NBS MONOGRAPH 25— SECTION 14

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

Standard X-ray Diffraction Powder Patterns

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[1] Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.

[2] Located at Boulder, Colorado 80302.

Standard X-ray Diffraction Powder Patterns
Section 14—Data for 68 Substances

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Joint Committee on
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ERRATA

A book has been published containing card images of NBS Standard X-ray Diffraction Powder Patterns[1]. During preparation of the book, some errors were found and corrected on the card images. A list of them is available on request. The corrections below are in addition to those included on the card images.

Circular 539

Vol. 1, p. 67 Density should be 2.749 g/cm^3
1, p. 78 In the test for chemical analysis, the word should be "thiocyanate."
2, p. 28 Previous erratum (Mono. 25, Sec. 5) changed the space group to Ia3. Change also the following indices: for d = 2.068, 1.808, 1.491, 1.1646, and 1.1110, use hkℓ = 431, 433, 543, 833, and 851 respectively.
3, p. 27 Previous erratum (Mono. 25, Sec. 5) changed the space group to Ia3. Change also the following indices: for d = 1.9301, 1.6885, and 1.3924, use hkℓ = 431, 433, and 543 respectively.
4, p. 67 In the lattice constants, the NBS values for "b" and "c" should be interchanged. Because "b" and "c" are so nearly equal, a few indices may also need to be changed.
5, p. 30 At hkℓ = 321, "d" should be 1.4479. At hkℓ = 631, "d" should be 0.7987.
6, p. 41 Delete "CdI_2-type structure." Insert "K_2GeF_6 is used as a structure type."
10, p. 4 Formula in title should be $AlPO_4$.

Monograph 25

Sec. 5, p. 11 At hkℓ = 002, d should be 4.401.
11, p. 39 Add this structural information: "The cubic cell given with Z = ½ is a pseudo-cell. The true cell with Z = 1 has random voids in the Hg position."
12, p. iii The formula for magnesium titanium oxide should be Mg_2TiO_4.
12, p. 42 The text and the references at the end should both have the year 1975 for the reference to McMurdie et al.
13, p. 26 At d = 1.648, the hkℓ's should be $\bar{4}42$,530.
13, p. 36 At d = 2.423, the intensity should be 20.
13, p. 79 Density should be 8.605.

[1]Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081, $150.00).

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

The following copies may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia, 22161. Where these publications are identified with a number, it must be used in ordering. They are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

Also, until the present supply is exhausted, the publication numbers marked by an asterisk are for sale from the Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402. Order Sections 11, 12, and 13 respectively, by catalog no. SN 003-003-01234-3, $1.55; SN 003-003-01376-5, $1.50; or C13.44:25/Sec. 13, $1.80. (Add 25% additional for other than U. S. mailing).

NBS Publication	Number
Circular 539, Volume 1	PB 178 902
Volume 2	PB 178 903
Volume 3	PB 178 904
Volume 4	PB 178 905
Volume 5	PB 178 906
Volume 6	PB 178 907
Volume 7	PB 178 908
Volume 8	PB 178 909
Volume 9	PB 178 910
Volume 10	PB 178 911

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Section 7	
Section 8	PB 194 872
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Section 10	COM 72-51079
*Section 11	COM 74-50183
*Section 12	COM 75-50162
*Section 13	

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 14. --- Data for 68 Substances

by

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Standard x-ray diffraction patterns are presented for 68 substances. Twenty-seven of these patterns represent experimental data and 41 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

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

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the Joint Committee on Powder Diffraction Standards,[1] the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 68 compounds (27 experimental and 41 calculated patterns), and is the twenty-fourth of the series of "Standard X-ray Diffraction Powder Patterns."[2]

EXPERIMENTAL POWDER PATTERNS

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the sample improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

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

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

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

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

[2]See previous page for other published volumes.

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

Calculated 2θ Angles, CuKα$_1$ λ = 1.540598Å

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

The new internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Cell parameter data were also collected for a single crystal from the boules ground to prepare the powder. The lattice parameters from the two methods agreed within 3 parts in 10^5 [Hubbard et al. 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation: λ(CuKα$_1$, peak)= 1.540598Å [Deslattes and Henins, 1973].

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

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

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

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and atomic weights published by IUPAC [1972].

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

position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (as shown in Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. Any intensity larger than 20 was rounded to the nearer multiple of 5. At least 3 patterns for intensity measurements were prepared for each sample to check reproducibility.

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 reflection 113(hexagonal) of corundum [Visser and de Wolff, 1964]. The ratio is tabulated for copper Kα radiation, for a 1:1 mixture by weight of the sample and corundum.

A new 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 ($x_s = 1-x_c$), intensities $I(\underline{h})$ and $I(\underline{k})$ are measured for several sets of reflections $\underline{h}$ 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

$$\frac{I(\underline{h}_0)}{I_c(113)} = \frac{x_c}{x_s} \cdot \frac{I_c^{rel}(\underline{k})}{I^{rel}(\underline{h})} \cdot \frac{I(\underline{h})}{I(\underline{k})}$$

and $(\underline{h}_0)$ indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection $(\underline{h}_0)$ will be the one with I=100 since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio, I/I_c. These values yield the tabulated average $\langle I/I_c \rangle$. From these data, an estimated standard deviation, Δ, (given in parentheses), was obtained from

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

where n is the number of measurements of the reference intensity ratio.

CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Clark, Smith and Johnson [1973] and modified at NBS.

Lattice parameters. Before the computations of the patterns, any necessary changes were made in the lattice constants in order to make them consistent with the revised value of $\lambda(CuK\alpha_1)$= 1.540598Å [Deslattes and Henins, 1973]. Both the altered and the original published values are given. A lattice constant arrangement which follows the conventions of Crystal Data has been referred to as the "CD cell." In several of the calculated patterns, the literature lattice constants, the atom positions, and hence the final patterns were not given in the CD arrangement. For cross-reference purposes, the CD cell was calculated separately and included in the text.

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

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

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

or

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

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

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

Structural information. The atom positions used in these calculated patterns varied somewhat in the degree of reliability. In our text, when the expression "the structure was determined by..." was used, the atomic parameters in the reference cited had been calculated from refinement of single crystal data. Otherwise, the atomic positions had been derived by analogy with similar compounds whose structure was known. In cases where isostructural relationships were used, the atoms were in fixed special positions or the ionic radii were closely related to the corresponding radii of the atoms in the known structure.

Integrated intensities. The theoretical integrated intensity of reflection i on the "absolute/relative" scale is computed from the right hand side of the equation:

$$\frac{I_i^{abs}}{K} = \frac{M_i Lp_i |F_i T_i|^2}{2\mu V^2}$$

where:

F is the structure factor
T is the thermal correction

$Lp = \frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$ is the Lorentz-polarization term

M is the multiplicity for the reflection i
μ is the linear absorption coefficient
V is the volume of the unit cell

When the largest integrated intensity was assigned a relative value of 100 and all other reflections were scaled relative to it, the intensities were placed on the relative intensity scale (I^{rel}). Relative intensities were rounded to the nearest integer value before being listed, and reflections with I^{rel} less than 0.7 were omitted.

Scale factor (integrated intensities). The scale factor, γ, was defined to convert the tabulated I^{rel} to the "absolute/relative" scale [Hubbard, Evans and Smith, 1976]. That is:

$$\gamma = \frac{M'Lp'|F'T'|^2}{200\mu V^2}$$

and

$$\frac{I^{abs}}{K} = \gamma I^{rel}$$

The primes denoted the values for the largest integrated intensity. In earlier Monographs (1969-1975), a different scale factor, k_{NBS}, was reported which is related to γ:

$$\frac{\gamma}{k_{NBS}} = \frac{1}{2\mu V^2}$$

From γ, the theoretical value of the Reference Intensity Ratio, I/I_c, was calculated:

$$I/I_c = \frac{\mu\gamma\rho_c}{\mu_c\gamma_c\rho}$$

where ρ is the density and the subscript c represents corundum (α-Al_2O_3).

For refined structures, the value of I/I_c was given. For those phases whose structures were postulated or were based only on analogy to other powder patterns, I/I_c was not included and any intensity above 20 was rounded further, to the nearer multiple of 5.

I/I_c and γ are each based on the single strongest reflection, not on the overlapping sum of superimposed reflections.

Peak intensities. The purpose of calculating peak intensities was to provide a tabulated pattern similar to what might be obtained from experimental diffractometer measurements. For each predicted reflection, Cauchy profiles centered at both the α_1 and the α_2 peak positions were calculated and summed, forming a simulated powder pattern. The full width at half-maximum (FWHM) was allowed to vary to represent the changing FWHM as a function of 2θ. [The values of the FWHM vs 2θ are given in the table below]. The resultant simulated powder pattern was then analyzed for peaks. In the regions of the predicted reflections several reflections could have identical or similar 2θ angles and produce only one composite peak in the simulated pattern. The 2θ angle of the composite peak was assigned the hkℓ of the reflection having the greatest contribution to the peak intensity. If any other peak contributed more than 10% of the intensity toward the composite peak intensity, a plus sign (+) was appended to the hkℓ. Peaks due solely to α_2 lines were omitted. If an α_1 peak and an α_2 peak overlapped, the α_1 reflection was listed only when it contributed a significant intensity (>10%) at the peak 2θ.

The peak search routine located peaks only at 2θ angles which were a multiple of 0.02°.

2θ CuKα1	FWHM	2θ CuKα1	FWHM
0°	0.12°	140	0.230
20	.12	145	.255
40	.12	150	.285
60	.125	155	.315
80	.130	160	.360
100	.135	162.5	.410
120	.155	165	.500
130	.185		

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Ammonium iron chloride hydrate, $(NH_4)_2FeCl_5 \cdot H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of an acid aqueous solution of NH_4Cl and $FeCl_3$.

Color
Deep reddish orange

Optical Data
Biaxial (+), $N_\alpha = 1.755$, $N_\beta = 1.77$, $N_\gamma = 1.82$. 2V is large.

Structure
Orthorhombic, Pmnb (62), Z=4, isostructural with $K_2FeCl_5 \cdot H_2O$ (erythrosiderite) [Bellanca, 1947]. The structure of $(NH_4)_2FeCl_5 \cdot H_2O$ was determined by Lindqvist [1946, 1948].

NBS lattice constants of this sample:

a = 9.925(3) Å
b = 13.713(3)
c = 7.039(2)

Volume
957.9 $Å^3$

Density
(calculated) 1.991 g/cm^3

Reference intensity
$I/I_{corundum} = 0.8$

References
Bellanca, A., (1947). Ric. Sci. Ricostr. 17, 1360.
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$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.26	8	011	14.13
5.74	100	101	15.43
5.64	95	120	15.71
5.29	9	111	16.73
4.96	60	200	17.87
4.92	80	021	18.03
4.39	5	121	20.19
4.01	6	220	22.13
3.836	12	031	23.17
3.579	5	131	24.86
3.515	5	002	25.32
3.492	4	221	25.49
3.426	6	040	25.99
3.410	4	012	26.11
3.082	17	041	28.95
3.034	18	231	29.42
2.989	25	122	29.87
2.983	25	320	29.93
2.945	12	141	30.32
2.869	35	202	31.15
2.820	95	240	31.70
2.812	85	212	31.80
2.787	65	032	32.09
2.742	4	321	32.63
2.685	5	132	33.34
2.648	5	222	33.83
2.617	4	241	34.24
2.557	4	051	35.07
2.481	65	400	36.17
2.456	50	042	36.55
2.432	4	232	36.93
2.382	5	142,340	37.73
2.313	11	013	38.91
2.308	9	411	38.99
2.227	4	160	40.47
2.214	20	421	40.73
2.202	12	242	40.96
2.174	11	061	41.50
2.163	15	052	41.73
2.114	13	152	42.73
2.082	11	431	43.42
2.042	19	133	44.32
1.991	6	261	45.53
1.984	4	252	45.68
1.932	7	441	46.99
1.907	10	520	47.66
1.881	8	162,360	48.34
1.854	25	171,432	49.10
1.811	6	352	50.34
1.782	7	053	51.22
1.764	5	271	51.78
1.745	25	442,014	52.40
1.7180	13	540	53.28
1.7150	8	512,080	53.38
1.6915	8	413	54.18
1.6696	6	541	54.95
1.6654	5	081	55.10
1.6429	8	181,034	55.92
1.6346	8	461	56.23
1.6304	9	452	56.39
1.6201	6	280,134	56.78
1.5434	5	542,314	59.88

Ammonium potassium iron chloride hydrate, (kremersite) $(NH_4,K)_2\ FeCl_5 \cdot H_2O$

Sample

The sample was prepared by slow evaporation at room temperature of a 1:1:1 molar aqueous solution of NH_4Cl, KCl and $FeCl_3$. The first crystals formed were used. From a plot of the cell parameters of the end members of the solid solution series, this sample was determined to be close to a 1:1 molar ratio of NH_4 to K. This is similar to the reported analysis of the natural mineral, kremersite, from Mt. Vesuvius [Palache et al., 1951].

Color

Deep reddish orange

Structure

Orthorhombic, Pmnb (62), Z=4, isostructural with $K_2FeCl_5 \cdot H_2O$ and $(NH_4)_2FeCl_5 \cdot H_2O$. The structure of $K_2FeCl_5 \cdot H_2O$ was determined by Bellanca[1947].

NBS lattice constants of this sample

a = 9.808(3)Å
b = 13.657(4)
c = 7.028(2)

Volume

941.4

Density

(calculated) 2.175 g/cm^3.

Reference Intensity

$I/I_{corundum} = 1.2$

References

Bellanca, A. (1947). Ric. Sci. Ricostr. 17, 1360.

Palache, C., Berman, H., and Frondel, C. (1951). Dana's System of Mineralogy (John Wiley & Sons, New York, 7th Ed.) pg. 101.

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

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.72	80	101	15.48
5.61	55	120	15.78
5.270	7	111	16.81
4.900	40	200,021	18.09
3.820	6	031	23.27
3.464	7	221	25.70
3.411	9	040	26.10
3.070	16	041	29.06
3.016	17	231	29.60
2.966	13	301	30.11
2.951	9	320	30.26
2.857	25	202	31.28
2.800	100	240	31.93
2.794	60	212	32.00
2.783	55	032	32.14
2.601	4	241	34.45
2.548	3	051	35.20
2.451	65	400,042	36.64
2.374	4	142	37.86
2.310	4	013	38.95
2.277	2	060	39.54
2.191	11	421,242	41.16
2.157	12	052	41.84
2.106	9	152	42.91
2.038	14	133	44.41
1.889	7	501	48.14
1.839	15	432	49.54
1.800	4	352	50.66
1.798	2	243	50.74
1.779	4	053	51.33
1.742	7	014	52.49
1.7327	13	442	52.79
1.6585	4	081	55.35
1.6541	3	204	55.51
1.6193	6	452	56.81

Ammonium strontium chromium oxide, $(NH_4)_2Sr(CrO_4)_2$

Sample
The sample was precipitated by adding a strong solution of $SrCl_2$ to one of $(NH_4)_2CrO_4$, following the method of Schwarz [1966]. This material gave somewhat broad peaks which suggest that the compound may be of lower symmetry.

Color
Dark orange yellow

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$ and many other double chromates and sulfates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

a = 5.758(1) Å
c = 22.027(4)

Volume
632.3 $Å^3$

Density
(calculated) 2.802 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.2(3)

Additional pattern
1. PDF card 19-70 [Schwarz, 1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 345, 230.

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

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
7.345	60	003	12.04
4.868	5	101	18.21
4.546	45	012	19.51
3.696	10	104	24.06
3.672	6	006	24.22
3.300	100	015	27.00
2.881	60	110	31.02
2.680	30	113	33.41
2.662	13	107	33.64
2.434	4	202	36.90
2.411	2	018	37.26
2.271	8	024	39.65
2.266	9	116	39.75
2.169	20	205	41.61
2.015	20	1·0·10	44.95
1.955	2	027	46.42
1.857	6	0·1·11,122	49.01
1.848	11	208	49.26
1.836	6	0·0·12	49.61
1.783	2	214	51.19
1.732	11	125	52.81
1.662	6	300	55.23
1.651	5	0·2·10	55.63
1.619	4	303,217	56.81
1.604	3	1·0·13	57.40
1.554	2	128	59.41
1.5481	2	1·1·12	59.68
1.4682	3	0·0·15	63.29
1.4392	5	220	64.72
1.4319	11	2·1·10	65.09

Barium vanadium oxide, $Ba_3(VO_4)_2$

Sample
Prepared by heating stoichiometric amounts of $BaCO_3$ and V_2O_5 at 825 °C, regrinding and reheating at 860 °C for 1½ hours, grinding again and heating on Méker burner (~1100 °C) for 10 minutes to improve crystallization.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$. The structure was determined by Zachariasen [1948] and refined by Süsse and Buerger [1970].

NBS lattice constants of this sample:

a = 5.7845(2) Å
c = 21.317(1)

Volume
617.73 $Å^3$

Density
(calculated) 5.176 g/cm^3

Reference intensity
$I/I_{corundum}$ = 4.7(4)

Additional patterns
1. PDF card 19-144 [Lubin & Rittershaus, Gen'l. Tel. and Electronics, N.Y. (1966)].
2. PDF card 25-1192 [Smith et al., 1974].
3. Zachariasen [1948].

References

Smith, D. K., et al., (1974). Annual Report to the Joint Committee on Powder Diffraction Standards.

Süsse, P., and Buerger, M. J., (1970). Z. Kristallogr. 131, 161.

Zachariasen, W. H., (1948). Acta Crystallogr. 1, 263.

