hitterman, R. L. (1966). Acta Crystallogr. 20, 842.

Ueki, T., Zalkin, A., and Templeton, D. H. (1966). Acta Crystallogr. 20, 836.

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
7.30	100	1 1 1	12.11
5.73	39	0 4 0	15.45
5.42	58	1 3 1	16.33
5.035	44	2 2 0	17.60
4.810	54	0 2 2	18.43
4.005	3	2 4 0	22.18
3.938	24	1 5 1	22.56
3.852	7	2 0 2	23.07
3.652	1	2 2 2	24.35
3.482	20	3 1 1	25.56
3.331	12	1 1 3	26.74
3.193M	28	3 3 1	27.92
3.193M		2 4 2	27.92
3.156	4	2 6 0	28.25
3.096	31	0 6 2	28.81
3.084	18	1 3 3	28.93
3.012	10	1 7 1	29.64
2.862	5	0 8 0	31.23
2.800	18	4 0 0	31.94
2.793	17	3 5 1	32.02
2.714	10	1 5 3	32.98
2.651	6	0 0 4	33.79
2.550M	11	3 1 3	35.16
2.550M		2 8 0	35.16
2.516	6	4 4 0	35.65
2.431	13	3 3 3	36.95
2.419	23	4 2 2	37.14
2.403	22	0 4 4	37.40
2.397	22	3 7 1	37.49
2.347	20	1 7 3	38.32
2.342	11	2 2 4	38.41
2.297	14	2 8 2	39.19
2.239	5	3 5 3	40.24
2.207	1	2 4 4	40.85
2.181	12	5 1 1	41.37
2.119	8	2 10 0	42.64
2.106	8	5 3 1	42.92
2.101	10	0 10 2	43.02
2.073	12	1 1 5	43.63
2.061	8	3 9 1	43.90
2.028	21	2 6 4	44.65
2.007	9	1 3 5	45.13
2.002	10	4 8 0	45.27
1.976	7	5 5 1	45.88
1.943	6	0 8 4	46.70
1.924	5	4 0 4	47.20
1.907	2	0 12 0	47.64
1.895	4	1 5 5	47.98
1.885	4	5 1 3	48.23
1.842	6	6 2 0	49.44
1.837+	9	3 1 5	49.58
1.837+		2 8 4	49.58
1.822	8	5 7 1	50.02
1.807M	4	3 9 3	50.47
1.807M		2 12 0	50.47
1.792M	7	3 11 1	50.93
1.792M		3 3 5	50.93
1.771	4	1 11 3	51.58
1.761	3	6 0 2	51.89
1.756	4	1 7 5	52.04

Titanium Carbide, TiC

CAS registry no.
12070-08-5

Sample
The sample was obtained from Kennametal, Latrobe, PA.

Color
Dark gray

Structure
Cubic, Fm3m (225), Z = 4. The structure of titanium carbide was qualitatively determined by von Schwarz and Summa [1932].

Lattice constant of this sample
$a = 4.3274(2)$ Å

Volume
81.037 Å^3

Density
(calculated) 4.911 g/cm^3

Figure of merit
$F_{10} = 121.6(0.008,10)$

Additional pattern
PDF card 6-614 [Cadoff and Nielsen, 1953]

References
Cadoff, I. and Nielsen, J. P. (1953). Trans. AIME 197, 248.

Schwarz, von, M. and Summa, O. (1932). Z. Elektrochem. 38, 743.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; temp. 25±1 °C
Internal standard W, $a = 3.16525$ Å

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
2.499	78	1 1 1	35.90
2.1637	100	2 0 0	41.71
1.5302	60	2 2 0	60.45
1.3047	30	3 1 1	72.37
1.2492	17	2 2 2	76.14
1.0818	10	4 0 0	90.80
.9927	13	3 3 1	101.78
.9677	25	4 2 0	105.50
.8834	23	4 2 2	121.38
.8327	16	5 1 1	135.34

Tungsten Oxide, WO_2

Synonym
Tungsten dioxide

CAS registry no.
12036-22-5

Sample
The sample was made at NBS by H. S. Parker by heating WO_3 in a W boat for 20 hours at 372 °C in an atmosphere of 95% N_2 and 5% H_2 gas. This was followed by heating at 590 °C for 90 hours under the same conditions.