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

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
7.09	4	003	12.47
4.878	11	101	18.17
4.537	3	012	19.55
3.651	12	104	24.36
3.247	100	015	27.45
2.893	75	110	30.88
2.487	4	021	36.09
2.439	7	202	36.82
2.369	9	009	37.95
2.353	3	018	38.22
2.267	11	024	39.72
2.243	6	116	40.17
2.160	40	205	41.79
1.962	25	1·0·10	46.24
1.934	4	027	46.95
1.886	3	211	48.20
1.833	10	119	49.71
1.785	3	214	51.14
1.731	25	125	52.85
1.670	13	300	54.92
1.624	12	0·2·10	56.64
1.543	1	128	59.90
1.511	2	306	61.30
1.457	4	0·1·14	63.85
1.446	10	220	64.38
1.421	4	0·0·15	65.66
1.416	13	2·1·10	65.92
1.386	1	131	67.53
1.3647	3	309	68.73
1.3445	1	134	69.91
1.3208	9	315	71.35
1.3010	2	2·0·14	72.61
1.2755	10	1·1·15	74.30
1.2438	1	042	76.53
1.2343	4	229	77.23
1.2324	2	318	77.37
1.2015	4	045	79.75
1.1864	3	1·2·14	80.97
1.1641	5	1·3·10	82.86
1.1235	1	324	86.57
1.1096	5	235	87.93
1.0947	4	1·0·19	89.44
1.0933	5	410	89.59
1.0824	6	3·0·15	90.74
1.0799	5	4·0·10	91.01
1.0425	3	0·1·20	95.27
1.0264	2	3·1·14	97.27
1.0239	2	0·2·19	97.57
1.0135	5	2·2·15	98.93
1.0114	7	3·2·10	99.22

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å			
d(Å)	I	hkℓ	2θ(°)
0.9927	2	419	101.78
.9809	2	2•0•20	103.49
.9753	2	505	104.34
.9653	4	2•1•19	105.87
.9641	4	330	106.06
.9288	4	1•2•20	112.07
.9242	3	425	112.91
.9174	2	2•3•14	114.21
.9067	2	0•5•10	116.32
.8802	2	155	122.12
.8729	1	1•3•19	123.87
.8665	1	4•1•15	125.50

Calcium iodate (lautarite), $Ca(IO_3)_2$

Sample
The preparation was begun by adding an aqueous solution of $Ca(NO_3)_2$ to one of HIO_3 to precipitate $Ca(IO_3)_2 \cdot 6H_2O$ which was then heated at 160°C. for six hours. It was heated again in a sealed glass tube at 240°C for several hours.

Color
Colorless

Structure
Monoclinic, $P2_1/n(14)$, Z=4, distorted perovskite type. [Gossner and Mussgnug, 1930]. The structure was determined by Gossner, [1937].

NBS lattice constants of this sample:

a = 7.280(1) Å
b = 11.304(2)
c = 7.148(1)
β = 106.36(2)°

Volume
564.4 $Å^3$

Density
(calculated) 4.588 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.45(4)

Additional Patterns
1. PDF card 1-386, labeled $Ca(IO_3)_2$ but data is for $Ca(IO_3)_2 \cdot H_2O$, brüggenite.

References
Gossner, B., (1937). Z. Krist. 96, 381.
Gossner, B., and Mussgnug, F., (1930). Z. Krist. 75, 410.

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

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
5.93	12	110	14.93
5.866	5	011	15.09
5.779	5	$\bar{1}01$	15.32
5.651	3	020	15.67
5.139	5	$\bar{1}11$	17.24
4.360	50	021	20.35
4.037	17	$\bar{1}21$,111	22.00
3.493	65	200	25.48
3.428	85	002	25.97
3.378	14	$\bar{2}11$	26.36
3.336	40	210,$\bar{1}12$	26.70
3.318	30	$\bar{1}30$	26.85
3.156	100	$\bar{1}31$	28.25
3.001	18	$\bar{2}21$	29.75
2.931	3	022	30.47
2.885	20	$\bar{2}02$	30.97
2.840	35	$\bar{1}31$	31.48
2.795	13	$\bar{2}12$	31.99
2.726	10	211	32.83
2.703	4	112	33.12
2.619	2	$\bar{1}40$	34.21
2.582	2	$\bar{2}31$	34.71
2.560	6	230,$\bar{1}32$	35.02
2.515	8	$\bar{2}21$	35.67
2.328	2	$\bar{1}13$	38.65
2.292	5	$\bar{2}32$	39.27
2.252	2	231	40.01
2.240	2	013,132	40.22
2.227	8	$\bar{3}21$	40.48
2.199	5	$\bar{3}12$	41.01
2.194	5	$\bar{1}23$	41.11
2.161	18	202	41.77
2.151	8	150	41.97
2.146	5	051	42.06
2.122	5	212	42.57
2.120	5	023	42.64
2.067	3	$\bar{2}23$	43.77
2.038	20	$\bar{3}31$,301	44.42
2.012	30	$\bar{1}33$,103	45.02
1.987	4	330,113	45.75
1.926	4	$\bar{3}03$	47.16
1.917	6	$\bar{3}21$	47.39
1.897	9	$\bar{1}52$,$\bar{3}13$	47.91
1.884	9	060	48.27
1.840	3	$\bar{3}41$	49.51
1.817	12	061	50.17
1.797	12	340	50.77
1.793	14	331	50.90
1.775	15	133	51.44
1.756	12	$\bar{3}42$,152	52.05
1.7500	11	$\bar{4}12$	52.23
1.7460	11	$\bar{2}43$,$\bar{2}04$	52.36
1.7255	11	410,$\bar{2}14$	53.03
1.7138	14	$\bar{3}33$	53.42
1.6863	4	213	54.36
1.6629	7	$\bar{2}61$	55.19
1.6582	8	260,$\bar{1}62$	55.36
1.6514	6	062	55.61
1.6078	1	053	57.25
1.5911	4	$\bar{3}52$,$\bar{3}43$	57.91
1.5836	4	$\bar{2}53$,$\bar{2}34$	58.21
1.5780	5	$\bar{2}62$	58.44
1.5735	5	170,411	58.62
1.5645	4	261	58.99
1.5602	4	034,162	59.17
1.5293	1	$\bar{4}41$,421	60.49

Calcium iodate hydrate, $Ca(IO_3)_2 \cdot 6H_2O$

Sample
The sample was prepared by adding an aqueous solution of $Ca(NO_3)_2$ to one of HIO_3. The loss in weight at 160°C indicated that it was a hexahydrate.

Color
Colorless

Optical Data
Biaxial, N_α=1.604, N_β=1.644, N_γ=1.686, 2V is large. [Winchell and Winchell, 1964].

Structure
Orthorhombic, Fdd2 (43) from precession patterns [Perloff, 1976]. Z=6 (from agreement of experimental and calculated densities).

NBS lattice constants of this sample

a = 14.866(3)Å
b = 23.015(5)
c = 6.392(1)

Volume
2187.1Å^3

Density
(calculated) 2.268 g/cm^2

Reference Intensity
$I/I_{corundum}$ = 2.4(3)

References
Perloff, A. (1976). Private communication.
Winchell, A. N., and Winchell, H. (1964). The Microscopical Characters of Artificial Inorganic Solid Substances (Academic Press, New York and London) p. 109.

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

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.75	50	040	15.39
5.69	60	111	15.55
4.65	100	131	19.04
3.86	25	311	23.02
3.714	40	400	23.94
3.625	11	151	24.54
3.538	5	420	25.14
3.489	55	331	25.51
3.406	20	260	26.14
3.121	40	440	28.58
3.078	6	022	28.99
2.983	5	351	29.93
2.936	40	202	30.42
2.878	25	080	31.05
2.867	30	171	31.17
2.842	8	222	31.45
2.676	19	511	33.46
2.669	15	460	33.55
2.616	55	242	34.25
2.544	13	531	35.25
2.517	16	371	35.64
2.455	3	062	36.57
2.370	3	422	37.93
2.343	18	191	38.39
2.331	6	262	38.60
2.275	8	640,480	39.59
2.234	1	442	40.34
2.198	7	2·10·0	41.03
2.142	3	391	42.15
2.101	15	113	43.02
2.081	9	660	43.43
2.055	11	282	44.03
2.048	8	462	44.18
2.034	12	133	44.51
2.007	5	711	45.14
1.971	11	1·11·1	46.02
1.956	7	4·10·0	46.38
1.951	19	313,731	46.52
1.930	6	622	47.05
1.917	1	0·12·0,153	47.39
1.896	4	333	47.95
1.868	9	0·10·2	48.71
1.853	25	642,482	49.12
1.846	20	751,3·11·1	49.33
1.802	2	353	50.62
1.775	11	173	51.43
1.744	4	662	52.42
1.728	4	513	52.96
1.719	3	771	53.25
1.690	6	533	54.25
1.683	8	373	54.49
1.669	7	4·10·2	54.96
1.653	6	5·11·1	55.55
1.606	8	2·12·2,2·14·0	57.34
1.599	4	004	57.61
1.566	2	931	58.95
1.562	3	880	59.11
1.549	3	224	59.65
1.532	6	573	60.37

Cesium iron chloride hydrate, $Cs_2FeCl_5 \cdot H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of a 2:1 molar aqueous solution of CsCl and $FeCl_3$.

Color
Deep reddish orange.

Structure
Orthorhombic, Amam(63), Z=4. Perloff [1976] by single crystal study found that $Cs_2FeCl_5 \cdot H_2O$ was isostructural with $Cs_2RuCl_5 \cdot H_2O$. The structure of $Cs_2RuCl_5 \cdot H_2O$ had been determined by Hopkins et al. [1966].

NBS lattice constants of this sample:

a = 8.070(1)Å
b = 17.326(2)
c = 7.436(1)

Volume
1039.8 $Å^3$

Density
(calculated) 3.302 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.9(2)

References
Hopkins, T. E., Zalkin, A., Templeton, D. H., and Adamson, M. G. (1966). Inorg. Chem. 5, 1431.
Perloff, A. (1976). Private communication.

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

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.83	8	011	12.95
5.91	7	120	14.97
5.21	4	111	17.00
4.565	40	031	19.43
4.335	6	040	20.47
4.037	45	200	22.00
3.973	100	131	22.36
3.816	5	140	23.29
3.719	25	002	23.91
3.660	4	220	24.30
3.476	12	211	25.61
3.418	3	022	26.05
3.143	10	122,051	28.37
3.024	20	231	29.52
2.950	75	240	30.27
2.888	8	060	30.94
2.822	55	042	31.68
2.736	95	202	32.71
2.721	45	160	32.89
2.665	5	142	33.60
2.571	4	320	34.87
2.502	2	311	35.86
2.479	4	251	36.20
2.454	4	013	36.59
2.349	2	071,260+	38.29
2.318	20	331	38.82
2.286	4	340	39.39
2.280	5	062	39.49
2.255	11	171	39.95
2.194	25	162	41.10
2.165	13	080	41.68
2.113	4	322	42.76
2.093	3	180	43.20
2.018	12	400,053	44.89
1.984	12	233	45.70
1.968	4	360	46.08
1.934	2	411	46.94
1.908	4	280	47.62
1.872	4	082	48.60
1.859	11	004	48.97
1.845	6	431	49.36
1.829	3	440	49.82
1.823	3	182	49.99
1.804	4	253	50.56
1.773	8	402,124	51.51
1.770	10	371	51.61
1.739	18	362,333	52.59
1.711	6	173	53.51
1.697	16	282,451	53.98
1.693	12	1•10•0	54.12
1.654	2	460	55.53
1.640	8	442	56.00
1.591	4	2•10•0	57.90
1.587	4	520	58.06
1.573	8	244	58.65
1.570	9	511,0•10•2	58.75
1.535	6	164	60.25
1.533	5	391	60.34
1.5207	6	093	60.87
1.5126	6	540	61.23
1.5101	6	433	61.34
1.4757	4	480	62.93
1.4565	3	3•10•0	63.86
1.4088	6	560	66.29

Copper phosphate, $Cu(PO_3)_2$

Sample
The sample was made by heating $CuCO_3$ and H_3PO_4 together at 760 °C for 45 minutes.

Color
Very pale green

Structure
Monoclinic, I2/a (15) or Ia (9), Z = 8, [Beucher and Grenier, 1968]. Those authors gave the cell in the settings C2/c (15) or Cc (9).

NBS lattice constants of this sample:

a = 11.584(2) Å
b = 8.081(2)
c = 9.569(2)
β = 107.91(2)°

Volume
852.3 $Å^3$

Density
(calculated) 3.452 g/cm^3

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

Additional patterns
1. PDF card 21-998 [Ball, 1968]
2. PDF card 25-1196 [Smith et al., 1974]

References

Ball, M. C., (1968). J. Chem. Soc. (London) 5A, 1113.
Beucher, M., and Grenier, J-C., (1968). Mater. Res. Bull. 3, 643.
Smith, D. K., et al., Annual Report to the Joint Committee on Powder Diffraction Standards, 1974.

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

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.52	7	110	13.56
6.046	55	011	14.64
5.507	5	200	16.08
4.565	20	$\bar{2}11$	19.43
4.205	4	$\bar{2}02$	21.11
4.101	35	$\bar{1}12$	21.65
3.716	30	$2\bar{1}1$	23.93
3.645	10	$\bar{1}21$	24.40
3.448	40	112	25.82
3.376	17	121	26.38
3.343	50	310	26.64
3.259	10	$\bar{2}20$	27.34
2.912	100	$\bar{2}22$	30.68
2.841	30	013	31.46
2.783	8	$\bar{3}21$	32.14
2.756	35	400	32.46
2.727	12	$\bar{4}11$	32.82
2.617	2	130	34.23
2.447	25	$\bar{2}22$	36.69
2.423	6	$\bar{2}31$	37.08
2.334	17	$\bar{4}11$	38.55
2.301	8	$\bar{3}23$	39.11
2.277	7	420,004	39.55
2.190	8	$\bar{3}14$	41.19
2.127	4	510	42.47
2.101	6	$\bar{4}04$	43.02
2.089	10	$\bar{4}02$	43.28
2.049	6	$\bar{2}24$	44.17
2.030	25	$\bar{2}33$	44.59
2.007	4	$\bar{5}21$	45.14
1.877	5	$\bar{5}23$	48.46
1.861	6	$\bar{2}15$	48.89
1.835	4	$\bar{3}32$	49.63
1.821	4	$\bar{2}42$	50.05
1.779	7	233	51.32
1.738	25	$512,\bar{3}34$ +	52.61
1.735	16	$\bar{6}22$	52.73
1.709	6	$\bar{6}04$	53.59
1.6724	5	620	54.85
1.6663	4	611	55.07
1.6378	6	$\bar{3}43$	56.11
1.6293	8	440	56.43
1.5906	8	051	57.93
1.5743	6	$\bar{6}24$	58.59
1.5600	13	$\bar{2}35,215$	59.18
1.5450	5	$710,\bar{4}06$	59.81
1.5411	4	$\bar{1}16$	59.98
1.5385	4	404	60.09
1.5204	9	$\bar{5}41,\bar{6}33$	60.88
1.5106	12	044	61.32
1.4932	3	$\bar{4}35$	62.11
1.4876	7	433,152	62.37
1.4827	5	$\bar{2}26$	62.60
1.4563	9	$\bar{5}16,444$	63.87

Lead chromium oxide, Pb_2CrO_5

Sample
The sample was prepared by T. Negas by heating PbO (massicot) and Cr_2O_3 together at 630-650 °C for 92 hours followed by regrinding and heating.

Color
Deep orange.

Structure
Monoclinic I2/m (12), Z = 4, isostructural with Pb_2SO_5. The structure has been studied by Ruckman et al. [1972]. These authors gave the cell in a setting in C2/m (12).

NBS lattice constants of this sample:

a = 12.728(1) Å
b = 5.6782(5)
c = 7.1414(6)
β = 95.23(1)°

Volume
513.96 $Å^3$

Density
(calculated) 7.061 g/cm^3

Reference Intensity
$I/I_{corundum}$ = 5.1(3)

Additional patterns
1. PDF card 26-832 [Ruckman et al., 1972].
2. Negas [1968].

References
Negas, T., (1968). J. Am. Ceram. Soc. 51, 716.
Ruckman, J. C., Morrison, R. T. W., and Buck, R. H. (1972). J. Chem. Soc. Dalton Trans. 1972, 426.

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

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.46	16	$\bar{1}01$	13.69
6.34	16	200	13.95
5.973	12	101	14.82
5.184	2	110	17.09
4.438	13	011	19.99
3.786	9	$\bar{3}01$	23.48
3.737	4	$\bar{2}11$	23.79
3.555	3	002	25.03
3.542	6	211	25.12
3.390	100	310	26.27
3.230	15	$\bar{2}02$	27.59
3.169	1	400	28.14
2.984	80	202,$\bar{1}12$	29.92
2.881	20	112	31.02
2.838	35	020	31.50
2.651	4	$\bar{4}11$	33.78
2.601	2	$\bar{1}21$	34.46
2.592	4	220	34.58
2.564	6	121	34.96
2.512	15	411	35.72
2.480	16	$\bar{4}02$	36.19
2.460	8	$\bar{5}01$	36.49
2.368	8	$\bar{1}03$,312	37.96
2.314	12	510	38.88
2.272	13	$\bar{3}21$	39.64
2.266	16	402	39.75
2.204	2	321	40.92
2.188	5	013	41.23
2.132	6	$\bar{2}22$	42.36
2.113	10	600	42.77
2.058	20	222	43.97
2.018	2	$\bar{5}12$	44.88
1.992	5	303	45.50
1.951	4	$\bar{6}11$	46.51
1.875	9	$\bar{4}13$	48.50
1.869	19	512,$\bar{4}22$	48.68
1.860	8	$\bar{5}21$	48.94
1.830	2	031	49.80
1.820	2	$\bar{1}23$	50.09
1.7972	1	521	50.76
1.7779	9	004	51.35
1.7708	11	$\bar{4}22$	51.57
1.7541	5	$\bar{2}04$	52.10
1.7469	1	602,231	52.33
1.7273	11	330	52.97
1.7177	5	701	53.29
1.6947	7	$\bar{6}20$	54.07
1.6654	11	$\bar{1}32$	55.10
1.6627	4	114	55.20
1.6473	3	132	55.76

d(Å)	I	hkℓ	2θ(°)
1.6304	5	$\bar{3}23$	56.39
1.6240	4	$\bar{3}14$	56.63
1.6076	8	$\bar{7}12$	57.26
1.5876	1	$\bar{6}13$	58.05
1.5841	2	800	58.19
1.5753	2	$\bar{6}22$	58.55
1.5682	3	431	58.84
1.5291	10	$\bar{5}23$,314	60.50
1.5197	8	$\bar{8}11$	60.91
1.5068	9	024,$\bar{7}03$	61.49
1.5020	4	712	61.71
1.4919	4	$\bar{2}24$	62.17
1.4789	2	033	62.78
1.4699	10	$\bar{5}14$,721	63.21
1.4593	4	613,$\bar{2}33$	63.72
1.4313	2	$\bar{5}23$	65.12
1.4260	2	$\bar{6}04$	65.39
1.4195	5	040	65.73
1.3991	2	105,$\bar{6}31$	66.81

Lead hydrogen arsenate (schultenite), $PbHAsO_4$

Sample
The sample was precipitated by adding a concentrated aqueous solution of $Pb(NO_3)_2$ to one of As_2O_5.

Color
Colorless

Optical data
Biaxial (+), N_α = 1.890, N_β = 1.910, N_γ = 1.976, 2V is medium.

Structure
Monoclinic, P2/a (13), Z = 2. [Claringbull, 1950].

NBS lattice constants of this sample:

a = 5.8421(6) Å
b = 6.7545(6)
c = 4.8575(6)
β = 95.40(1)°

Volume
190.83 $Å^3$

Density
(calculated) 6.041 g/cm^3

Reference intensity
$I/I_{corundum}$ = 7.6(2)

Additional patterns
1. PDF card 11-141 [Claringbull, 1950]
2. Hanawalt et al., [1938]

References

Claringbull, G. F., (1950). Mineral. Mag. 29, 287.
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 Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.74	25	010	13.12
4.833	12	001	18.34
4.410	18	110	20.12
3.931	4	011	22.60
3.376	100	$\bar{1}11$,020	26.38
3.149	70	111	28.32
2.919	13	120	30.60
2.909	25	200	30.71
2.769	6	021	32.30
2.671	5	210	33.52
2.603	4	$\bar{2}01$	34.43
2.555	16	$\bar{1}21$	35.10
2.450	5	121	36.65
2.419	11	002	37.14
2.395	5	201	37.53
2.276	1	012	39.56
2.252	6	030	40.00
2.204	16	$\bar{2}20$	40.92
2.187	7	$\bar{1}12$	41.24
2.100	3	130	43.04
2.061	6	$\bar{2}21$	43.89
2.041	3	031	44.34
1.967	11	$\bar{0}22$	46.12
1.951	12	$\bar{2}02$,$\bar{1}31$	46.51
1.9024	6	131	47.77
1.8751	2	$\bar{2}12$	48.51
1.8636	4	310	48.83
1.8203	2	$\bar{1}22$	50.07
1.7939	10	$\bar{3}11$	50.86
1.7802	14	230	51.28
1.7200	1	$\bar{2}12$	53.21
1.7029	1	$\bar{2}31$	53.79
1.6886	11	040,311 +	54.28
1.6820	6	320	54.51
1.6484	5	032	55.72
1.6410	2	$\bar{2}31$	55.99
1.6298	3	$\bar{3}21$	56.41
1.6217	2	$\bar{1}40$	56.72
1.6123	2	$\bar{1}32$,003	57.08
1.5939	< 1	041	57.80
1.5740	5	222	58.60
1.5590	3	$\bar{1}32$	59.22
1.5497	10	$\bar{1}41$,321 +	59.61
1.5254	5	141	60.66
1.4806	5	113	62.70
1.4749	5	$\bar{2}32$	62.97
1.4606	2	240	63.66
1.4542	3	023,400	63.97
1.4404	2	$\bar{1}23$	64.66
1.4346	2	$\bar{3}31$	64.95
1.4157	1	312	65.93
1.3954	2	232	67.01
1.3842	2	042,123	67.63
1.3788	2	$\bar{3}31$	67.93
1.3634	< 1	$\bar{1}42$	68.80
1.3507	2	050	69.54
1.3353	2	$\bar{4}20$	70.46
1.3167	1	$\bar{4}21$	71.61
1.3102	< 1	$\bar{0}33$	72.02
1.3010	3	$\bar{4}02$,051	72.61
1.2774	3	$\bar{4}12$,$\bar{3}13$ +	74.17
1.2592	1	421,223	75.43
1.2503	2	$\bar{3}41$	76.06
1.2251	3	250,242	77.92
1.2132	4	341	78.83
1.1990	2	$\bar{2}51$	79.95
1.1972	1	402	80.09
1.1791	2	052,412	81.58
1.1766	2	251	81.79
1.1679	2	313	82.53
1.1586	2	$\bar{1}43$	83.34
1.1564	2	$\bar{3}42$	83.54

Lithium silicate, Li_2SiO_3

Sample
The sample was prepared by heating a 1:1 molar mixture of Li_2CO_3 and dried silica gel at 860 °C for 5 minutes; the material was ground and reheated for 5 minutes at 860 °C. A final heating for several minutes at about 1200 °C followed.

Color
Colorless

Structure
Orthorhombic, $Ccm2_1(36)$, Z = 4, [Seeman, 1956], isostructural with Na_2SiO_3, low $(Na,Li)SiO_3$ [West, 1976] and Li_2GeO_3 [Völlenkle and Wittman, 1968].

NBS lattice constants of this sample:

a = 5.3975(6) Å
b = 9.3974(6)
c = 4.6615(5)

Volume
236.44 $Å^3$

Density
(calculated) 2.527 g/cm^3

Additional patterns
1. PDF card 15-519 [Lam, Sheffield, England].
2. West [1976].

References
Seemann, H. (1956). Acta Crystallogr. 9, 251.
Völlenkle, H., and Wittmann, A. (1968). Monatsh. Chem. 99, 244.
West, A. R. (1976). J. Am. Ceram. Soc. 59, 118.

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

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.69	100	020,110	18.91
3.301	65	111	26.99
2.708	65	130	33.05
2.700	45	200	33.15
2.342	19	131,220	38.41
2.331	20	002	38.60
2.091	7	221	43.24
2.085	5	022,112	43.36
1.7747	4	150	51.45
1.7667	9	310,132	51.70
1.7638	8	202	51.79
1.6563	7	241	55.43
1.6522	7	311,222	55.58
1.5665	12	060	58.91
1.5605	15	330	59.16
1.4747	3	113	62.98
1.4105	1	242	66.20
1.4079	1	312	66.34
1.3547	3	260	69.31
1.3475	5	133	69.73
1.3001	5	062,350	72.67
1.2965	8	332,401 +	72.90
1.2544	3	171	75.77
1.2495	2	421	76.12
1.1747	2	080	81.95
1.1710	2	262	82.27
1.1681	2	243,402	82.52
1.1350	3	352,441	85.48
1.0770	<1	280	91.32
1.0759	<1	370	91.44
1.0700	<1	204	92.09
1.0488	1	082	94.52
1.0452	1	511	94.95
1.0441	<1	044	95.08
1.0253	1	190	97.40
1.0212	2	263	97.93
1.0188	1	403	98.24
1.0013	1	191	100.58
0.9984	2	461,173	100.98
0.9778	<1	282	103.96
0.9769	<1	372	104.10
0.9738	1	244	104.57
0.9727	<1	314	104.73
0.9397	<1	0·10·0	110.12
0.9384	<1	192	110.34
0.9348	1	532,443 +	110.98
0.9337	1	334	111.18

Lithium tantalum oxide, $LiTaO_3$

Sample
The sample was prepared as a precipitate by adding LiOH to a solution of hydrolyzed Ta_2O_5. This was further crystallized by heating at 860°C overnight.

Color
Colorless

Structure
Hexagonal, R3c (161), Z=6, by analogy with $LiNbO_3$ which was studied by Bailey [1952].

NBS lattice constants of this sample:

a = 5.1530(4) Å
c = 13.755(2)

Volume
316.30 $Å^3$

Reference intensity
$I/I_{corundum}$ = 11.8(5)

Density
(calculated) 7.430 g/cm^3

Additional pattern
1. PDF card 9-187 [Lapickij and Simanov, 1955].

References
Bailey, P., thesis, Bristol (1952) quoted by Megaw, H. D. (1954). Acta Cryst. 7, 187.
Lapickij, A. V. and Simanov, J. P. (1955). Zh. Fiz. Khim. 29, 1201.

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

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
3.745	100	012	23.74
2.723	40	104	32.86
2.577	25	110	34.79
2.292	4	006	39.28
2.245	3	113	40.13
2.122	14	202	42.57
1.871	16	024	48.62
1.712	20	116	53.48
1.638	14	122	56.12
1.604	6	018	57.41
1.5139	11	214	61.17
1.4874	6	300	62.38
1.3621	3	208	68.88
1.3145	3	119,1·0·10	71.75
1.2883	3	220	73.44
1.2481	3	306	76.22
1.2183	4	312	78.44
1.2043	4	128	79.53
1.1710	2	0·2·10	82.27
1.1648	4	134	82.80
1.1463	1	0·0·12	84.44
1.1231	3	226	86.61
1.10. 2	1	042	88.78
1.0664	2	2·1·10	92.50
1.0471	2	137,1·1·12	94.72
1.0126	2	232	99.06
1.0047	2	318,1·2·11	100.12
0.9812	2	324	103.45
.9740	2	410	104.54

Manganese phosphate, $Mn(PO_3)_2$

Sample
The sample was prepared by melting $MnCl_2$ with H_3PO_4 in molar proportions of 1:2.

Color
Pale pink

Structure
Monoclinic, I2/a (15) or Ia (9), Z = 8 [Beucher and Grenier, 1968]. Those authors gave the cell in the settings C2/c (15) or Cc (9).

NBS lattice constants of this sample

a = 11.359(2) Å
b = 8.472(2)
c = 10.176(2)
β = 112.06°(2)

Volume
907.57 $Å^3$

Density
(calculated) 3.116 g/cm^3

Reference intensity
$I/I_{corundum}$ = 0.89(11)

Additional pattern
1. PDF card 21-554 [Lee and Browne, 1968].

References
Beucher, M., and Grenier, J. C., (1968). Mater. Res. Bull. 3, 643.
Lee, J. D., and Browne, L. S., (1968). J. Chem. Soc. A 559.

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

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.29	30	011	14.06
5.26	4	200	16.85
4.71	13	002	18.81
4.65	13	$\bar{2}11$	19.07
4.348	35	$\bar{1}12$	20.41
3.613	20	211	24.62
3.468	30	112	25.67
3.300	10	220	27.00
3.242	35	$\bar{3}10$	27.49
3.065	100	$\bar{2}22$	29.11
2.998	3	202	29.78
2.947	20	013	30.30
2.728	3	$\bar{1}30$	32.80
2.681	4	$\bar{4}11$	33.39
2.632	20	400	34.03
2.521	5	$\bar{2}31$	35.59
2.446	20	$\bar{2}22$	36.71
2.424	7	$\bar{3}23$	37.06
2.358	3	$\bar{0}04$	38.13
2.331	9	$\bar{3}14,\bar{4}22$	38.59
2.236	11	$\bar{4}11,420$	40.30
2.218	2	$\bar{4}04$	40.64
2.200	2	$\bar{3}30$	41.00
2.175	4	$\bar{2}24$	41.48
2.145	19	$\bar{2}33$	42.09
2.118	4	040	42.66
2.001	6	$\bar{4}02$	45.29
1.979	5	$\bar{2}15$	45.81
1.965	2	$\bar{4}24,240$	46.16
1.928	3	$\bar{5}23$	47.11
1.890	3	$\bar{4}33$	48.10
1.864	4	$\bar{4}15$	48.82
1.839	6	$\bar{3}34$	49.54
1.802	7	$\bar{1}25,233$	50.60
1.767	5	$\bar{5}32$	51.70
1.735	4	224	52.71
1.728	11	$242,\bar{6}22$	52.93
1.687	2	$\bar{4}42$	54.35
1.667	10	$051,\bar{5}12$	55.05
1.6503	12	$440,\bar{4}06$	55.65

Nickel phosphate, $Ni(PO_3)_2$

Sample
The sample was prepared by heating a 1:2 molar mixture of $NiCO_3$ and H_3PO_4 at about 700°C for 15 hours. It was reground and heated to 1000°C for 15 hours.

Color
Light yellowish green

Structure
Monoclinic, I2/a(15) or Ia(9), Z=8, [Beucher and Grenier, 1968]. These authors gave the cell in the settings C2/c(15) or Cc(9).

NBS lattice constants of this sample:

a = 11.086(3)Å
b = 8.227(2)
c = 9.832(3)
β = 112.74(3)°

Volume
826.9 $Å^3$

Density
(calculated) 3.480 g/cm^3

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

Additional pattern
1. PDF card 19-835 (Sarver, 1966].

References
Beucher, M. and Grenier, J. C. (1968). Mater. Res. Bull. 3, 643.
Sarver, J. F. (1966). Trans. Brit. Ceram. Soc. 65, 191.

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

d(Å)	I	hkℓ	2θ(°)
6.39	7	110	13.84
6.08	50	011	14.55
5.11	3	200	17.33
4.53	20	$\bar{2}11$	19.56
4.321	3	$\bar{2}02$	20.54
4.209	40	$\bar{1}12$	21.09
3.711	5	$\bar{1}21$	23.96
3.493	19	211	25.48
3.339	30	112	26.68
3.205	11	220	27.81
3.148	30	310	28.33
3.049	4	022	29.27
2.979	100	$\bar{2}22$	29.97
2.836	25	013	31.52
2.748	2	$\bar{3}21$	32.56
2.650	2	130	33.80
2.612	4	$\bar{4}11$	34.31
2.557	25	400,$\bar{1}23$	35.06
2.451	4	$\bar{2}31$	36.64
2.359	25	$\bar{3}23$	38.11
2.263	8	$\bar{3}14$	39.81
2.220	2	123	40.60
2.165	13	411	41.69
2.135	3	330,$\bar{5}12$	42.29
2.106	3	$\bar{2}24$	42.90
2.081	20	$\bar{2}33$	43.44
2.057	4	040	43.99
2.001	2	$\bar{1}41$	45.28
1.936	4	141	46.90
1.929	7	402,$\bar{5}21$	47.07
1.912	5	$\bar{2}15$	47.52
1.882	2	$\bar{5}23$	48.33
1.856	2	$\bar{2}42$	49.03
1.848	2	$\bar{6}02$	49.26
1.8102	3	$\bar{4}15$	50.37
1.7968	3	$\bar{3}41$	50.77
1.7857	4	$\bar{3}34$	51.11
1.7638	2	$\bar{6}11$	51.79
1.7392	9	$\bar{1}43$,233 +	52.58
1.7215	5	$\bar{5}32$	53.16
1.6858	7	$\bar{6}22$,521	54.38
1.6740	3	$\bar{3}43$,242	54.79
1.6704	3	224	54.92
1.6193	7	051	56.81
1.5976	10	$\bar{2}35$	57.65
1.5759	1	$\bar{2}44$,$\bar{2}51$	58.52
1.5577	2	$\bar{1}16$	59.27
1.5534	4	125	59.45
1.5233	7	044	60.74

Potassium barium chromium oxide, $K_2Ba(CrO_4)_2$

Sample
The sample was prepared by heating $K_2Cr_2O_7$ and $BaCO_3$ in a 1:1 molar ratio at 750 °C for 1 hour followed by grinding and heating for 18 hours at 750 °C.

Color
Light greenish yellow

Structure
Hexagonal, $R\bar{3}m(166)$. Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double sulfates and chromates [Schwarz, 1966]. The structure of $Sr_3(PO_4)_2$ was determined by Wilhelmi [1967] and $(NH_4)_2Pb(SO_4)_2$ was determined by Møller [1954].

NBS lattice constants of this sample:

a = 5.7292(5) Å
c = 21.512(3)

Volume
611.51 $Å^3$

Density
(calculated) 3.645 g/cm^3

Reference intensity
$I/I_{corundum}$ = 3.3(2)

Additional pattern
1. PDF card 19-937 [Schwarz, 1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 41.
Wilhelmi, K.-A., (1967). Ark. Kemi 26, 157.

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

d(Å)	I	hkℓ	2θ(°)
7.16	15	003	12.36
4.83	4	101	18.36
4.503	30	012	19.70
3.642	3	104	24.42
3.590	2	006	24.78
3.251	100	015	27.41
2.864	70	110	31.21
2.661	14	113	33.65
2.612	8	107	34.31
2.464	2	021	36.43
2.416	3	202	37.18
2.390	7	009	37.61
2.252	11	024	40.00
2.238	8	116	40.26
2.149	30	205	42.01
1.973	20	1·0·10	45.95
1.868	2	211	48.70
1.848	4	122	49.27
1.836	5	119	49.60
1.8234	3	208	49.98
1.7926	3	0·0·12	50.90
1.7188	15	125	53.25
1.6538	9	300	55.52
1.6253	7	0·2·10	56.58
1.6118	3	303	57.10
1.6007	2	217	57.53
1.5200	3	1·1·12	60.90
1.5017	2	306	61.72
1.4676	2	0·1·14	63.32
1.4321	9	220	65.08
1.4134	10	2·1·10	66.05
1.4045	1	223	66.52
1.3766	2	0·2·13	68.05
1.3731	1	131	68.25
1.3650	2	312	68.71
1.3600	2	309	69.00
1.3533	1	1·2·11	69.39
1.3108	5	315	71.98
1.2823	7	1·1·15	73.84
1.2561	1	137	75.65
1.2289	2	229	77.63
1.2260	1	0·1·17	77.85
1.2157	2	3·0·12	78.64

Potassium barium molybdenum oxide, $K_2Ba(MoO_4)_2$

Sample
The sample was made by melting together MoO_3, K_2CO_3 and $BaCO_3$ in a molar ratio of 2:1:1, followed by grinding and reheating.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $K_2Pb(SO_4)_2$, $Sr_3(PO_4)_2$ and other double chromates and sulfates [Trunin et al., 1975]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

$a = 6.0051(4)$ Å
$c = 21.324(2)$

Volume
665.96 Å^3

Density
(calculated) 4.004 g/cm^3

Reference intensity
$I/I_{corundum} = 4.2(3)$

Additional pattern
1. Trunin et al. [1975].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Trunin, A. S., Shter, G. E., and Serezhkin, V. N., (1975). Russ. J. Inorg. Chem. 20, 1227.