Color
Dark brown

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. Distorted rutile structure. The structure was studied by Magnéli et al. [1952] and by Magnéli and Andersson [1955]. The structure was discussed by Roger et al. [1969].

Lattice constants of this sample

a = 5.5754(7) Å
b = 4.8995(12)
c = 5.5608(9)
β = 118.869(12)°

a/b = 1.1380
c/b = 1.1350

Volume
133.03 $Å^3$

Density
(calculated) 10.78 g/cm^3

Figure of merit
F_{30} = 28.8(0.016,67)

Additional pattern
PDF card 5-431 [Magnéli et al., Univ. of Uppsala, Sweden]

References

Magnéli, A. and Andersson, G. (1955). Acta Chem. Scand. 9, 1378.

Magnéli, A., Andersson, G., Blomberg, B., and Kihlborg, L. (1952). Anal. Chem. 24, 1998.

Roger, D. B., Shannon, R. D., Sleight, A. W., and Gillson, J. L. (1969). Inorg. Chem. 8, 841.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
4.795	1	-1 0 1	18.49
3.452	100	0 1 1	25.79
2.831	2	1 0 1	31.58
2.449M	20	1 1 1	36.66
2.449M		0 2 0	36.66
2.442	30	2 0 0	36.77
2.437	27	0 0 2	36.86
2.423	34	-2 1 1	37.07
2.398	17	-2 0 2	37.48
2.184	2	2 1 0	41.30
2.154	1	-2 1 2	41.91
1.853	2	1 2 1	49.13
1.833	3	-3 0 1	49.70
1.7324M	18	2 1 1	52.80
1.7324M		1 1 2	52.80
1.7282	31	2 2 0	52.94
1.7167	14	-3 1 1	53.32
1.7123M	10	-2 2 2	53.47
1.7123M		-1 1 3	53.47
1.5987	1	-3 0 3	57.61
1.5481M	10	1 3 0	59.68
1.5481M		0 3 1	59.68
1.5448	10	3 1 0	59.82
1.5408	10	0 1 3	59.99
1.4670	2	-3 2 1	63.35
1.4157	3	2 0 2	65.93
1.4094	5	-2 3 1	66.26
1.3934	4	-4 0 2	67.12
1.3900	5	-2 0 4	67.31
1.3588	1	3 0 1	69.07
1.3388	1	-3 2 3	70.25
1.2993	2	-4 1 1	72.72
1.2856	3	-4 1 3	73.62
1.2251+	5	2 3 1	77.92
1.2251+		0 4 0	77.92
1.2171	2	0 0 4	78.53
1.2140	3	-2 3 3	78.77
1.2109	3	-4 2 2	79.01
1.2087	3	-2 2 4	79.18
1.1982	2	-4 0 4	80.01
1.1879M	2	1 4 0	80.85
1.1879M		0 4 1	80.85
1.1529	2	3 3 0	83.85
1.1513	5	0 3 3	83.99

Synonym
Uranium mononitride

CAS registry no.
25658-43-9

Sample
The sample was obtained from the Battelle Memorial Institute, Columbus, OH.

Color
Dark gray

Structure
Cubic, Fm3m (225), Z = 4. The structure was determined by Rundle et al. [1948] and confirmed by Mueller and Knott [1958].

Lattice constant of this sample
$a = 4.8897(2)$ Å

Volume
116.91 Å^3

Density
(calculated) 14.318 g/cm^3

Figure of merit
$F_{13} = 93.2(0.011,13)$

Additional patterns
PDF card 11-315 [Mueller and Knott, Argonne National Laboratory, Lemont, IL]

Kempter et al. [1959]

$CuK\alpha_1$ $\lambda = 1.540598$ Å; temp. 25±1 °C Internal standard W, $a = 3.16524$ Å					
d(Å)	I^{rel}, $\sigma = \pm 3$	h	k	ℓ	2θ(°)
2.825	100	1	1	1	31.65
2.445	82	2	0	0	36.72
1.7291	52	2	2	0	52.91
1.4749	58	3	1	1	62.97
1.4119	18	2	2	2	66.13
1.2224	11	4	0	0	78.12
1.1219	22	3	3	1	86.72
1.0935	25	4	2	0	89.57
.9981	19	4	2	2	101.02
.9410	22	5	1	1	109.89
.8644	8	4	4	0	126.04
.8265	26	5	3	1	137.50
.8149	20	6	0	0	141.90

References

Kempter, C. P., McGuire, J. C., and Nadler, M. R. (1959). Anal. Chem. 31, 156.