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

d(Å)	I	hkℓ	2θ(°)
7.104	9	003	12.45
5.055	7	101	17.53
4.677	20	012	18.96
3.719	4	104	23.91
3.552	3	006	25.05
3.296	100	015	27.03
3.001	90	110	29.75
2.765	8	113	32.35
2.629	7	107	34.08
2.370	1	009	37.94
2.338	2	024	38.48
2.220	35	205	40.61
1.973	25	1·0·10	45.97
1.933	2	122	46.96
1.861	2	208,119	48.90
1.844	2	214	49.37
1.785	20	125	51.12
1.734	11	300	52.76
1.684	2	303	54.43
1.649	9	0·2·10	55.70
1.530	3	1·1·12	60.46
1.5009	8	220	61.76
1.4450	10	2·1·10	64.43
1.4295	2	312	65.21
1.4214	2	0·0·15	65.63
1.3664	6	315	68.63
1.3036	2	137	72.44
1.2852	7	1·1·15	73.65
1.2438	4	045	76.53
1.1945	4	1·3·10	80.31
1.1860	2	0·2·16,232	81.01
1.1491	4	235	84.19
1.1351	4	410	85.47
1.1206	2	413	86.85
1.1106	3	327	87.83
1.0993	4	3·0·15	88.97
1.0445	2	0·1·20	95.04
1.0323	2	2·2·15	96.52

Potassium calcium sulfate hydrate (syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$

Sample
The sample was prepared by mixing equal volumes of saturated aqueous solutions of $CaSO_4$ and K_2SO_4, and evaporating slowly at room temperature. The first crystals formed were used. The crystals were acicular.

Color
Colorless

Optical data
N_α=1.500, N_γ=1.518 [Aruja, 1958].

Structure
Monoclinic, $P2_1/m$ (11), Z=2 [Laszkiewicz, 1936] The structure of $K_2Ca(SO_4)_2 \cdot H_2O$ has been refined by Corazza and Sabelli[1967] and by Gorogotskaya et al. [1968].

NBS lattice constants of this sample

a = 9.777(2)Å
b = 7.147(2)
c = 6.250(2)
β = 104.01(2)°

Volume
423.7Å^3

Density
(calculated) 2.574 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.05(6)

Additional patterns
1. PDF card 11-117 [Aruja, 1958],

2. Baynham and Raistrick [1960].

References

Aruja, E. (1958). Mineral Mag. 31, 943.
Baynham, J. W. and Raistrick, B. (1960). In Chemistry and Technology of Fertilizers (Reinhold, N. Y.). ACS Monogr. Ser. 148, Chap. 21, p. 358.
Corazza, E. and Sabelli, K. (1967). Z. Krist. 124, 398.
Gorogotskaya, L. I., Podberezskaya, N. V. and Borisov, S. V. (1968). Zh. Strukt. Khim., SSSR, 9 #1, 86.
Laszkiewicz, A. (1936). Arch. Mineral. 12, 8.

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

d(Å)	I	hkℓ	2θ(°)
9.49	40	100	9.31
5.71	55	110	15.51
4.74	16	200	18.71
4.624	40	011	19.18
4.496	30	$\bar{1}11$	19.73
3.954	20	210	22.47
3.887	30	111	22.86
3.572	30	020	24.91
3.347	35	120	26.61
3.165	75	300	28.17
3.114	17	$\bar{3}01,\bar{1}02$	28.64
3.036	35	002	29.40
2.891	30	$\bar{2}02,310$	30.91
2.855	100	$\bar{1}12,220$	31.31
2.827	50	121	31.62
2.791	20	012	32.04
2.741	55	$\bar{2}21$	32.64
2.704	15	102	33.10
2.560	2	301	35.02
2.513	30	$\bar{3}02$	35.70
2.447	7	221	36.69
2.411	8	311	37.26
2.371	20	400,$\bar{3}12$	37.91
2.355	25	$\bar{3}21$	38.18
2.312	16	022,130	38.93
2.288	7	$\bar{4}11$	39.34
2.250	4	410,$\bar{2}22$	40.04
2.129	5	230	42.42
2.081	14	321,$\bar{2}31$	43.46
2.046	17	$\bar{2}03,\bar{4}12$	44.23
2.002	9	$\bar{4}21$	45.27
1.974	8	420	45.90
1.965	25	302	46.15
1.9498	20	$\bar{5}01$	46.54
1.9447	20	013,231	46.67
1.9028	12	330	47.76
1.8968	13	500,$\bar{3}31$	47.92
1.8924	12	$\bar{1}32$	48.04
1.8333	6	510,$\bar{4}22$	49.69
1.7870	20	132,040	51.07
1.7763	7	421,$\bar{2}23$	51.40
1.7444	4	331	52.41
1.6755	7	520	54.74
1.6293	2	$\bar{6}01$	56.43
1.5812	6	$\bar{4}23,600$	58.31
1.5559	11	340	59.35
1.5436	5	610	59.87
1.5293	7	$\bar{6}12$	60.49
1.4781	4	133	62.82
1.4518	8	$\bar{5}23$	64.09

Potassium calcium sulfate hydrate (syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$ - (continued)

d(Å)	I	hkℓ	2θ(°)
1.4466	6	$60\bar{1},\bar{4}04$	64.35
1.4278	5	$\bar{2}24,\bar{1}24$ +	65.30
1.3964	3	$\bar{7}0\bar{1},\bar{6}13$	66.96
1.3701	4	$\bar{4}42$	68.42
1.3494	6	522	69.62
1.3413	4	$62\bar{1}$	70.10
1.3314	4	$710,\bar{5}14$	70.70
1.3217	8	$342,\bar{5}33$	71.30
1.3085	5	$\bar{3}43$	72.13
1.2803	5	$\bar{3}34$	73.98
1.2669	3	$\bar{5}24$	74.89

Potassium iron chloride hydrate (erythrosiderite), $K_2FeCl_5 \cdot H_2O$

Sample
The sample was made by slow evaporation at room temperature of an acid solution of KCl and $FeCl_3$.

Optical Data
Biaxial (+), $N_\alpha = 1.712$, $N_\beta = 1.75$, $N_\gamma = 1.795$
2V is medium large.

Color
Deep reddish orange

Structure
Orthorhombic, Pmnb (62), Z=4, isostructural with $(NH_4)_2FeCl_5 \cdot H_2O$. The structure was determined by Bellanca [1947].

NBS lattice constants of this sample:

a = 9.706(3)Å
b = 13.585(3)
c = 7.018(1)

Volume
925.3 Å

Density
(calculated) 2.364 g/cm^3

Reference intensity
$I/I_{corundum} = 1.9$

Additional patterns
1. PDF card 25-1160, natural mineral [Mandarino, Toronto, Ontario].

Reference
Bellanca, A. (1947). Ric. Sci. Ricostr. 17, 1360.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
5.68	35	101	15.59
5.566	40	120	15.91
5.248	4	111	16.88
4.878	14	021	18.17
3.832	2	211	23.19
3.541	2	131	25.13
3.507	2	002	25.38
3.440	10	221	25.88
3.397	12	012,040	26.21
3.208	2	112,140	27.79
3.056	14	041	29.20
2.993	19	231	29.83
2.969	5	122	30.07
2.934	8	301	30.44
2.920	10	320	30.59
2.841	16	202	31.46
2.782	100	212,240	32.15
2.589	3	241	34.62
2.440	25	042	36.81
2.427	40	400	37.01
2.365	2	142	38.02
2.306	2	013	39.02
2.244	3	322,113	40.16
2.211	4	023	40.77
2.180	5	242	41.39
2.149	12	052	42.00
2.099	6	152	43.07
2.078	4	033	43.51
2.032	8	133	44.55
1.995	2	351	45.43
1.970	6	261	46.04
1.911	3	233	47.54
1.902	6	062,441	47.79
1.890	3	143	48.10
1.872	8	501,071	48.61
1.868	6	162,520	48.72
1.826	12	432,323	49.91
1.789	4	352	51.01
1.7711	3	262	51.56
1.7484	3	333	52.28
1.7404	5	014	52.54
1.7209	10	442	53.18
1.7123	4	114	53.47
1.6982	6	072,080	53.95
1.6730	4	172,180 +	54.83
1.6560	2	460,343	55.44
1.6500	4	081,204	55.66
1.6392	3	541	56.06
1.6349	5	034,423	56.22
1.6084	8	452	57.23
1.5621	3	281	59.09

Potassium lead chromium oxide, $K_2Pb(CrO_4)_2$

Sample
The sample was prepared by melting a 1:1 molar mixture of K_2CrO_4 and $PbCrO_4$.

Color
Strong yellow

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with Sr_3PO_4 and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was determined by Møller [1954].

NBS lattice constants of this sample:

a = 5.7173(7) Å
c = 21.031(3)

Volume
595.35 $Å^3$

Density
(calculated) 4.329 g/cm^3

Reference intensity
$I/I_{corundum} = 3.8(2)$

Additional pattern
1. PDF card 19-971 [Schwarz, 1966]

References
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 345, 230.

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

d(Å)	I	hkℓ	2θ(°)
6.99	30	003	12.65
4.82	19	101	18.39
4.47	40	012	19.83
3.604	8	104	24.68
3.505	2	006	25.39
3.204	100	015	27.82
2.859	85	110	31.26
2.647	20	113	33.84
2.571	8	107	34.87
2.457	4	021	36.54
2.336	6	009	38.50
2.240	11	024	40.23
2.216	11	116	40.69
2.133	30	205	42.34
1.935	19	1·0·10	46.92
1.863	4	211	48.83
1.842	5	122	49.45
1.809	5	119	50.41
1.802	5	208	50.62
1.764	2	214	51.80
1.753	2	0·0·12	52.13
1.7102	19	125	53.54
1.6508	9	300	55.63
1.6066	7	303	57.30
1.6033	7	0·2·10	57.43
1.5884	3	217	58.02
1.4935	3	1·1·12,306	62.10
1.4380	2	0·1·14	64.78
1.4293	7	220	65.22
1.3978	10	2·1·10	66.88
1.3621	2	312	68.88
1.3053	6	315	72.33
1.2586	6	1·1·15	75.47

Potassium lead molybdenum oxide, $K_2Pb(MoO_4)_2$

Sample
The sample was prepared by melting together K_2CO_3, $PbCO_3$ and MoO_3, at about 850 °C.

Color
Yellowish white

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3. The similarity of the cell size, powder patterns, and chemistry of $K_2Pb(MoO_4)_2$, $Sr_3(PO_4)_2$, $K_2Pb(SO_4)_2$ (palmierite), and $(NH_4)_2Pb(SO_4)_2$ strongly suggests an isostructural relationship. The structure of $(NH_4)_2Pb(SO_4)_2$ has been studied by Møller [1954].

NBS lattice constants of this sample:

a = 5.9853(2) Å
c = 20.987(1)

Polymorphism
Belyaev [1961] reports a polymorphic transformation of $K_2Pb(MoO_4)_2$ at 765 °C. No evidence of this was seen in the present work.

Volume
651.09 $Å^3$

Density
(calculated) 4.631 g/cm^3

Reference intensity
$I/I_{corundum}$ = 4.0(3)

References
Belyaev, I.N. (1961). Russ. J. Inorg. Chem. 6, 602.
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.

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

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.99	25	003	12.66
4.648	40	012	19.08
3.687	2	104	24.12
3.262	100	015	27.32
2.993	85	110	29.83
2.752	18	113	32.51
2.595	8	107	34.54
2.332	3	009	38.57
2.325	3	024	38.70
2.274	3	116	39.60
2.205	30	205	40.89
1.960	4	027	46.28
1.945	18	1·0·10	46.65
1.925	7	122	47.17
1.843	3	208	49.41
1.7750	25	125	51.44
1.7485	3	0·0·12	52.28
1.7279	12	300	52.95
1.6775	3	303	54.67
1.6397	4	217	56.04
1.6312	7	0·2·10	56.36
1.5694	2	128	58.79
1.5099	3	1·1·12	61.35
1.4961	8	220	61.98
1.4632	2	223	63.53
1.4398	5	0·1·14	64.69
1.4319	9	2·1·10	65.09
1.4245	4	312	65.47
1.3991	2	0·0·15	66.81
1.3602	8	315	68.99
1.2961	2	137	72.93
1.2675	4	1·1·15	74.85
1.2382	3	045	76.94
1.2292	1	3·0·12	77.61
1.2010	1	0·1·17	79.79
1.1860	5	1·3·10	81.01
1.1619	1	048	83.05
1.1442	5	235	84.63
1.1368	3	2·2·12	85.31
1.1312	3	410	85.84
1.1166	1	413	87.24
1.1054	2	327	88.35
1.1028	3	4·0·10	88.61
1.0874	2	3·0·15	90.21

Potassium lead sulfate (palmierite), $K_2Pb(SO_4)_2$

Sample
The sample was prepared by melting a 1:1 molar mixture of K_2SO_4 and $PbSO_4$, grinding and reheating at 450 °C overnight.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample

a = 5.4950(6) Å
c = 20.849(4)

Volume
545.18 $Å^3$

Density
(calculated) 4.363 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.77(10)

Additional pattern
1. PDF card 20-902 [Schwarz, 1966]

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 41.

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

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.948	35	003	12.73
4.641	25	101	19.11
4.333	45	012	20.48
3.515	18	104	25.32
3.477	3	006	25.60
3.138	100	015	28.42
2.749	70	110	32.54
2.557	35	113	35.07
2.526	13	107	35.51
2.366	9	021	38.00
2.318	10	202,009	38.82
2.287	3	018	39.36
2.166	25	024	41.67
2.156	30	116	41.86
2.068	35	205	43.74
1.910	25	1·0·10	47.57
1.860	2	027	48.94
1.792	10	211	50.92
1.772	20	122,119	51.54
1.760	7	0·1·11	51.92
1.7575	8	208	51.99
1.7373	4	0·0·12	52.64
1.7002	3	214	53.88
1.6516	20	125	55.60
1.5861	11	300	58.11
1.5684	8	0·2·10	58.83
1.5464	5	303	59.75
1.5397	4	217	60.04
1.5195	2	1·0·13	60.92
1.4823	3	2·0·11	62.62
1.4802	3	128	62.72
1.4686	5	1·1·12	63.27
1.4428	6	306	64.54
1.4212	3	0·1·14	65.64
1.3900	2	0·0·15	67.31
1.3734	10	220	68.23
1.3617	14	2·1·10	68.90
1.3479	2	223	69.71
1.3296	2	0·2·13	70.81
1.3169	1	131	71.60
1.3088	3	312,309	72.11
1.3046	3	1·2·11	72.38
1.2792	2	134	74.05
1.2622	<1	2·0·14	75.22
1.2582	9	315	75.50
1.2403	13	1·1·15	76.79
1.2067	2	137	79.34
1.1974	2	2·1·13	80.08
1.1878	2	401,0·1·17	80.86
1.1820	3	042	81.34

Potassium strontium sulfate (kalistrontite), $K_2Sr(SO_4)_2$

Sample
Two and one-half grams of $SrCl_2 \cdot 6H_2O$ in 10 mL H_2O was added dropwise to 20 g K_2SO_4 in 100 mL H_2O at the boiling point and refluxed with stirring for 4 days. The precipitate was filtered at the boiling point, squeezed on blotting paper and dried in dessicator. The crystallinity was improved by heating the precipitate to 600 °C for 3 days.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates, and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

a = 5.4630(3) Å
c = 20.843(1)

Volume
538.73 $Å^3$

Density
(calculated) 3.310 g/cm^3

Reference intensity
$I/I_{corundum}$ = 3.3(2)

Additional patterns
1. PDF card 15-123 Voronova [1962].
2. PDF card 19-996 Schwarz [1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.
Voronova, M. L., (1962). Zap. Vses. Mineral. Obshchest. 91, 712.

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

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.94	15	003	12.75
4.617	1	101	19.21
4.308	17	012	20.60
3.472	1	006	25.64
3.128	100	015	28.51
2.731	65	110	32.77
2.543	11	113	35.27
2.520	4	107	35.60
2.352	2	021	38.24
2.316	8	009	38.85
2.308	6	202	39.00
2.153	17	024	41.92
2.148	19	116	42.03
2.0576	25	205	43.97
1.9077	18	1·0·10	47.63
1.7818	3	211	51.23
1.7664	5	119	51.71
1.7622	2	122	51.84
1.7516	3	208	52.18
1.7364	3	0·0·12	52.67
1.6915	<1	214	54.18
1.6435	12	125	55.90
1.5772	7	300	58.47
1.5641	5	0·2·10	59.01
1.5376	2	303	60.13
1.4657	1	1·1·12	63.41
1.4358	2	306	64.89
1.4201	1	0·1·14	65.70
1.3892	2	0·0·15	67.35
1.3655	8	220	68.68
1.3570	9	2·1·10	69.17
1.3400	1	223	70.18
1.3273	1	0·2·13	70.95
1.3033	1	309	72.46
1.3007	2	1·2·11	72.63
1.2723	<1	134	74.52
1.2513	5	315	75.99
1.2384	8	1·1·15	76.93
1.2008	<1	137	79.81
1.1765	1	229	81.80
1.1677	<1	3·0·12	82.55
1.1533	<1	404	83.81
1.1441	1	1·2·14	84.64
1.1410	1	0·2·16	84.93
1.1379	2	045	85.21
1.1105	3	1·3·10	87.84
1.0737	1	2·2·12	91.68
1.0661	1	1·1·18	92.53
1.0506	3	235	94.31
1.0426	4	3·0·15	95.26
1.0324	2	410	96.51
1.0287	1	4·0·10	96.97
1.0210	1	413	97.97
1.0180	1	0·1·20	98.35

Rubidium barium chromium oxide, $Rb_2Ba(CrO_4)_2$

Sample
The sample was prepared by heating a 1:1 molar mixture of $Rb_2Cr_2O_7$ and $BaCO_3$ together at 750° for 1 hour. This was followed by grinding, and reheating at 750° for 48 hours.

Color
Light greenish yellow

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double sulfates, chromates, and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

$a = 5.8107(6)$ Å
$c = 22.210(3)$

Volume
649.4 $Å^3$

Density
(calculated) 4.144 g/cm^3

Reference Intensity
$I/I_{corundum} = 5.8(2)$

Additional pattern
1. PDF card 19-1066 [Schwarz, 1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.

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

d(Å)	I	hkℓ	2θ(°)
7.39	2	003	11.96
4.90	6	101	18.09
4.58	4	012	19.38
3.731	4	104	23.83
3.326	100	015	26.78
2.905	65	110	30.75
2.705	2	113	33.09
2.683	2	107	33.37
2.500	2	021	35.89
2.467	5	009	36.39
2.455	4	202	36.58
2.430	2	018	36.97
2.291	9	024	39.29
2.287	12	116	39.37
2.189	25	205	41.21
2.031	20	1·0·10	44.57
1.972	1	027	45.99
1.895	2	211	47.96
1.881	5	119	48.34
1.876	3	122	48.49
1.850	1	0·0·12	49.20
1.799	1	214	50.70
1.748	15	125	52.28
1.677	7	300	54.68
1.665	8	0·2·10	55.10
1.528	1	306	60.56
1.513	1	0·1·14	61.19
1.480	2	0·0·15	62.71
1.453	7	220	64.02
1.4448	10	2·1·10	64.44
1.3869	1	309	67.48
1.3314	5	315	70.70
1.3196	8	1·1·15	71.43
1.2520	2	229	75.94
1.2102	3	045	79.06
1.1819	4	1·3·10	81.35

Rubidium iron chloride hydrate, $Rb_2FeCl_5 \cdot H_2O$

Sample
The sample was prepared by slow evaporation at room temperature. Since the material was incongruently soluble, a 1:1 molar aqueous solution of RbCl and $FeCl_3$ was prepared with some additional HCl. The first crystals formed were used.

Color
Deep reddish orange

Structure
Orthorhombic, Pmnb (62), Z = 4, isostructural with $K_2FeCl_5 \cdot H_2O$ and $(NH_4)_2FeCl_5 \cdot H_2O$. The structure of $K_2FeCl_5 \cdot H_2O$ was determined by Bellanca [1947].

NBS lattice constants of this sample:

a = 9.923(3) Å
b = 13.836(4)
c = 7.092(2)

Volume
973.8 $Å^3$

Density
(calculated) 2.879 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.7(2)

Reference
Bellanca, A.,(1947). Rec. Sci. Recostr. 17, 1360.

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

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.92	6	020	12.78
6.31	3	011	14.02
5.78	30	101	15.33
5.68	30	120	15.58
5.34	4	111	16.60
4.960	8	200,021	17.87
3.904	8	211	22.76
3.870	4	031	22.96
3.602	4	131	24.70
3.504	50	221	25.40
3.462	25	040	25.71
3.436	20	012	25.91
3.109	17	041	28.69
3.050	30	231	29.26
3.006	8	122	29.70
2.996	7	301	29.80
2.885	25	202	30.97
2.836	90	240	31.52
2.826	100	212	31.63
2.814	70	032	31.77
2.635	8	241	33.99
2.479	55	400,042	36.21
2.403	3	142	37.40
2.308	2	411,060	38.99
2.238	3	023	40.26
2.218	2	421	40.65
2.180	18	052	41.38
2.130	6	152	42.40
2.108	7	213	42.87
2.089	2	431	43.28
2.058	5	133	43.96
2.010	14	412	45.06
2.004	15	261	45.20
1.997	9	252	45.38
1.940	12	441	46.79
1.936	14	233	46.88
1.912	7	501	47.51
1.860	15	432	48.92
1.820	3	352	50.07
1.800	2	262	50.66
1.776	4	333	51.41
1.773	5	004	51.50
1.758	8	014	51.97
1.753	13	442	52.13
1.730	6	080	52.88
1.698	3	413	53.96
1.679	6	081,522	54.61
1.6696	4	204,362	54.95
1.6552	5	034	55.47
1.6378	12	452	56.11

Rubidium lead chromium oxide, $Rb_2Pb(CrO_4)_2$

Sample
The sample was prepared by melting a mixture of Rb_2CrO_4 and $PbCrO_4$, at about 730 °C.

Color
Slight orange yellow

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates, and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

a = 5.8037(4) Å
c = 21.827(3)

Volume
636.70 $Å^3$

Density
(calculated) 4.773 g/cm^3

Reference intensity
$I/I_{corundum}$ = 5.3(3)

Additional pattern
1. PDF card 19-1077 [Schwarz, 1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.

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

d(Å)	I	hkℓ	2θ(°)
7.273	12	003	12.16
4.897	25	101	18.10
4.567	10	012	19.42
3.699	9	104	24.04
3.638	4	006	24.45
3.296	100	015	27.03
2.904	75	110	30.76
2.696	7	113	33.21
2.650	2	107	33.80
2.497	5	021	35.93
2.426	5	009	37.03
2.283	13	024	39.43
2.270	12	116	39.68
2.178	25	205	41.43
2.002	17	1·0·10	45.26
1.957	2	027	46.34
1.892	5	211	48.04
1.871	3	122	48.63
1.861	5	119	48.89
1.849	1	208	49.24
1.819	1	0·0·12	50.12
1.794	2	214	50.85
1.742	18	125	52.49
1.675	8	300	54.75
1.648	5	0·2·10	55.73
1.632	1	303	56.32
1.558	2	2·0·11	59.26
1.5216	2	306	60.83
1.4889	2	0·1·14	62.31
1.4546	7	0·0·15	63.95
1.4506	6	220	64.15
1.4329	8	2·1·10	65.04
1.3912	2	131	67.24
1.3784	2	309	67.95
1.3720	2	1·2·11	68.31
1.3507	1	134	69.54
1.3276	5	315	70.93
1.3008	5	1·1·15	72.62
1.2447	1	229	76.46
1.2242	1	404	77.99
1.2074	3	045	79.28
1.1747	3	1·3·10	81.95
1.1519	<1	321	83.94
1.1149	2	235	87.41
1.0987	3	3·0·15	89.03
1.0969	3	410	89.22

Sodium magnesium sulfate hydrate (loeweite), $Na_{12}Mg_7(SO_4)_{13}\cdot 15H_2O$

Sample

The sample was prepared by evaporation of an aqueous solution of a 6:7 molar ratio of Na_2SO_4 and $MgSO_4$ at 95 °C. The precipitate was filtered off while the solution was hot. The composition of this phase was originally given as $Na_2Mg(SO_4)_2\cdot 2.5H_2O$. It was corrected by Kühn and Ritter [1958]. The sample contained about 15% of bloedite [$Na_2Mg(SO_4)_2\cdot 4H_2O$]. This pattern has been confirmed by computer calculation using structure data from Fang and Robinson [1970]. The sample was colorless.

Intensities

The intensities given in the table have been calculated from the data of Fang and Robinson [1970], and thus represent the intensities which would be obtained from a sample free from bloedite.

Structure

Hexagonal, $R\bar{3}$ (148), Z = 3, isostructural with $Na_{12}Mn_7(SO_4)_{13}\cdot 15H_2O$ [Schneider and Zemann, 1959]. The structure of loeweite was determined by Fang and Robinson [1970].

NBS lattice constants of this sample:

a = 18.866(2) Å
c = 13.434(2)

A least squares refinement based on 43 unique reflections free from bloedite gave lattice constants which did not differ from those above by more than 0.005 A.

Volume

4140.9 $Å^3$

Density

(calculated) 2.364 g/cm^3

Reference intensity

$I/I_{corundum} = 0.56(3)$

Additional patterns

1. PDF card 21-1139 [Madsen, 1966]
2. PDF card 24-1107 [Heide, Min. Inst. Jena, 1967]. This pattern has the formula incorrectly given as $Na_2Mg(SO_4)_2\cdot 2.5H_2O$.

References

Fang, J. H., and Robinson, P. D., (1970). Am. Mineralogist 55, 378.

Kuhn, R., and Ritter, K.-H. (1958). Kali Steinsalz 2, 238.

Madsen, B. M., (1966). U. S. Geol. Surv. Prof. Pap. 550B, 125.

Schneider, W. (1960). Z. Anorg. Allg. Chem. 303, 113.

Schneider, W., and Zemann, J. (1959). Beitr. Mineral. Petrogr. 6, 201.

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

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
10.37	100	101	8.52
9.42	18	110	9.38
6.98	26	021	12.68
6.21	14	012	14.26
5.61	28	211	15.78
5.45	32	300	16.26
5.19	5	202	17.07
4.55	8	122	19.49
4.471	10	003	19.84
4.294	65	131	20.67
4.046	62	113	21.95
3.904	2	401	22.76
3.759	31	312	23.65
3.612	9	321	24.63
3.563	4	410	24.97
3.493	2	042	25.48
3.458	52	303	25.74
3.277	45	232	27.19
3.251	23	223	27.41
3.175	41	051	28.08
3.144	10	330	28.36
3.109	4	024	28.69
3.012	6	241	29.64
2.949	3	214	30.28
2.942	21	502	30.36
2.868	22	511	31.16
2.806	17	422	31.87
2.790	23	413	32.06
2.723	22	600	32.86
2.698	47	134	33.18
2.635	15	431	34.00
2.617	17	520	34.24
2.552	1	205	35.14
2.499	1	324	35.90
2.494	3	342	35.98
2.451	10	161	36.64
2.356	5	440	38.16
2.343	1	054	38.39
2.335	5	612	38.52
2.311	4	315	38.94
2.273	1	244	39.62
2.259	2	523	39.87
2.211	15	514	40.78
2.206	15	072	40.87
2.180	6	116	41.39
2.163	3	710	41.72
2.097	2	434	43.10
2.070	9	306	43.69
2.066	11	541	43.78
2.023	16	226	44.76

d(Å)	I	hkℓ	2θ(°)
1.999	8	452	45.34
1.954	4	802	46.43
1.917	8	354	47.38
1.900	4	345	47.84
1.896	4	416	47.95
1.870	3	633	48.65
1.856	1	461	49.03
1.839	6	182	49.54
1.833	4	217	49.69
1.805	4	642	50.51
1.783	3	820	51.18
1.776	6	544	51.42
1.761	3	075	51.87
1.739	8	553,407	52.60
1.716	2	274	53.34
1.708	3	327	53.61
1.699	5	191	53.92
1.694	4	740	54.08
1.6821	3	903	54.51
1.6702	2	018	54.93
1.6557	8	823,057	55.45
1.6503	8	455	55.65
1.6448	6	208	55.85
1.6362	5	464	56.17
1.6301	6	247	56.40
1.6100	5	832	57.17
1.5869	4	0·10·2	58.08
1.5750	5	318	58.56
1.5576	2	185	59.28

Sodium manganese sulfate hydrate, $Na_{12}Mn_7(SO_4)_{13}\cdot 15H_2O$

Sample
The sample was prepared by evaporation of an aqueous solution of 4:3 molar mixture of Na_2SO_4 and $MnSO_4$ at 95 °C. The crystals were filtered off while the solution was hot.

Color
Pale pink

Optical data
Uniaxial (—), $N_e = 1.501$, $N_o = 1.520$

Structure
Hexagonal, $R\bar{3}$ (148), Z = 3, isostructural with $Na_{12}Mg_7(SO_4)_{13}\cdot 15H_2O$ (loeweite). The structure has been studied by Schneider [1960].

NBS lattice constants of this sample:

a = 19.126(2) Å
b = 13.529(3)

Volume
4285.7 $Å^3$

Density
(calculated) 2.533 g/cm^3

Reference intensity
$I/I_{corundum} = 0.66(7)$

Reference
Schneider, W. (1960). Z. Anorg. Allg. Chem. 303, 113.

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

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
10.47	55	101	8.44
9.57	25	110	9.23
7.07	85	021	12.51
6.25	35	012	14.15
5.683	30	211	15.58
5.525	30	300	16.03
4.784	20	220	18.53
4.595	25	122	19.30
4.510	35	003	19.67
4.350	80	131	20.40
4.079	70	113	21.77
3.803	16	312	23.37
3.660	30	321	24.30
3.616	14	410	24.60
3.531	14	042	25.21
3.494	80	303	25.47
3.312	90	104,232	26.90
3.282	18	223	27.15
3.218	70	051	27.70
3.189	18	330	27.96
3.132	11	024	28.48
3.051	7	241	29.25
2.977	35	214,502	29.99
2.907	55	511	30.73
2.843	40	422	31.44
2.820	45	413	31.70
2.760	50	600	32.41
2.723	100	134,152	32.86
2.669	9	015,431	33.55
2.651	30	520	33.78
2.603	8	333	34.43
2.527	10	324,342	35.50
2.483	9	125,161	36.14
2.391	9	440	37.59
2.367	25	054,612	37.99
2.329	17	315,351	38.62
2.285	5	523	39.40
2.265	8	045,621	39.76
2.254	18	006	39.96
2.233	55	514,072	40.36
2.194	11	116,710	41.11
2.122	6	434	42.57
2.113	6	443	42.75
2.095	20	505,541	43.15
2.089	16	306,630	43.28
2.046	17	425,081	44.23
2.039	30	226	44.39
2.022	15	164,452	44.78
2.001	6	155,271	45.29
1.979	8	802	45.81
1.973	9	713	45.95
1.938	19	354,722	46.83
1.920	14	107,345	47.31
1.913	10	416,550	47.48
1.893	10	633	48.01
1.882	4	027,461	48.33
1.864	6	182	48.83
1.846	6	615,731	49.32
1.841	8	336,900	49.48
1.829	9	642	49.83
1.796	10	544,372	50.80
1.781	12	137,075	51.26
1.761	15	553	51.89
1.736	4	274	52.67
1.722	13	327,191	53.15
1.717	13	526,740	53.31
1.704	6	903	53.75
1.681	16	814,562	54.54
1.678	14	823	54.66
1.670	12	057,455	54.94
1.657	12	208,464	55.40
1.620	8	921,725 +	56.78
1.608	10	0·10·2	57.24
1.604	7	743	57.39
1.586	12	318,292	58.10

Acetanilide, $C_6H_5NHCOCH_3$

Synonym
N - phenylacetamide

Structure
Orthorhombic, Pbca (61), Z = 8. The structure was determined by Brown and Corbridge [1954] and refined by Brown [1966].

Atom positions
All atoms were in general positions.

Lattice constants
a = 19.641 A
b = 9.483
c = 7.979
(published values: a = 19.640, b = 9.483, c = 7.979 [Brown and Corbridge, 1954]).

CD cell: a = 9.483, b = 19.641, c = 7.979, space group Pcab; a/b = 0.4828, c/b = 0.4063

Volume
1486. A^3

Density
(measured) 1.206 g/cm^3
(calculated) 1.208 g/cm^3

Thermal parameters
Isotropic: overall B = 5.0

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.471 \times 10^{-3}$
I/I_c (calculated) = 0.50

Additional pattern
1. PDF card 18-1501 [Billig, B. and Greenberg, B., Polytechnic Inst. of Brooklyn]

References

Brown, C. J. and Corbridge, D. E. C. (1954). Acta Crystallogr. 7, 711.
Brown, C. J. (1966). Acta Crystallogr. 21, 442.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
9.82	100	2 0 0	9.00
6.82	38	2 1 0	12.98
5.82	81	1 1 1	15.20
5.18	31	2 1 1	17.10
4.91	3	4 0 0	18.06
4.74	6	0 2 0	18.72
4.46	26	3 1 1	19.88
4.36	27	4 1 0	20.36
4.27	5	2 2 0	20.80
4.07	40	0 2 1	21.80
3.99	58	1 2 1	22.26
3.91	29	1 0 2	22.74
3.82	9	4 1 1	23.24
3.76	36	2 2 1	23.62
3.70	73	2 0 2	24.06
3.61	25	1 1 2	24.62
3.44	47	2 1 2	25.86
3.41	8	3 0 2	26.12
3.30	6	5 1 1	25.98
3.20	17	3 1 2	27.82
3.09	7	4 0 2*	28.84
3.05	15	0 2 2	29.24
3.02	30	1 2 2	29.60
2.884	1	6 1 1	30.98
2.815	6	2 3 1	31.76
2.766	4	3 2 2	32.34
2.693	3	6 2 0	33.24
2.687	3	5 1 2	33.32
2.657	2	4 3 0	33.70
2.592	6	4 2 2	34.58
2.539	4	1 1 3	35.32
2.532	4	6 0 2	35.42
2.478	3	2 1 3	36.22
2.445	1	6 1 2	36.72
2.410	2	5 2 2	37.28
2.377	5	8 1 0	37.82
2.353	1	5 3 1	38.22
2.311	3	7 2 1*	38.94
2.304	4	1 2 3	39.06
2.295	5	7 0 2	39.22
2.273	6	6 3 0*	39.62
2.258	2	2 2 3*	39.90
2.214	2	2 4 1	40.72
2.186	4	3 2 3*	41.26
2.097	1	4 2 3	43.10
2.065	2	7 2 2	43.80
2.055	2	9 1 1	44.02
2.024	2	1 3 3	44.74
1.967	1	5 4 1*	46.12
1.943	3	3 3 3*	46.72

Calculated Pattern (Peak heights)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.919	3	6	4	0+	47.32
1.915	3	9	0	2+	47.44
1.892	2	7	1	3+	48.06
1.884	2	8	3	1+	48.28
1.880	2	4	3	3+	48.38
1.870	3	10	1	1+	48.64
1.838	1	0	2	4+	49.56
1.813	1	2	5	1+	50.28
1.808	2	2	2	4+	50.44
1.771	4	3	2	4+	51.58
1.748	2	5	1	4	52.30
1.744	2	8	3	2	52.42
1.708	1	3	4	3+	53.60
1.668	1	10	3	0	55.00
1.664	1	2	3	4+	55.16
1.658	1	3	5	2	55.38

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
9.82	100	2	0	0	9.00
6.82	39	2	1	0	12.97
5.83	85	1	1	1	15.18
5.18	33	2	1	1	17.09
4.91	3	4	0	0	18.05
4.74	6	0	2	0	18.70
4.47	28	3	1	1	19.87
4.36	29	4	1	0	20.35
4.27	5	2	2	0	20.79
4.08	43	0	2	1	21.79
3.99	61	1	2	1	22.26
3.99	4	0	0	2	22.27
3.91	31	1	0	2	22.73
3.83	8	4	1	1	23.23
3.76	39	2	2	1	23.61
3.70	82	2	0	2	24.06
3.61	28	1	1	2	24.61
3.46	2	3	2	1	25.73
3.44	53	2	1	2	25.85
3.41	1	4	2	0	26.11
3.41	5	3	0	2	26.14
3.30	6	5	1	1	26.97
3.21	20	3	1	2	27.80
3.10	4	4	0	2	28.81
3.09	3	6	1	0	28.83
3.05	16	0	2	2	29.23
3.02	34	1	2	2	29.59
3.01	2	2	3	0	29.67
2.885	1	6	1	1	30.97
2.828	2	5	2	1	31.61

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.815	6	2	3	1	31.76
2.767	4	3	2	2	32.33
2.694	3	6	2	0	33.23
2.685	1	5	1	2	33.35
2.658	2	4	3	0	33.69
2.592	8	4	2	2	34.57
2.552	1	6	2	1	35.13
2.549	1	7	1	1	35.17
2.539	4	1	1	3	35.32
2.531	3	6	0	2	35.44
2.478	3	2	1	3	36.22
2.445	1	6	1	2	36.73
2.410	2	5	2	2	37.27
2.377	5	8	1	0	37.82
2.371	1	0	4	0	37.92
2.353	1	5	3	1	38.22
2.317	1	3	3	2	38.83
2.311	2	7	2	1	38.94
2.304	2	1	2	3	39.07
2.295	5	7	0	2	39.22
2.278	1	8	1	1	39.53
2.274	4	6	3	0	39.60
2.273	2	0	4	1	39.63
2.258	1	2	2	3	39.90
2.257	1	1	4	1	39.90
2.214	3	2	4	1	40.72
2.187	2	6	3	1	41.25
2.186	3	3	2	3	41.26
2.145	1	5	1	3	42.09
2.097	1	4	2	3	43.09
2.066	3	7	2	2	43.79
2.055	2	9	1	1	44.03
2.024	3	1	3	3	44.73
1.967	1	5	4	1	46.11
1.943	2	3	3	3	46.70
1.942	2	1	1	4	46.73
1.923	1	10	1	0	47.22
1.920	2	6	4	0	47.30
1.915	1	9	0	2	47.45
1.893	1	6	2	3	48.03
1.891	2	7	1	3	48.06
1.884	1	8	3	1	48.26
1.880	1	4	3	3	48.38
1.877	1	9	1	2	48.47
1.871	1	3	1	4	48.63
1.870	2	10	1	1	48.66
1.839	1	0	2	4	49.54
1.813	1	2	5	1	50.27
1.807	1	2	2	4	50.46
1.776	1	3	5	1	51.41

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.772	2	8	1	3	51.53
1.770	3	3	2	4	51.59
1.763	1	1	4	3	51.83
1.748	2	5	1	4	52.29
1.744	1	8	3	2	52.43
1.722	1	4	2	4	53.15
1.708	2	3	4	3	53.60
1.668	1	10	3	0	55.00
1.663	1	2	3	4	55.20
1.657	1	3	5	2	55.40
1.633	1	10	3	1	56.29

Allobarbital, $C_{10}H_{12}N_2O_3$

Synonyms
5,5 - diallylbarbituric acid, Dial

Structure
Monoclinic, C2/c (15), Z = 8. The structure was determined by Escobar [1975].