Mueller, M. H. and Knott, H. W. (1958). Acta Crystallogr. 11, 751.

Rundle, R. E., Baenziger, N. C., Wilson, A. S., and McDonald, R. A., (1948). J. Amer. Chem. Soc. 70, 98.

Uranyl Acetate Hydrate, $C_4H_6O_6U \cdot 2H_2O$

Synonym
Uranyl acetate dihydrate

CAS registry no.
20154-66-9

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

Color
Bright greenish yellow

Structure
Orthorhombic, $Pna2_1$ (33), Z = 4. [Mentzen and Giorgio, 1970] [Amirthalingham et al., 1959]

Lattice constants of this sample
a = 9.630(2) Å
b = 14.883(2)
c = 6.823(2)

a/b = 0.6470
c/b = 0.4584

Volume
977.91 Å^3

Density
(calculated) 2.881 g/cm^3

Figure of merit
F_{30} = 38.7(0.016,49)

Additional patterns
PDF card 14-744 [Hanawalt et al., 1938]

PDF card 23-714 [Mentzen and Giorgio, 1970]

References
Amirthalingham, V., Chandran, O. V., and Padmanabham, V. M. (1959). Acta Crystallogr. 12, 821.

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

Mentzen, B. and Giorgio, G. (1970). J. Inorg. Nucl. Chem. 32, 1509.

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

d(Å)	I^{rel} σ = ±6	hkℓ	2θ(°)
8.09	63	1 1 0	10.93
7.44	15	0 2 0	11.89
6.22	94	0 1 1	14.22
5.90	65	1 2 0	15.01
5.221	22	1 1 1	16.97
4.581	100	2 1 0	19.36
4.462	47	1 2 1	19.88
4.412	31	1 3 0	20.11
3.936	60	2 0 1	22.57
3.805	3	2 1 1	23.36
3.706	43	1 3 1	23.99
3.470	22	1 4 0	25.65
3.456	18	2 3 0	25.76
3.410	37	0 0 2	26.11
3.140M	13	1 1 2	28.40
3.140M		3 1 0	28.40
3.092	9	1 4 1	28.85
2.949M	24	1 2 2	30.28
2.949M		3 2 0	30.28
2.852	7	3 1 1	31.34
2.845	7	1 5 0	31.42
2.737	28	2 1 2	32.69
2.727	30	0 5 1	32.81
2.703	31	2 4 1	33.12
2.698M	28	1 3 2	33.18
2.698M		3 3 0	33.18
2.606	1L	2 2 2	34.39
2.532	21	2 5 0	35.43
2.510	17	3 3 1	35.75
2.481	9	0 6 0	36.17
2.430	11	3 4 0	36.96
2.408	38	4 0 0	37.32
2.374M	1L	4 1 0	37.86
2.374M		2 5 1	37.86
2.292	3	4 2 0	39.28
2.265	9	1 6 1	39.77
2.245	20	4 1 1	40.14
2.230M	10	3 2 2	40.42
2.230M		2 4 2	40.42
2.189	7	1 1 3	41.20
2.122	15	1 2 3	42.57
2.099	11	2 6 1	43.07
2.076	9	1 7 0	43.56
2.057	10	2 0 3	43.99
2.031	13	0 7 1	44.58
2.020	19	1 3 3	44.83
2.006	10	0 6 2	45.16
1.986	8	1 7 1	45.65
1.980	14	3 4 2	45.80
1.963M	14	1 6 2	46.20
1.963M		3 6 0	46.20
1.910	5	5 1 0	47.58
1.865	1L	5 2 0	48.78
1.860	4	0 8 0	48.92
1.841	4	3 1 3	49.47
1.826	3	1 8 0	49.90
1.804	14	4 5 1	50.54
1.800M	17	3 2 3	50.68
1.800M		2 4 3	50.68
1.796	17	5 3 0	50.79

CAS registry no.
7440-65-5

Sample
The sample was obtained from the United Mineral and Chemical Corp., New York, NY. The part used was filed off with a file cleaned by dipping it for 10 seconds in a nitric acid solution.

Color
Dark gray

Structure
Hexagonal, Pb_3/mmc (194), Z = 2. The structure was done by Bommer [1939].

Lattice constants of this sample
a = 3.6471(3) Å
c = 5.7285(6)

c/a = 1.5707

Volume
65.988 $Å^3$

Density
(calculated) 4.474 g/cm^3

Figure of merit
F_{21} = 89.6(0.011,22)

Additional pattern
PDF card 12-702 [U.S. Bureau of Mines, Albany, OR].

Reference
Bommer, H. (1939). Z. Elektrochem. 45, 357.

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

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
3.159	26	1 0 0	28.23
2.865	25	0 0 2	31.19
2.765	100	1 0 1	32.35
2.122	12	1 0 2	42.58
1.8234	14	1 1 0	49.98
1.6338	12	1 0 3	56.26
1.5797	2	2 0 0	58.37
1.5378	14	1 1 2	60.12
1.5229	11	2 0 1	60.77
1.4323	2	0 0 4	65.07
1.3831	2	2 0 2	67.69
1.3041	2	1 0 4	72.41
1.2171	3	2 0 3	78.53
1.1937	1	2 1 0	80.38
1.1685	5	2 1 1	82.48
1.1262	3	1 1 4	86.31
1.1019	1	2 1 2	88.70
1.0770	2	1 0 5	91.32
1.0610	1	2 0 4	93.10
1.0529	1	3 0 0	94.04
1.0121	3	2 1 3	99.12

Zinc Acetate Hydrate, $C_4H_6O_4Zn \cdot 2H_2O$

Synonym
Zinc acetate dihydrate

CAS registry no.
5970-45-6

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

Color
Colorless

Optical data
Biaxial (+), $N_\alpha = 1.49$, $N_\beta = 1.490$, $N_\gamma = 1.556$. 2V is large

Structure
Monoclinic, C2/c (15), Z = 4. [Whitney and Corvin, 1949]. The structure was determined by Van Niekerk et al. [1953].

Lattice constants of this sample
a = 14.431(5) Å
b = 5.340(3)
c = 10.981(4)
β = 99.88(3)°

a/b = 2.7024
c/b = 2.0564

Volume
833.6 $Å^3$

Density
(calculated) 1.749 g/cm^3

Figure of merit
$F_{30} = 28.4(0.014,74)$

Additional pattern
PDF card 14-902 [Whitney and Corvin, 1949]
Mislabeled $Zn(C_2H_3O_2) \cdot 2H_2O$

References
Van Niekerk, J. N., Schoening, F. R. L., and Talbot, J. H. (1953). Acta Crystallogr. 6, 720.

Whitney, J. and Corvin, I. (1949). Anal. Chem. 21, 645.

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

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
7.10	100	2 0 0	12.46
5.411	2	0 0 2	16.37
5.004	3	1 1 0	17.71
4.714	8	-2 0 2	18.81
4.645	9	-1 1 1	19.09
4.436	23	1 1 1	20.00
3.987	21	2 0 2	22.28
3.789	10	-1 1 2	23.46
3.545	23	3 1 0	25.10
3.245	20	3 1 1	27.46
3.158	7	-3 1 2	28.24
2.846	3	1 1 3	31.41
2.805	1	3 1 2	31.88
2.688	4	-2 0 4	33.30
2.509	2	5 1 0	35.76
2.421	4	-5 1 2	37.10
2.403	3	2 2 1	37.39
2.366	4	5 1 1	38.00
2.296	2	-3 1 4	39.21
2.223	1	-5 1 3	40.54
2.155	4	5 1 2	41.89
2.137	3	-4 2 1	42.25
2.054	4	4 2 1	44.06
2.030	11	-1 1 5	44.59
1.997M	4	2 2 3	45.38
1.997M		-5 1 4	45.38
1.961	2	-3 1 5	46.26
1.924	2	-7 1 1	47.20
1.8203	1	7 1 1	50.07
1.8038M	2	-7 1 3	50.56
1.8038M		0 0 6	50.56
1.7827	1	2 2 4	51.20
1.7600	1	4 2 3	51.91
1.7135	2	6 2 1	53.43

Zirconium Fluoride, ZrF_4

Synonym
Zirconium tetrafluoride

CAS registry no.
7783-64-4

Sample
The sample was from Alfa Products, Thiokol/ Ventron Division, Danvers, MA. It was heated to 300 °C for 3 days to dehydrate a small amount of the hydrate which was present.

Color
Colorless

Structure
Monoclinic, I2/a (15), Z = 12 [Schulze, 1934, Zachariasen, 1949]. The structure was determined by Burbank and Bensey [1956].