Atom positions
There was some disorder in the structure, with one carbon randomly occupying 2 sites in the proportion of 4 to 1. All other atoms were in general positions [ibid.].

Lattice constants
a = 14.570 Å
b = 7.289
c = 20.618
β = 99.83°
(published values: a = 14.569(6), b = 7.289(4), c = 20.617(7), β = 99.83(4)° [Escobar, 1975]).

CD cell: a = 20.618, b = 7.289, c = 14.570, β = 99.83°, space group A2/a; a/b = 2.8286, c/b = 1.9989

Volume
2157.5 Å^3

Density
(measured) 1.278
(calculated) 1.282

Thermal parameters
Isotropic: overall B = 4.0

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.627 \times 10^{-3}$
I/I_c (calculated) = 0.65

Additional pattern
1. PDF card 5-158 [Huang, 1951]

References
Escobar, C. (1975). Acta Crystallogr. B31, 1059.
Huang, T.-Y. (1951). Acta Pharm. Int. 2, 43.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
10.16	6	0 0 2	8.70
7.17	3	2 0 0	12.34
6.50	100	1 1 0	13.62
6.39	52	-2 0 2	13.84
6.05	51	1 1 1	14.62
5.68	16	-1 1 2	15.60
5.43	26	2 0 2	16.30
5.29	25	1 1 2	16.76
5.08	44	0 0 4	17.46
4.88	33	-1 1 3	18.18
4.52	2	-2 0 4	19.62
4.16	6	-1 1 4	21.34
4.03	34	-3 1 1	22.02
4.00	14	3 1 0	22.20
3.917	3	-3 1 2	22.68
3.821	7	3 1 1	23.26
3.681	12	-3 1 3	24.16
3.642	22	0 2 0	24.42
3.587	10	0 2 1	24.80
3.553	6	3 1 2	25.04
3.386	6	-3 1 4	26.30
3.329	4	1 1 5	26.76
3.285	14	-2 0 6	27.12
3.248	52	2 2 0*	27.44
3.216	15	4 0 2*	27.72
3.169	5	2 2 1*	28.14
3.102	6	-1 1 6	28.76
3.026	11	2 2 2*	29.50
2.944	18	3 1 4	30.34
2.877	2	2 0 6	31.06
2.845	2	2 2 3	31.42
2.788	2	-3 1 6	32.08
2.714	9	4 0 4*	32.98
2.692	4	-5 1 2	33.26
2.671	3	5 1 0	33.52
2.639	6	-2 2 5*	33.94
2.595	1	5 1 1	34.54
2.555	4	-4 2 2	35.10
2.534	5	-2 0 8	35.40
2.481	2	0 2 6	36.18
2.447	3	2 2 5	36.70
2.429	5	-1 1 8	36.98
2.420	5	3 1 6	37.12
2.405	3	-4 2 4	37.36
2.399	3	1 3 0	37.46
2.388	3	-1 3 1	37.64
2.371	4	1 3 1	37.92
2.346	3	-1 3 2	38.34
2.323	2	-6 0 4	38.74
2.317	2	1 3 2	38.84

Calculated Pattern (Peak heights)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.275	1	2	0	8*	39.58
2.245	1	6	0	2	40.14
2.223	2	5	1	4	40.54
2.184	2	-1	1	9	41.30
2.179	2	4	2	4	41.40
2.172	4	-3	3	1	41.54
2.167	4	3	3	0	41.64
2.082	2	1	1	9*	43.42
2.046	2	-4	2	7	44.24
2.033	1	0	0	10*	44.54
2.006	1	-5	1	8	45.16
2.000	2	-6	2	3*	45.30
1.984	1	-7	1	3*	45.68
1.959	1	-6	2	4	46.32
1.952	1	-7	1	4*	46.48
1.923	1	-4	2	8*	47.22
1.913	1	-4	0	10*	47.48
1.861	1	-5	3	2	48.90
1.853	1	3	3	5*	49.12
1.848	1	6	2	3	49.26
1.843	1	-7	1	6	49.42
1.822	1	1	3	7*	50.02
1.813	1	4	2	7*	50.30
1.791	2	-8	0	4*	50.96
1.766	2	2	4	0	51.72
1.746	1	7	1	4	52.36
1.714	1	-2	0	12*	53.40
1.710	1	-8	0	6*	53.54
1.690	1	-2	4	4*	54.22
1.683	1	5	3	4	54.46
1.630	1	-4	4	1*	56.42
1.624	2	-4	4	2*	56.62
1.608	1	-4	4	3*	57.24
1.595	1	2	4	5*	57.76

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
10.16	6	0	0	2	8.70
7.18	3	2	0	0	12.32
6.50	100	1	1	0	13.61
6.40	45	-2	0	2	13.83
6.33	4	-1	1	1	13.97
6.06	53	1	1	1	14.62
5.68	16	-1	1	2	15.60
5.44	27	2	0	2	16.28
5.29	26	1	1	2	16.74
5.08	47	0	0	4	17.45
4.88	36	-1	1	3	18.16
4.53	3	-2	0	4	19.60
4.16	6	-1	1	4	21.34
4.04	37	-3	1	1	22.01
4.00	11	3	1	0	22.21
3.917	3	-3	1	2	22.68
3.823	8	3	1	1	23.25
3.682	12	-3	1	3	24.15
3.645	25	0	2	0	24.40
3.587	11	0	2	1	24.80
3.553	6	3	1	2	25.04
3.386	6	-3	1	4	26.30
3.331	3	1	1	5	26.74
3.286	14	-2	0	6	27.11
3.250	37	2	2	0	27.42
3.248	33	-2	2	1	27.44
3.247	1	3	1	3	27.45
3.216	13	4	0	2	27.72
3.209	3	0	2	3	27.78
3.171	3	2	2	1	28.12
3.167	1	-2	2	2	28.16
3.103	7	-1	1	6	28.75
3.028	10	2	2	2	29.48
3.022	4	-2	2	3	29.53
2.961	7	0	2	4	30.16
2.945	21	3	1	4	30.33
2.878	3	2	0	6	31.04
2.845	2	2	2	3	31.42
2.788	2	-3	1	6	32.08
2.730	1	-1	1	7	32.78
2.720	7	4	0	4	32.90
2.713	5	0	2	5	32.99
2.705	1	-5	1	1	33.10
2.704	1	-4	0	6	33.10
2.691	3	-5	1	2	33.27
2.671	2	5	1	0	33.52
2.646	2	2	2	4	33.85
2.639	5	-2	2	5	33.94
2.596	1	5	1	1	34.53
2.554	5	-4	2	2	35.10

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.534	6	-2	0	8	35.40
2.481	2	0	2	6	36.18
2.447	3	2	2	5	36.69
2.430	5	-1	1	8	36.97
2.420	4	3	1	6	37.13
2.404	3	-4	2	4	37.37
2.396	1	1	3	0	37.51
2.387	2	-1	3	1	37.65
2.371	4	1	3	1	37.91
2.347	3	-1	3	2	38.33
2.323	2	-6	0	4	38.74
2.317	1	1	3	2	38.84
2.275	1	2	0	8	39.58
2.245	1	6	0	2	40.14
2.223	2	5	1	4	40.55
2.185	2	-1	1	9	41.28
2.180	1	4	2	4	41.39
2.172	5	-3	3	1	41.54
2.166	1	3	3	0	41.66
2.083	1	1	1	9	43.41
2.080	1	-2	2	8	43.46
2.046	2	-4	2	7	44.23
2.031	1	0	0	10	44.57
2.006	1	-5	1	8	45.15
2.000	1	6	2	0	45.30
1.997	1	-6	2	3	45.37
1.985	1	-7	1	3	45.67
1.959	1	-6	2	4	46.32
1.923	1	-4	2	8	47.24
1.861	1	-5	3	2	48.90
1.848	1	6	2	3	49.27
1.842	1	-7	1	6	49.43
1.826	1	5	1	7	49.90
1.791	2	-8	0	4	50.96
1.766	2	2	4	0	51.71
1.746	1	7	1	4	52.37
1.714	1	-2	0	12	53.40
1.690	1	-2	4	4	54.22
1.683	1	5	3	4	54.47
1.670	1	-1	1	12	54.94
1.630	1	-4	4	1	56.42
1.624	1	-4	4	2	56.63
1.608	1	-4	4	3	57.23
1.595	1	2	4	5	57.74

Calcium carbonate, aragonite, $CaCO_3$

Structure
Orthorhombic, Pnma (62), Z = 4. The structure was determined by Bragg [1924] and refined by de Villiers [1971]. Aragonite is isostructural with strontianite ($SrCO_3$) and witherite ($BaCO_3$) [de Villiers, 1971].

Atom positions
4(c) 4 calcium
4(c) 4 carbon
4(c) 4 oxygen(1)
8(d) 8 oxygen(2)

Polymorphism
There are 2 hexagonal polymorphs, calcite and vaterite; the 3 forms may coexist in synthetic samples.

Lattice constants
a = 5.740(1)
b = 4.9614(6)
c = 7.966(1)
This cell was refined from NBS data [Swanson, Fuyat and Ugrinic, 1954, and on PDF card 5-453]

CD cell: a=5.740(1), b=7.966(1), c=4.9614(6), space group, Pnam, a/b = 0.7206, c/b = 0.6228

Volume
226.9 $Å^3$

Density
(calculated) 2.931 g/cm^3

Thermal parameters
Anisotropic [de Villiers, 1971]

Scattering factors
Ca^{2+}, C^0 [International Tables, 1962]
O^{2-} [Suzuki, 1960]

Scale factors (integrated intensities)
$\gamma = 0.220 \times 10^{-3}$
I/I_c (calculated) = 0.98

Additional patterns
1. PDF card 5-453 [Powder Diffraction Data 1976]
2. PDF card 24-25 [Smith et al., 1973]

References

Bragg, W. L. (1924). Proc. Roy. Soc. A105, 16.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204.
Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081), p. 16.
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Suzuki, T. (1960). Acta Crystallogr. 13, 279.
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de Villiers, J. P. R. (1971). Am. Mineralogist 56, 758.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.653	1	1 0 1	19.06
4.211	5	0 1 1	21.08
3.980	2	0 0 2	22.32
3.394	100	1 1 1	26.24
3.271	62	1 0 2	27.24
2.8698	4	2 0 0	31.14
2.7315	11	1 1 2	32.76
2.6995	62	2 0 1	33.16
2.4821	43	2 1 0+	36.16
2.4100	18	1 0 3	37.28
2.3708	42	2 1 1	37.92
2.3411	31	0 1 3	38.42
2.3283	24	2 0 2	38.64
2.1893	15	1 2 1	41.20
2.1682	1	1 1 3	41.62
2.1055	22	0 2 2	42.92
1.9911	6	0 0 4	45.52
1.9771	69	1 2 2	45.86
1.9498	1	2 0 3	46.54
1.8813	34	1 0 4	48.34
1.8769	38	2 2 0	48.46
1.8268	3	2 2 1	49.88
1.8139	28	2 1 3	50.26
1.7591	4	1 1 4	51.94
1.7416	28	3 1 1	52.50
1.7282	11	1 2 3	52.94
1.7246	18	3 0 2	53.06
1.6979	2	2 2 2	53.96
1.6359	2	2 0 4	56.18
1.6296	1	3 1 2	56.42
1.6190	2	0 3 1	56.82
1.5585	6	1 3 1	59.24
1.5350	2	1 0 5	60.24
1.5318	1	2 2 3	60.38
1.5168	1	0 1 5	61.04
1.4991	6	1 2 4	61.84
1.4759	3	1 3 2	62.92
1.4663	7	1 1 5	63.38
1.4329	1	2 3 0+	65.04
1.4121	4	4 0 1	66.12
1.4102	4	2 3 1	66.22
1.4038	4	0 3 3	66.56
1.3786	1	4 1 0	67.94
1.3659	4	2 2 4	68.66
1.3583	5	4 1 1	69.10
1.3501	2	4 0 2	69.58
1.3410	3	2 1 5	70.12
1.3278	2	0 0 6	70.92
1.3055	1	1 2 5	72.32
1.3024	1	4 1 2	72.52

Calculated Pattern (Peak heights)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.2611	6	2	3	3	75.30
1.2404	7	0	4	0+	76.78
1.2360	9	3	3	1	77.10
1.2235	6	4	1	3	78.04
1.2146	2	2	2	5	78.72
1.2057	8	3	2	4+	79.42
1.1937	1	3	3	2	80.38
1.1888	6	3	1	5	80.78
1.1706	9	0	2	6	82.30
1.1643	1	4	0	4	82.84
1.1598	3	1	4	2	83.24
1.1470	1	1	2	6	84.38
1.1385	1	2	4	0	85.16
1.1359	1	5	0	1	85.40
1.1333	1	4	1	4	85.64
1.1318	1	3	3	3	85.78
1.1269	2	2	4	1	86.24
1.1251	4	1	3	5	86.42
1.1164	1	1	0	7	87.26
1.1075	2	5	1	1	88.14
1.1031	1	5	0	2+	88.58
1.0978	1	3	2	5	89.12
1.0947	2	2	4	2	89.44
1.0890	1	1	1	7	90.04
1.0839	1	2	2	6	90.58
1.0739	1	4	3	1	91.66
1.0655	2	2	3	5	92.60
1.0595	1	3	3	4	93.28
1.0579	1	2	0	7	93.46
1.0539	1	4	2	4+	93.92
1.0465	1	2	4	3	94.80
1.0425	1	4	1	5	95.28
1.0356	4	1	4	4+	96.12
1.0330	4	5	2	1	96.44
1.0180	1	1	2	7+	98.34
1.0079	4	5	2	2	99.68
1.0070	3	3	4	2	99.80
1.0035	4	4	3	3	100.28
.9986	1	3	2	6	100.96
.9957	1	0	0	8	101.36
.9946	1	5	0	4	101.52
.9884	1	2	4	4	102.40
.9840	2	3	3	5	103.04
.9811	2	1	0	8	103.46
.9795	1	4	2	5	103.70
.9739	2	2	3	6+	104.54
.9732	1	2	2	7	104.66
.9706	2	1	5	1	105.06
.9648	1	1	4	5	105.96
.9624	1	1	1	8	106.34

Calculated Pattern (Peak heights)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.9596	3	3	1	7	106.78
.9568	3	6	0	0	107.24
.9520	1	4	3	4	108.02
.9497	1	6	0	1	108.40
.9407	1	2	0	8	109.94
.9378	1	2	5	0	110.44
.9365	1	5	3	1	110.68
.9315	3	2	5	1+	111.58
.9295	3	0	5	3	111.94
.9252	1	1	3	7	112.72
.9231	1	5	2	4	113.12
.9175	1	1	5	3+	114.18
.9154	2	5	1	5	114.60
.9132	2	4	4	2	115.02
.9123	3	1	2	8	115.20
.9063	2	0	4	6+	116.40
.9001	1	6	0	3	117.70
.8961	1	4	3	5	118.54
.8926	1	6	2	0	119.30
.8912	2	2	3	7	119.62
.8856	2	6	1	3	120.88
.8843	2	2	5	3	121.18
.8796	1	2	2	8	122.26
.8776	2	4	1	7+	122.74
.8755	2	3	5	1	123.24
.8712	1	0	1	9+	124.30
.8643	2	2	4	6	126.06
.8601	1	3	5	2	127.16
.8523	1	5	3	4	129.32
.8489	1	4	4	4	130.30
.8460	1	6	2	3	131.14
.8439	1	1	3	8	131.78
.8419	3	3	3	7	132.40
.8391	1	4	2	7	133.26
.8378	1	5	4	1	133.68
.8360	1	3	5	3	134.26
.8338	3	2	1	9+	135.00
.8320	2	3	2	8	135.58
.8269	1	0	6	0	137.36
.8243	1	5	4	2	138.30
.8202	1	6	0	5	139.84
.8161	1	4	5	0	141.42
.8157	1	7	0	1	141.58
.8142	1	6	2	4+	142.20
.8118	2	4	5	1	143.20
.8116	2	5	3	5	143.28
.8096	2	0	6	2	144.14
.8082	1	2	5	5+	144.76
.8049	1	7	1	1	146.28
.8031	1	7	0	2+	147.14