Lattice constants of this sample
a = 9.5585(13) Å
b = 9.9512(13)
c = 7.7071(14)
β = 94.520(1)°

a/b = 0.9605
c/b = 0.7745

Volume
730.81 Å^3

Density
(calculated) 4.559 g/cm^3

Polymorphism
Gaudreau [1965] prepared two other forms of ZrF_4 by heating $(NH_4)_3$ ZrF_7 under various conditions. These forms were called alpha and gamma. Gaudreau called the form reported in the present work beta.

Figure of merit
F_{30} = 74.9(0.010,40)

Additional patterns
PDF card 17-926 [Burbank and Bensey, 1956]

Amirthalirgam and Muralidharan [1964]

Brunton [1965]

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

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
6.88	18	1 1 0	12.86
6.083	12	0 1 1	14.55
4.971	3	0 2 0	17.83
4.762	15	2 0 0	18.62
3.889	94	-1 2 1	22.85
3.875	100	-2 1 1	22.93
3.842	12	0 0 2	23.13
3.641	55	2 1 1	24.43
3.441M	99	2 2 0	25.87
3.441M		-1 1 2	25.87
3.276	36	1 1 2	27.20
3.133	7	1 3 0	28.47
3.112	17	-2 0 2	28.66
3.043M	38	0 3 1	29.33
3.043M		0 2 2	29.33
3.025	25	3 1 0	29.50
2.638	1L	-2 2 2	33.95
2.582	3	-3 2 1	34.71
2.530	2	2 3 1	35.45
2.494	5	2 2 2	35.98
2.479M	5	0 1 3	36.21
2.479M		3 2 1	36.21
2.470	3	-3 1 2	36.35
2.461	2	-1 3 2	36.48
2.382	2	4 0 0	37.74
2.310	1	-1 4 1	38.96
2.294M	1L	3 1 2	39.24
2.294M		3 3 0	39.24
2.284	1L	1 4 1	39.42
2.272	1L	-2 1 3	39.64
2.267	1L	-4 1 1	39.73
2.251	1L	-1 2 3	40.02
2.205	1	2 4 0	40.90
2.1722	1	4 1 1	41.54
2.1344	2	2 1 3	42.31
2.0994	1	-4 0 2	43.05
2.0883	1	0 4 2	43.29
2.0266	3	0 3 3	44.68
2.0218	4	-3 3 2	44.79
1.9566	13	4 0 2	46.37
1.9482	8	1 5 0	46.58
1.9423	8	-2 4 2	46.73
1.9349	16	-4 2 2	46.92
1.9264	12	0 5 1	47.14
1.9199M	34	0 0 4	47.31

References

Amirthalirgam, V. and Muralidharan, K. V. (1964). J. Inorg. Nucl. Chem. 26, 2038.

Brunton, G. (1965). J. Inorg. Nucl. Chem. 27, 1173.

Burbank, R. D. and Bensey, F. N. (1956). AEC Report K1280.

Gaudreau, B. (1965). Rev. Chim. Miner. 2, 1.

Schulze, G. E. R. (1934). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 89, 477.

Zachariasen, W. H. (1949). Acta Crystallogr. 2, 388.

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.9199M		-3 4 1	47.31
1.9085	29	-2 3 3	47.61
1.8824	5	2 4 2	48.31
1.8715	14	5 1 0	48.61
1.8483	21	4 3 1	49.26
1.8316	12	-2 0 4	49.74
1.8258	10	2 3 3	49.91
1.7919M	41	3 2 3	50.92
1.7919M		0 2 4	50.92
1.7873	26	-4 1 3	51.06
1.7740	18	2 5 1	51.47
1.7625	7	-5 2 1	51.83
1.7484	20	-1 5 2	52.28
1.7367M	16	1 4 3	52.66
1.7367M		-5 1 2	52.66
1.7206	2	4 4 0	53.19
1.7064	5	5 2 1	53.67
1.6872	1L	3 5 0	54.33
1.6801	6	-3 1 4	54.58
1.6588	4	0 6 0	55.34
1.6527	5	5 3 0	55.56

Zirconium Oxide Chloride Hydrate, $ZrOCl_2 \cdot 8H_2O$

Synonym
Zirconium oxychloride octahydrate

Sample
The sample was made by slow evaporation at room temperature of an aqueous solution of $ZrOCl_2$.