Calculated Pattern (Peak heights)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.8017	3	1	6	2	147.82
.8006	1	2	2	9	148.38
.7977	1	5	1	7	149.90
.7966	1	0	0	10	150.46
.7946	1	2	6	0	151.60
.7927	1	7	1	2	152.70
.7906	2	6	3	3	154.00
.7890	1	1	0	10	155.00
.7849	2	4	3	7	157.90
.7834	1	7	0	3	159.00

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.657	1	1	0	1	19.04
4.211	5	0	1	1	21.08
3.983	2	0	0	2	22.30
3.395	100	1	1	1	26.22
3.272	62	1	0	2	27.23
2.8700	4	2	0	0	31.14
2.7317	10	1	1	2	32.76
2.7001	65	2	0	1	33.15
2.4843	34	2	1	0	36.13
2.4807	18	0	2	0	36.18
2.4100	18	1	0	3	37.28
2.3716	45	2	1	1	37.91
2.3411	31	0	1	3	38.42
2.3285	21	2	0	2	38.64
2.1894	16	1	2	1	41.20
2.1678	1	1	1	3	41.63
2.1057	24	0	2	2	42.92
1.9915	4	0	0	4	45.51
1.9769	79	1	2	2	45.87
1.9491	1	2	0	3	46.56
1.8815	34	1	0	4	48.34
1.8768	21	2	2	0	48.46
1.8604	1	3	0	1	48.92
1.8268	2	2	2	1	49.88
1.8141	32	2	1	3	50.25
1.7592	4	1	1	4	51.94
1.7420	33	3	1	1	52.49
1.7286	8	1	2	3	52.93
1.7247	15	3	0	2	53.06
1.6977	3	2	2	2	53.96

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.6362	3	2	0	4	56.17
1.6290	1	3	1	2	56.44
1.6193	2	0	3	1	56.81
1.5584	7	1	3	1	59.24
1.5530	1	0	2	4	59.47
1.5352	2	1	0	5	60.23
1.5326	1	2	2	3	60.35
1.5169	1	0	1	5	61.04
1.4991	7	1	2	4	61.84
1.4884	1	3	2	1	62.34
1.4760	4	1	3	2	62.92
1.4666	8	1	1	5	63.37
1.4350	1	4	0	0	64.93
1.4329	1	2	3	0	65.04
1.4161	1	3	2	2	65.91
1.4123	4	4	0	1	66.11
1.4103	3	2	3	1	66.21
1.4038	4	0	3	3	66.56
1.3785	1	4	1	0	67.95
1.3658	4	2	2	4	68.66
1.3636	1	1	3	3	68.79
1.3583	6	4	1	1	69.10
1.3501	2	4	0	2	69.58
1.3483	1	2	3	2	69.68
1.3411	3	2	1	5	70.11
1.3293	1	3	1	4	70.83
1.3277	2	0	0	6	70.93
1.3054	1	1	2	5	72.33
1.3027	1	4	1	2	72.50
1.2610	8	2	3	3	75.30
1.2421	3	4	2	0	76.65
1.2403	7	0	4	0	76.78
1.2360	10	3	3	1	77.10
1.2235	7	4	1	3	78.04
1.2146	2	2	2	5	78.72
1.2058	9	3	2	4	79.41
1.2050	4	2	0	6	79.47
1.1937	1	3	3	2	80.38
1.1887	7	3	1	5	80.79
1.1858	1	4	2	2	81.02
1.1709	1	2	1	6	82.27
1.1706	11	0	2	6	82.30
1.1642	1	4	0	4	82.85
1.1598	4	1	4	2	83.23
1.1470	1	1	2	6	84.38
1.1386	1	2	4	0	85.15
1.1363	1	5	0	1	85.36
1.1335	1	4	1	4	85.63
1.1318	1	3	3	3	85.78
1.1271	2	2	4	1	86.22

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.1251	4	1	3	5	86.41
1.1251	1	4	2	3	86.41
1.1163	1	1	0	7	87.27
1.1092	1	0	1	7	87.97
1.1076	3	5	1	1	88.13
1.1031	1	5	0	2	88.58
1.1029	1	1	4	3	88.61
1.0979	1	3	2	5	89.11
1.0947	2	2	4	2	89.44
1.0890	2	1	1	7	90.03
1.0839	2	2	2	6	90.58
1.0740	1	4	3	1	91.66
1.0654	2	2	3	5	92.61
1.0594	1	3	3	4	93.28
1.0579	1	2	0	7	93.46
1.0539	1	4	2	4	93.92
1.0537	1	5	0	3	93.94
1.0528	1	0	4	4	94.05
1.0464	1	2	4	3	94.80
1.0425	2	4	1	5	95.28
1.0356	5	1	4	4	96.12
1.0346	2	2	1	7	96.24
1.0330	2	5	2	1	96.43
1.0189	1	1	3	6	98.23
1.0180	1	1	2	7	98.35
1.0079	4	5	2	2	99.68
1.0070	3	3	4	2	99.81
1.0035	4	4	3	3	100.28
.9985	1	3	2	6	100.97
.9957	1	0	0	8	101.35
.9946	2	5	0	4	101.52
.9884	1	2	4	4	102.40
.9840	2	3	3	5	103.04
.9811	2	1	0	8	103.47
.9796	1	4	2	5	103.69
.9745	1	4	0	6	104.45
.9739	2	2	3	6	104.55
.9731	1	2	2	7	104.67
.9705	2	1	5	1	105.07
.9699	1	5	2	3	105.17
.9648	1	1	4	5	105.96
.9625	1	1	1	8	106.33
.9596	5	3	1	7	106.78
.9567	3	6	0	0	107.26
.9520	1	4	3	4	108.02
.9498	1	6	0	1	108.38
.9407	1	2	0	8	109.93
.9384	1	4	4	0	110.34
.9378	1	2	5	0	110.45
.9365	2	5	3	1	110.67

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.9319	2	4	4	1	111.49
.9314	1	5	0	5	111.59
.9314	2	2	5	1	111.59
.9295	2	0	5	3	111.94
.9252	1	1	3	7	112.72
.9232	1	5	2	4	113.11
.9224	1	3	4	4	113.25
.9175	1	1	5	3	114.18
.9154	2	5	1	5	114.59
.9134	1	4	4	2	114.99
.9128	1	2	5	2	115.10
.9123	4	1	2	8	115.20
.9071	1	4	2	6	116.26
.9064	2	0	4	6	116.40
.9000	1	6	0	3	117.71
.8961	2	4	3	5	118.54
.8926	1	6	2	0	119.31
.8912	2	2	3	7	119.63
.8870	1	6	2	1	120.54
.8856	3	6	1	3	120.88
.8843	3	2	5	3	121.17
.8833	1	3	0	8	121.40
.8796	2	2	2	8	122.26
.8777	1	1	5	4	122.72
.8776	1	4	1	7	122.74
.8755	3	3	5	1	123.24
.8748	1	1	0	9	123.42
.8714	1	0	1	9	124.26
.8710	1	6	2	2	124.35
.8696	1	3	1	8	124.70
.8643	4	2	4	6	126.06
.8623	1	6	0	4	126.58
.8601	1	3	5	2	127.17
.8523	1	5	3	4	129.31
.8496	1	6	1	4	130.10
.8489	1	4	4	4	130.31
.8461	1	6	2	3	131.13
.8458	1	2	0	9	131.21
.8438	1	1	3	8	131.82
.8423	1	0	5	5	132.28
.8419	6	3	3	7	132.41
.8396	1	4	3	6	133.11
.8391	2	4	2	7	133.27
.8378	1	5	4	1	133.67
.8361	1	3	5	3	134.25
.8338	5	2	1	9	135.00
.8334	2	1	5	5	135.14
.8321	3	3	2	8	135.55
.8297	1	1	4	7	136.36
.8281	1	6	3	0	136.93

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2Θ(°) λ = 1.540598Å
.8269	1	0	6	0	137.36
.8250	1	1	2	9	138.04
.8243	2	5	4	2	138.30
.8237	1	6	3	1	138.53
.8202	1	6	0	5	139.84
.8162	1	4	5	0	141.40
.8157	1	7	0	1	141.59
.8145	1	6	2	4	142.07
.8142	1	1	6	1	142.21
.8119	4	4	5	1	143.15
.8115	4	5	3	5	143.31
.8096	1	0	6	2	144.13
.8086	1	4	4	5	144.61
.8082	1	5	0	7	144.77
.8082	1	2	5	5	144.77
.8056	1	3	5	4	145.96
.8049	1	2	4	7	146.28
.8049	2	7	1	1	146.29
.8032	2	7	0	2	147.11
.8031	1	5	4	3	147.15
.8017	7	1	6	2	147.82
.8005	1	2	2	9	148.40
.7995	1	4	5	2	148.91
.7977	3	5	1	7	149.89
.7966	1	0	0	10	150.47
.7946	3	2	6	0	151.60
.7930	1	3	1	9	152.52
.7928	1	7	1	2	152.61
.7905	5	6	3	3	154.01
.7890	2	1	0	10	154.98
.7848	5	4	3	7	157.90
.7835	1	7	0	3	158.94

Calcium oxide (lime), CaO

Structure
Cubic, Fm3m (225), Z = 4, isostructural with NaCl [Davey and Hoffman, 1920].

Atom positions
4(a) 4 calcium
4(b) 4 oxygen

Lattice constants
a = 4.8108 Å
(published value, 4.8105 [Swanson and Tatge, 1953, and on PDF card 4-777])

Volume
111.34 $Å^3$

Density
(calculated) 3.345 g/cm^3

Thermal parameters
Isotropic: calcium B = 0.5; oxygen B = 1.0

Scattering factors
O^{2-} [Suzuki, 1960]
Ca^{2+} [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.611 \times 10^{-3}$
I/I_c (calculated) = 4.56

Additional pattern
1. PDF card 4-777 [Powder Diffraction Data, 1976].

References

Davey, W. P. and Hoffman, E. O. (1920). Phys. Rev. 15, 333.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 204.

Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081), p. 8.

Suzuki, T. (1960). Acta Crystallogr. 13, 279.

Swanson, H. E. and Tatge, E. (1953). Nat'l. Bur. Std. U.S. Circ. 539, 1, 43.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.7777	36	1 1 1	32.20
2.4051	100	2 0 0	37.36
1.7008	49	2 2 0	53.86
1.4504	14	3 1 1	64.16
1.3887	13	2 2 2	67.38
1.2026	5	4 0 0	79.66
1.1037	5	3 3 1	88.52
1.0757	14	4 2 0	91.46
.9820	11	4 2 2	103.34
.9259	5	5 1 1+	112.60
.8504	4	4 4 0	129.86
.8132	7	5 3 1	142.62
.8018	11	4 4 2+	147.78

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.7775	36	1 1 1	32.20
2.4054	100	2 0 0	37.35
1.7009	54	2 2 0	53.86
1.4505	16	3 1 1	64.15
1.3888	15	2 2 2	67.38
1.2027	6	4 0 0	79.65
1.1037	6	3 3 1	88.52
1.0757	17	4 2 0	91.46
.9820	14	4 2 2	103.33
.9258	5	5 1 1	112.61
.9258	2	3 3 3	112.61
.8504	8	4 4 0	129.85
.8132	16	5 3 1	142.62
.8018	22	4 4 2	147.77
.8018	6	6 0 0	147.77

Cerium zinc, $CeZn_3$

Structure
Orthorhombic, Amma (63), Z = 4, from powder data. The pattern is nearly identical to that of $PrZn_3$ (space group Pnma) except that for $CeZn_3$, all hkℓ reflections having k+ℓ = 2n+1 were absent, suggesting a change to the A-centered lattice [Bruzzone et al., 1970].

Atom positions
The structure was determined with all atoms in positions 4(c) of Pnma.

Lattice constants
a = 6.644 A
b = 4.627
c = 10.437
[Bruzzone et al., 1970]

CD cell: a = 6.644, b = 10.437, c = 4.627, space group Amam. a/b = 0.6366, c/b = 0.4433.

Volume
320.9 A^3

Density
(calculated) 6.961 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Ce^0, Zn^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.512 \times 10^{-3}$

References

Bruzzone, G., Fornasini, M.L. and Merlo, F. (1970). J. Less-Common Metals 22, 253.
Cromer, D. H. and Mann, J. B. (1968). Acta Crystallogr. A24, 361.

Calculated Pattern (Peak heights)

d(A)	I	hkℓ	2θ(°) λ = 1.540598A
4.227	5	0 1 1	21.00
4.103	5	1 0 2	21.64
3.567	10	1 1 1	24.94
3.321	10	2 0 0	26.82
2.611	100	2 1 1+	34.32
2.564	65	1 1 3	34.96
2.429	15	1 0 4	36.98
2.313	35	0 2 0	38.90
2.132	30	2 1 3	42.36
2.039	15	3 0 2	44.40
2.015	1	1 2 2	44.94
1.962	5	3 1 1	46.24
1.898	5	2 2 0	47.88
1.731	15	0 2 4	52.84
1.689	5	3 0 4	54.28
1.684	5	1 0 6	54.44
1.675	10	1 2 4	54.76
1.661	5	4 0 0	55.26
1.651	10	2 1 5	55.62
1.546	5	4 1 1	59.76
1.530	10	3 2 2	60.48
1.4432	1	3 1 5	64.52
1.4258	1	4 1 3	65.40
1.4193	1	0 1 7	65.74
1.4012	1	4 0 4	66.70
1.3872	15	1 1 7+	67.46
1.3793	5	1 3 3	67.90
1.3680	5	3 0 6	68.54
1.3641	5	3 2 4	68.76
1.3607	5	1 2 6	68.96
1.3494	5	4 2 0	69.62
1.2978	5	2 3 3	72.82
1.2803	1	1 0 8	73.98
1.2677	1	5 1 1	74.84
1.2144	1	2 0 8	78.74
1.1989	10	5 1 3+	79.96
1.1841	1	5 0 4	81.16
1.1774	5	3 2 6	81.72
1.1620	1	2 3 5	83.04
1.1568	1	0 4 0	83.50
1.1238	1	4 3 1+	86.54
1.1203	1	1 2 8	86.88
1.1073	1	6 0 0	88.16
1.0752	1	2 2 8+	91.52
1.0721	1	0 3 7+	91.86
1.0655	1	2 1 9	92.60
1.0583	5	1 3 7+	93.42
1.0443	1	1 4 4+	95.06
1.0193	1	6 0 4	98.18
1.0111	1	3 2 8	99.26

Calculated Pattern (Peak heights)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.0061	1	3 4 2	99.92
1.0020	1	5 3 1	100.48
.9989	1	6 2 0	100.92
.9963	1	2 0 10	101.28
.9699	5	5 1 7	105.16
.9671	5	5 3 3	105.60
.9543	1	3 4 4	107.64
.9514	1	0 2 10	108.12
.9491	1	4 4 0	108.50
.9338	1	7 0 2+	111.16
.9328	1	6 2 4	111.34
.9295	1	0 1 11	111.94
.9146	1	2 2 10	114.76
.8951	1	2 1 11	118.76
.8928	1	2 3 9	119.26
.8921	1	4 4 4+	119.42
.8882	1	2 5 1	120.28
.8863	1	1 5 3	120.72
.8833	5	3 4 6+	121.40
.8741	1	3 2 10	123.58
.8659	1	7 2 2+	125.64
.8636	1	2 5 3+	126.24
.8343	5	5 3 7	134.82
.8332	1	7 0 6+	135.20
.8323	1	7 2 4	135.50
.8255	1	4 2 10	137.84
.8198	1	2 5 5	139.96
.8149	1	8 1 1	141.90
.8111	1	4 1 11	143.50
.8092	1	3 0 12+	144.34
.8081	1	0 3 11+	144.80
.8061	1	3 4 8+	145.72
.7999	1	6 4 0	148.72
.7958	1	8 1 3	150.94
.7889	1	7 1 7	155.06
.7874	1	7 3 3+	156.10
.7854	1	2 3 11+	157.50
.7839	1	7 2 6	158.62

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.230	5	0 1 1	20.98
4.104	5	1 0 2	21.64
3.568	10	1 1 1	24.93
3.322	10	2 0 0	26.82
2.613	100	2 1 1	34.30
2.609	30	0 0 4	34.34
2.565	80	1 1 3	34.95
2.429	20	1 0 4	36.98
2.313	45	0 2 0	38.90
2.132	35	2 1 3	42.35
2.039	20	3 0 2	44.40
2.015	1	1 2 2	44.94
1.962	5	3 1 1	46.23
1.903	1	0 1 5	47.76
1.898	5	2 2 0	47.88
1.739	1	0 0 6	52.57
1.732	1	3 1 3	52.80
1.731	15	0 2 4	52.85
1.688	5	3 0 4	54.29
1.683	1	1 0 6	54.48
1.675	10	1 2 4	54.75
1.661	5	4 0 0	55.26
1.651	10	2 1 5	55.62
1.546	5	4 1 1	59.77
1.530	15	3 2 2	60.48
1.4871	1	1 3 1	62.40
1.4432	1	3 1 5	64.52
1.4260	1	4 1 3	65.39
1.4191	5	0 1 7	65.75
1.4012	1	4 0 4	66.70
1.3903	1	0 2 6	67.29
1.3878	15	1 1 7	67.43
1.3865	10	2 3 1	67.50
1.3793	10	1 3 3	67.90
1.3680	5	3 0 6	68.54
1.3639	5	3 2 4	68.78
1.3609	1	1 2 6	68.95
1.3493	5	4 2 0	69.63
1.2979	5	2 3 3	72.81
1.2802	1	1 0 8	73.99
1.2677	1	5 1 1	74.84
1.2143	1	2 0 8	78.74
1.1989	10	5 1 3	79.95
1.1985	1	4 2 4	79.99
1.1949	1	3 1 7	80.28
1.1841	1	5 0 4	81.16
1.1775	10	3 2 6	81.71
1.1621	5	2 3 5	83.04
1.1567	5	0 4 0	83.51
1.1241	1	3 0 8	86.51

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.1237	1	4	3	1	86.56
1.1201	1	1	2	8	86.90
1.1073	1	6	0	0	88.16
1.0823	1	3	3	5	90.76
1.0790	1	4	1	7	91.11
1.0752	1	2	2	8	91.52
1.0749	1	4	3	3	91.55
1.0720	1	0	3	7	91.87
1.0712	1	6	1	1	91.96
1.0655	5	2	1	9	92.60
1.0583	5	1	3	7	93.42
1.0575	5	0	4	4	93.51
1.0541	1	5	2	4	93.91
1.0443	1	1	4	4	95.05
1.0437	1	0	0	10	95.13
1.0193	1	6	0	4	98.17
1.0111	1	3	2	8	99.26
1.0061	5	3	4	2	99.93
1.0021	1	5	3	1	100.48
.9988	5	6	2	0	100.93
.9957	1	2	0	10	101.36
.9700	5	5	1	7	105.15
.9670	5	5	3	3	105.61
.9543	1	3	4	4	107.65
.9514	1	0	2	10	108.13
.9492	1	4	4	0	108.48
.9441	1	3	0	10	109.35
.9338	1	7	0	2	111.15
.9328	1	6	2	4	111.34
.9295	1	0	1	11	111.94
.9146	1	2	2	10	114.75
.8951	1	2	1	11	118.76
.8928	1	2	3	9	119.26
.8920	1	4	4	4	119.43
.8920	1	7	0	4	119.45
.8882	5	2	5	1	120.28
.8863	5	1	5	3	120.71
.8837	1	4	0	10	121.30
.8833	5	3	4	6	121.40
.8741	1	3	2	10	123.58
.8730	1	6	1	7	123.85
.8659	1	7	2	2	125.63
.8636	1	2	5	3	126.25
.8583	1	1	4	8	127.66
.8376	1	2	4	8	133.76
.8343	5	5	3	7	134.81
.8332	1	7	0	6	135.19
.8322	1	7	2	4	135.51
.8274	1	5	4	4	137.16
.8255	5	4	2	10	137.84

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.8198	1	2	5	5	139.97
.8149	5	8	1	1	141.90
.8111	5	4	1	11	143.49
.8081	1	0	3	11	144.79
.8061	1	3	4	8	145.70
.8060	1	4	5	1	145.77
.8022	1	1	3	11	147.56
.7999	5	6	4	0	148.73
.7958	5	8	1	3	150.93
.7907	1	2	2	12	153.90
.7903	1	3	5	5	154.17
.7890	1	7	1	7	155.03
.7874	1	4	5	3	156.06
.7874	1	7	3	3	156.10
.7863	1	0	5	7	156.87
.7855	1	1	1	13	157.43
.7852	1	2	3	11	157.61
.7839	5	7	2	6	158.63

Cerium zinc, $CeZn_5$

Structure
Hexagonal, P6/mmm (191), Z = 1, isostructural with $CaCu_5$, from powder data [Lott and Chiotti, 1966].