Color
Colorless

Structure
Tetragonal, $P\bar{4}2_1c$ (114), Z = 8. [Clearfield and Vaughan, 1956]. The structure was refined by Mak [1968].

Lattice constants of this sample
a = 17.094(3) Å
c = 7.713(2)

c/a = 0.4512

Volume
2253.8

Density
(calculated) 1.899 g/cm^3

Figure of merit
F_{30} = 35.2(0.015,58)

Reference intensity
$I/I_{corundum}$ = 1.22(12)

Additional pattern
PDF card 21-1499 [Dept. of Physics, University College, Cardiff, Wales]

References
Clearfield, A. and Vaughan, P. A. (1956). Acta Crystallogr. 9, 555.

Mak, T. C. W. (1968). Can. J. Chem. 46, 3491.

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

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
12.10	100	1 1 0	7.30
8.53	15	2 0 0	10.36
7.66	4	2 1 0	11.55
7.03	65	1 0 1	12.58
6.05	10	2 2 0	14.63
5.417	11	3 1 0	16.35
4.739	1	3 2 0	18.71
4.429	7	3 1 1	20.03
4.141	8	4 1 0	21.44
4.028	52	3 3 0	22.05
3.857	14	0 0 2	23.04
3.828	12	4 2 0	23.22
3.679	17	1 1 2	24.17
3.423M	27	4 2 1	26.01
3.423M		4 3 0	26.01
3.356	4	5 1 0	26.54
3.192	10	3 0 2	27.93
3.173	21	5 2 0	28.10
3.126	43	4 3 1	28.53
3.021	11	4 4 0	29.54
2.936	10	5 2 1	30.42
2.848	9	6 0 0	31.39
2.810	3	6 1 0	31.82
2.740	10	5 3 1	32.65
2.672M	1	6 0 1	33.51
2.672M		5 4 0	33.51
2.641	2	6 1 1	33.91
2.558	7	4 3 2	35.05
2.547	5	6 3 0	35.21
2.525	5	5 4 1	35.53
2.451	4	5 2 2	36.64
2.419M	3	6 3 1	37.14
2.419M		7 1 0	37.14
2.378	5	4 4 2	37.80
2.345	5	3 0 3	38.36
2.327	7	7 0 1	38.66
2.321	8	3 1 3	38.76
2.291	4	6 0 2	39.30
2.267	9	6 4 1	39.73
2.259	13	3 2 3	39.88
2.245M	6	7 2 1	40.13
2.245M		7 3 0	40.13
2.205	5	4 0 3	40.90
2.189	6	6 5 0	41.21
2.155	2	7 3 1	41.88
2.133	10	4 2 3	42.34
2.124	12	6 3 2	42.52
2.119	12	7 4 0	42.63
2.053	13	4 3 3	44.07
2.047	16	5 5 2	44.20
2.014	2	6 6 0	44.98
2.007	6	7 2 2	45.14
2.000	6	8 3 0	45.30
1.987	5	7 5 0	45.62
1.933	9	5 3 3	46.98
1.925	8	7 5 1	47.17
1.854	8	7 6 0	49.10
1.834	3	9 1 1	49.66
1.811	8	8 5 0	50.34

INORGANIC NAMES

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.

m - Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

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$C_6H_{15}NdO_{12}S_3 \cdot 9H_2O$	Neodymium ethylsulfate hydrate	9	41
$C_7H_5BrO_2$	o-Bromobenzoic acid	16m	22
$C_7H_5ClO_2$	m-Chlorobenzoic acid	16m	30
$C_7H_5FO_2$	p-Fluorobenzoic acid	16m	36
$C_7H_9NO_2S$	Methyl sulfonanilide	9m	78
$C_7H_{12}O_4$	Pimelic acid	7m	153
$C_8H_4Hg_2O_4$	Mercury o-phthalate	10m	113
$C_8H_5KO_4$	Potassium hydrogen o-phthalate	4m	30
$C_8H_5O_4Tl$	Thallium hydrogen phthalate	16m	75
$C_8H_7N_3O_7$	2,4,6-Trinitrophenetole	8m	152
$C_8H_8O_3$	p-Anisic acid	16m	11
C_8H_9NO	Acetanilide (calc. pattern)	14m	38
C_8H_9NO	Acetanilide	16m	7
$C_8H_{11}N_2NaO_3$	Sodium barbital	16m	157
$C_8H_{12}N_2O_3$	Barbital, form I	15m	126
$C_8H_{12}N_2O_3$	Barbital, form II	15m	128
$C_8H_{12}N_2O_3$	Barbital, form IV	15m	130
$C_9H_{14}N_2O_3$	Metharbital	15m	177
$C_{10}H_{12}N_2O_3$	Allobarbital	14m	41
$C_{10}H_{16}ClNO$	(-)-Ephedrine hydrochloride	16m	124
$C_{11}H_{16}N_2O_3$	Vinbarbital, form I	16m	162
$C_{11}H_{18}N_2O_3$	Amobarbital, form I	15m	114
$C_{11}H_{18}N_2O_3$	Amobarbital, form II	15m	117
$C_{12}H_{10}N_2$	Azobenzene	7m	86
$C_{12}H_{12}N_2 \cdot 2HCl$	Benzidine hydrochloride	18m	14
$C_{12}H_{12}N_2O_3$	Phenobarbital, form III	16m	144
$C_{12}H_{16}Cl_2CuN_8$	Copper tetrapyrazole chloride	8m	31
$C_{12}H_{16}Cl_2N_8Ni$	Nickel tetrapyrazole chloride	8m	44
$C_{12}H_{16}CuN_{10}O_6$	Copper tetraimidazole nitrate	13m	24
$C_{12}H_{16}N_2$	(N,N)-Dimethyltryptamine	14m	109
$C_{12}H_{16}N_2O$	Bufotenine	15m	133
$C_{12}H_{16}N_2O$	Psilocin	16m	152
$C_{12}H_{22}O_{11}$	Sucrose	11m	66
$C_{12}H_{26}N_2O_4$	Hexamethylenediammonium adipate	7m	121
$C_{13}H_{21}ClN_2O_2$	Procaine hydrochloride	16m	149
$C_{13}H_{21}N_2O_4P$	Psilocybin methanolate	16m	154
$C_{14}H_{11}FO$	4-Acetyl-2'-fluorodiphenyl	8m	91
$C_{14}H_{20}ClN_3S$	Methapyrilene hydrochloride	14m	112
$C_{15}H_{12}N_2O$	β-Carbamazepine	18m	24
$C_{15}H_{12}O_2$	Dibenzoylmethane	7m	115
$C_{16}H_{13}ClN_2O$	Diazepam	14m	106
$C_{16}H_{13}N$	N-Phenyl-2-naphthylamine	6m	29
$C_{17}H_{19}ClN_2S$	Chlorpromazine	14m	60
$C_{17}H_{20}ClNO_3 \cdot 3H_2O$	Morphine hydrochloride hydrate	16m	133
$C_{17}H_{22}ClNO_4$	L-Cocaine hydrochloride	16m	114
$C_{17}H_{26}ClN$	Phencyclidine hydrochloride	16m	141
$C_{18}H_{22}BrNO_3 \cdot 2H_2O$	Codeine hydrobromide hydrate	16m	117
$C_{18}H_{24}CdN_{14}O_6$	Cadmium hexaimidazole nitrate	8m	23
$C_{18}H_{24}N_{14}NiO_6$	Nickel hexaimidazole nitrate	7m	27
$C_{18}H_{28}N_2O_4S$	(+)-Amphetamine sulfate	15m	119
$C_{19}H_{22}ClNO_4 \cdot 2H_2O$	Naloxone hydrochloride hydrate	16m	136
$C_{19}H_{22}N_2O$	Cinchonine	17m	26
$C_{19}H_{25}ClN_2$	Imipramine hydrochloride	16m	129
$C_{20}H_{26}ClNO_3$	Benactyzine hydrochloride	16m	92
$C_{20}H_{34}$	α-Dihydrophyllocladene, hartite (or bombiccite)	16m	122
$C_{21}H_{23}ClFNO_2$	Haloperidol	16m	127
$C_{21}H_{30}O_2$	Cannabidiol	16m	111
$C_{22}H_{25}ClN_2OS \cdot 2H_2O$	Clopenthixol hydrate	17m	28
$C_{22}H_{30}O_4$	Δ^9-Tetrahydrocannabinolic acid B	16m	160
$C_{24}H_{32}N_2O_2Pd$	Palladium bis-(N-isopropyl-3-ethylsalicylaldiminate)	7m	144
$C_{25}H_{15}N_6$	N-Methylphenazinium-7,7,8,8-tetracyanoquinodimethanide	7m	146
$C_{33}H_{40}N_2O_9$	Reserpine	8m	123

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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
Mercury acetate	$C_4H_6Hg_2O_4$	17m	51
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 (α-HMX)	$C_4H_8N_8O_8$	11m	100
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (β-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	56
Picric acid	$C_6H_3N_3O_7$	16m	56
Pimelic acid	$(CH_2)_5(CO_2H)_2$	7m	153
Potassium formate-formic acid complex	$KO_2CH \cdot HO_2CH$	9m	93
Potassium hydrogen o-phthalate	$C_6H_4(COOH)(COOK)$	4m	30
Potassium hydrogen oxalate hydrate	$C_4H_3KO_8 \cdot 2H_2O$	17m	60
Potassium oxalate hydrate	$K_2C_2O_4 \cdot H_2O$	9m	39
Potassium oxalate perhydrate	$K_2C_2O_4 \cdot H_2O_2$	9m	96
Potassium sodium tartrate hydrate	$C_4H_4KNaO_6 \cdot 4H_2O$	15m	55
Procaine hydrochloride	$C_{13}H_{21}ClN_2O_2$	16m	149
Psilocin	$C_{12}H_{16}N_2O$	16m	152
Psilocybin methanolate	$C_{13}H_{21}N_2O_4P$	16m	154
Reserpine	$C_{33}H_{40}N_2O_9$	8m	123
Rubidium oxalate perhydrate	$Rb_2C_2O_4 \cdot H_2O_2$	9m	102
Silver oxalate	$Ag_2C_2O_4$	9m	47
Sodium acetate hydrate	$C_2H_3NaO_2 \cdot 3H_2O$	15m	66
Sodium barbital	$C_8H_{11}N_2NaO_3$	16m	157
Sodium glutamate hydrate	$C_5H_8NNaO_4 \cdot H_2O$	17m	70
Sodium hydrogen oxalate hydrate	$C_2HNaO_4 \cdot H_2O$	17m	72
Sodium oxalate	$Na_2C_2O_4$	6m	70
Sodium D-tartrate hydrate	$(CHOH\text{-}CO_2Na)_2 \cdot 2H_2O$	11m	110
Strontium formate	$Sr(CHO_2)_2$	8	55
Strontium formate hydrate	$Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic)	8	56
Sucrose	$C_{12}H_{22}O_{11}$	11m	66
Tartaric acid, D-	$(CHOHCO_2H)_2$	7m	168
Δ^9-Tetrahydrocannabinolic acid B	$C_{22}H_{30}O_4$	16m	160
Thallium hydrogen phthalate	$C_8H_5O_4Tl$	16m	75
Thiosemicarbazide	CH_5N_3S	17m	81
Thiourea	CH_4N_2S	17m	83
Trimethylammonium chloride	$(CH_3)_3NHCl$	9m	113
2,4,6-Trinitrophenetole	$C_2H_5OC_6H_2(NO_2)_3$	8m	152
Uranyl acetate hydrate	$C_4H_6O_6U \cdot 2H_2O$	18m	76
Urea	$CO(NH_2)_2$	7	61
Uric acid, phase 1, (calc. pattern)	$C_5H_4N_4O_3$	8m	154
Uric acid (phase 1)	$C_5H_4N_4O_3$	16m	78
Vinbarbital, form I	$C_{11}H_{16}N_2O_3$	16m	162
Zinc acetate hydrate	$C_4H_6O_4 \cdot 2H_2O$	18m	78
Zinc diimidazole chloride	$Zn(C_3H_4N_2)_2Cl_2$	7m	123
Zinc glutamate hydrate,	$Zn(O_2CCHNH_2CH_2CH_2CO_2) \cdot 2H_2O$	7m	170

*Natural mineral

*U.S. GOVERNMENT PRINTING OFFICE : 1981 0-340-997/ 1826

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Section 18 - Data for 58 Substances

5. AUTHOR(S) Marlene C. Morris, Howard F. McMurdie, Eloise H. Evans, Boris Paretzkin, Harry S. Parker, Nicolas C. Panagiotopoulos, and Camden R. Hubbard

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

Standard x-ray powder diffraction patterns are presented for 58 substances. These experimental patterns, useful for identification, were obtained by diffractometer methods. The lattice constants were refined by least-squares methods, and reflections were assigned Miller indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

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

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