Atom positions [ibid.]
1(a) 1 cerium
2(c) 2 zinc
3(g) 3 zinc

Lattice constants
A composition range exists from 70.00 to 71.97 wt.% of zinc, and the constants vary accordingly. For 70 wt.% Zn:

a = 5.4166 Å
c = 4.2649

(published values: a = 5.4163, c = 4.2647 Å [ibid., Table 1])

Volume
108.4 $Å^3$

Density
(calculated) 7.156 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Ce^0, Zn^0 [Cromer and Mann, 1968], corrected for anomalous dispersion [Cromer and Liberman, 1970].

Scale factors (integrated intensities)
$\gamma = 0.786 \times 10^{-3}$

Additional patterns
1. Green [1973]
2. Lott and Chiotti [1966]

References

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Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Green, M. L. (1973). J. Less-Common Metals 32, 391.
Lott, B. G. and Chiotti, P. (1966). Acta Crystallogr. 20, 733.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.69	2	1 0 0	18.92
4.26	4	0 0 1	20.82
3.16	45	1 0 1	28.26
2.707	30	1 1 0	33.06
2.345	35	2 0 0	38.36
2.286	100	1 1 1	39.38
2.132	25	0 0 2	42.36
2.055	12	2 0 1	44.02
1.676	11	1 1 2	54.74
1.637	9	2 1 1	56.14
1.578	16	2 0 2	58.44
1.564	5	3 0 0	59.02
1.468	18	3 0 1	63.30
1.360	3	1 0 3	68.98
1.354	12	2 2 0	69.34
1.261	5	3 0 2	75.32
1.259	10	1 1 3	75.46
1.245	3	3 1 1	76.48
1.216	1	2 0 3	78.64
1.173	2	4 0 0	82.12
1.143	11	2 2 2	84.72
1.131	1	4 0 1	85.88
1.109	2	2 1 3	87.98
1.066	1	0 0 4	92.52
1.052	4	3 0 3	94.16
1.043	2	3 2 1	95.16
1.028	3	4 0 2	97.12
1.024	2	4 1 0	97.62
.995	7	4 1 1	101.40
.993	4	1 1 4	101.76
.971	2	2 0 4	105.04
.960	1	3 1 3	106.76
.923	2	4 1 2	113.18
.887	2	4 2 0	120.66
.883	3	3 3 1	121.42
.881	3	3 0 4	121.94
.858	1	3 2 3	127.72
.839	1	1 0 5	133.24
.838	5	2 2 4	133.72
.831	5	4 1 3	136.04
.827	1	5 1 1	137.48
.819	3	4 2 2	140.44
.814	2	1 1 5	142.46
.789	2	4 0 4	155.06

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.69	2	1	0	0	18.90
4.26	4	0	0	1	20.81
3.16	40	1	0	1	28.26
2.708	30	1	1	0	33.05
2.345	35	2	0	0	38.35
2.286	100	1	1	1	39.38
2.132	25	0	0	2	42.35
2.055	12	2	0	1	44.03
1.675	12	1	1	2	54.74
1.637	10	2	1	1	56.13
1.578	17	2	0	2	58.45
1.564	5	3	0	0	59.03
1.468	20	3	0	1	63.30
1.361	3	1	0	3	68.97
1.354	14	2	2	0	69.34
1.261	4	3	0	2	75.31
1.259	11	1	1	3	75.46
1.244	4	3	1	1	76.49
1.216	1	2	0	3	78.63
1.173	3	4	0	0	82.12
1.143	14	2	2	2	84.73
1.131	1	4	0	1	85.88
1.109	2	2	1	3	87.98
1.066	2	0	0	4	92.52
1.052	6	3	0	3	94.16
1.043	2	3	2	1	95.16
1.028	3	4	0	2	97.11
1.024	2	4	1	0	97.62
.995	10	4	1	1	101.41
.992	2	1	1	4	101.87
.971	3	2	0	4	105.05
.960	2	3	1	3	106.75
.923	3	4	1	2	113.17
.916	1	5	0	1	114.43
.903	1	3	3	0	117.14
.886	3	4	2	0	120.67
.883	4	3	3	1	121.42
.881	2	3	0	4	121.96
.868	1	4	2	1	125.12
.858	2	3	2	3	127.72
.839	1	1	0	5	133.24
.838	9	2	2	4	133.71
.831	2	3	3	2	135.81
.831	10	4	1	3	136.03
.827	2	5	1	1	137.48
.819	7	4	2	2	140.45
.814	5	1	1	5	142.45
.789	5	4	0	4	155.06
.783	2	5	0	3	159.30

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with rhombohedral modification of U_2Zn_{17}, from powder data and qualitative single crystal analysis [Lott and Chiotti, 1966].

Atom positions
The structures of several analogous compounds have been refined and the atomic parameters are very similar [Johnson et al., 1969]. The parameters for Ce_2Zn_{17} were not available, but the ratios of the cell edges c/a and of the atomic radii r_{Ce}/r_{Zn} are close to the corresponding ratios for Nb_2Be_{17} for which there is refined structure data [Zalkin et al., 1959]. The atomic positions for Nb_2Be_{17} were used here for Ce_2Zn_{17}.

6(c)	6 cerium	18(f)	18 zinc(F)
6(c)	6 zinc(C)	18(h)	18 zinc(H)
9(d)	9 zinc(D)		

Lattice constants [Lott and Chiotti]
a = 9.0713(5) Å
c = 13.2852(5)
(published values: a = 9.0708, c = 13.2844)

Volume
946.8 $Å^3$

Density
(calculated) 7.322 g/cm^3

Thermal parameters
Isotropic: Zn(C), B = .81; Zn(D), B = 1.32; Zn(F), B = .74; Zn(H), B = 1.04 [Johnson et al., 1969]. For Ce, B = .54, from their values for Pr [ibid.]

Scattering factors
Ce^0, Zn^0 [Cromer and Mann, 1968], corrected for dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)
$\gamma = 0.344 \times 10^{-3}$

References
Cromer, D.T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
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Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.767	5	0 2 1	23.60
3.381	6	2 0 2	26.34
3.169	25	1 1 3	28.14
3.058	9	1 0 4	29.18
2.8970	2	2 1 1	30.84
2.7106	7	1 2 2	33.02
2.6182	40	3 0 0	34.22
2.5364	20	0 2 4	35.36
2.5185	4	0 1 5	35.62
2.2674	65	2 2 0	39.72
2.2544	100	0 3 3+	39.96
2.2140	50	0 0 6+	40.72
2.2016	17	2 0 5	40.96
2.1504	1	1 3 1	41.98
2.0180	35	2 2 3	44.88
1.9894	6	1 1 6	45.56
1.9804	6	1 2 5	45.78
1.9427	2	4 0 1	46.72
1.8835	1	0 4 2	48.28
1.8448	2	1 0 7	49.36
1.8220	2	1 3 4	50.02
1.7860	3	3 2 1	51.10
1.7392	2	2 3 2	52.58
1.7090	2	0 2 7	53.58
1.6909	6	3 0 6+	54.20
1.5989	11	4 1 3+	57.60
1.5844	20	2 2 6+	58.18
1.5291	1	5 0 2	60.50
1.5119	4	3 3 0	61.26
1.4917	5	2 3 5	62.18
1.4309	12	3 3 3	65.14
1.4204	3	0 5 4	65.68
1.4034	4	1 1 9+	66.58
1.3800	2	1 5 2	67.86
1.3555	4	2 4 4+	69.26
1.3521	3	5 0 5	69.46
1.3093	14	6 0 0	72.08
1.3064	10	3 2 7	72.26
1.2987	4	5 1 4	72.76
1.2959	4	4 2 5	72.94
1.2859	16	0 3 9+	73.60
1.2680	1	0 4 8+	74.82
1.2585	1	0 2 10+	75.48
1.2484	1	3 3 6	76.20
1.2462	2	1 5 5	76.36
1.2371	2	2 2 9	77.02
1.2102	3	2 5 3+	79.06
1.1339	5	4 4 0	85.58
1.1324	3	5 1 7	85.72
1.1269	9	0 6 6+	86.24

Calculated Pattern (Peak heights)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.1186	5	4	1	9+	87.04
1.1071	3	0	0	12+	88.18
1.0984	1	4	4	3	89.06
1.0752	1	2	6	2+	91.52
1.0632	1	3	5	4	92.86
1.0562	6	3	3	9	93.66
1.0351	2	6	2	4	96.18
1.0339	1	5	3	5	96.32
1.0197	2	3	0	12+	98.12
1.0130	3	7	1	3+	99.00
1.0093	4	4	4	6	99.50
1.0081	2	2	6	5	99.66
.9949	3	2	2	12	101.48
.9898	1	6	3	0+	102.20
.9660	5	6	3	3+	105.76
.9574	2	2	5	9+	107.14
.9449	1	6	2	7	109.22
.9416	1	0	8	4	109.78
.9407	1	4	5	5	109.94
.9220	1	2	7	4	113.32
.8932	1	3	3	12	119.18
.8888	3	3	2	13+	120.14
.8863	2	8	1	4	120.72
.8821	1	3	4	11+	121.68
.8689	1	1	8	5	124.88
.8572	4	8	2	0+	127.96
.8505	3	7	1	9+	129.84

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
3.767	7	0	2	1	23.60
3.381	9	2	0	2	26.34
3.169	40	1	1	3	28.14
3.059	15	1	0	4	29.17
2.8978	3	2	1	1	30.83
2.7108	11	1	2	2	33.02
2.6187	70	3	0	0	34.21
2.5362	40	0	2	4	35.36
2.5170	4	0	1	5	35.64
2.2678	100	2	2	0	39.71
2.2541	85	3	0	3	39.97
2.2541	85	0	3	3	39.97
2.2142	60	0	0	6	40.72
2.2136	30	2	1	4	40.73
2.2008	18	2	0	5	40.98
2.1501	1	1	3	1	41.99
2.0185	60	2	2	3	44.87
1.9898	10	1	1	6	45.55
1.9800	10	1	2	5	45.79
1.9429	4	4	0	1	46.72
1.8834	3	0	4	2	48.28
1.8448	3	1	0	7	49.36
1.8218	3	1	3	4	50.03
1.7859	6	3	2	1	51.10
1.7394	5	2	3	2	52.57
1.7143	1	4	1	0	53.40
1.7089	3	0	2	7	53.59
1.6908	6	3	0	6	54.21
1.6908	5	0	3	6	54.21
1.6848	1	3	1	5	54.41
1.5991	7	2	1	7	57.59
1.5987	8	4	1	3	57.61
1.5987	7	1	4	3	57.61
1.5843	25	2	2	6	58.18
1.5841	12	3	2	4	58.19
1.5603	1	0	5	1	59.17
1.5290	2	5	0	2	60.50
1.5119	7	3	3	0	61.26
1.4915	9	2	3	5	62.19
1.4311	1	1	3	7	65.13
1.4308	25	3	3	3	65.15
1.4203	5	0	5	4	65.69
1.4037	7	1	1	9	66.57
1.4031	2	5	1	1	66.60
1.3802	3	1	5	2	67.85
1.3555	1	4	1	6	69.26
1.3555	1	1	4	6	69.26
1.3554	6	2	4	4	69.27
1.3524	2	5	0	5	69.44
1.3093	25	6	0	0	72.08

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.3069	7	3 2 7	72.23
1.2986	7	5 1 4	72.76
1.2960	4	4 2 5	72.93
1.2859	14	3 0 9	73.60
1.2859	15	0 3 9	73.60
1.2855	2	4 3 1	73.63
1.2681	2	0 4 8	74.81
1.2585	2	0 2 10	75.48
1.2486	2	3 3 6	76.19
1.2462	3	1 5 5	76.36
1.2371	3	2 2 9	77.02
1.2103	2	0 5 7	79.06
1.2101	2	5 2 3	79.07
1.2101	3	2 5 3	79.07
1.1694	1	2 4 7	82.41
1.1339	11	4 4 0	85.58
1.1323	4	5 1 7	85.73
1.1270	9	6 0 6	86.23
1.1270	9	0 6 6	86.23
1.1186	4	4 1 9	87.04
1.1186	4	1 4 9	87.04
1.1183	1	3 5 1	87.07
1.1071	5	0 0 12	88.18
1.1066	1	5 3 2	88.23
1.1066	1	0 7 2	88.23
1.0985	2	4 4 3	89.05
1.0858	1	6 2 1	90.38
1.0751	1	2 6 2	91.53
1.0632	3	3 5 4	92.85
1.0563	1	3 1 11	93.64
1.0562	11	3 3 9	93.66
1.0405	1	7 1 0	95.51
1.0352	5	6 2 4	96.17
1.0338	2	5 3 5	96.33
1.0197	1	0 3 12	98.12
1.0197	2	3 0 12	98.12
1.0134	1	1 0 13	98.95
1.0130	3	7 1 3	99.01
1.0130	3	1 7 3	99.01
1.0093	8	4 4 6	99.50
1.0080	3	2 6 5	99.67
1.0030	1	5 4 1	100.35
.9949	6	2 2 12	101.48
.9900	1	2 4 10	102.17
.9898	2	6 3 0	102.20
.9672	1	5 1 10	105.57
.9663	3	2 1 13	105.72
.9660	2	3 5 7	105.76
.9659	4	6 3 3	105.78
.9659	4	3 6 3	105.78

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.9627	2	5 4 4	106.29
.9575	3	5 2 9	107.13
.9575	3	2 5 9	107.13
.9448	2	6 2 7	109.23
.9417	1	0 8 4	109.77
.9407	2	4 5 5	109.94
.9299	1	0 7 8	111.87
.9252	1	1 3 13	112.72
.9220	2	2 7 4	113.32
.9211	1	8 0 5	113.50
.9173	1	8 1 1	114.23
.9108	1	1 8 2	115.50
.8932	2	3 3 12	119.17
.8890	4	3 2 13	120.11
.8888	3	5 4 7	120.16
.8887	1	5 5 3	120.18
.8861	4	8 1 4	120.75
.8821	2	3 4 11	121.67
.8819	1	7 3 1	121.72
.8689	2	1 8 5	124.87
.8572	11	8 2 0	127.97
.8567	2	0 5 13	128.10
.8565	1	2 7 7	128.15
.8564	1	9 0 3	128.17
.8564	2	0 9 3	128.17
.8505	5	7 1 9	129.84
.8505	4	1 7 9	129.84

Cesium cerium chloride, Cs_2CeCl_6

Structure
Hexagonal, $P\bar{3}m1$ (164), Z=1 [Kaatz and Marcovich, 1966].

Atom positions
1(a) 1 cerium
2(d) 2 cesium
6(ℓ) 6 chlorine

Lattice constants [ibid.]
a = 7.476(2) A
c = 6.039(2)

c/a = 0.8078

Volume
292.3 $Å^3$

Density
(calculated) 3.52 g/cm^3
[Kaatz and Marcovich, 1966].

Thermal parameters
Isotropic [Kaatz and Marcovich, 1966].

Scattering factors
Cl^- [Dawson, 1960]
Cs^+, Ce^{4+} [Thomas and Umeda, 1957]

Scale factors (integrated intensities)
$\gamma = 0.648 \times 10^{-3}$

References
Dawson, B. (1960). Acta Crystallogr. 13, 403.
Kaatz, T. and Marcovich, M. (1966). Acta Crystallogr. 21, 1011.
Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 6, 293.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
6.47	2	100	13.68
6.04	4	001	14.66
4.41	100	011	20.10
3.74	29	110	23.80
3.24	2	200	27.54
3.18	6	111	28.06
3.02	6	002	29.56
2.852	6	201+	31.34
2.736	12	102+	32.70
2.267	22	121	39.72
2.208	14	202+	40.84
2.158	5	300	41.82
2.032	1	301+	44.56
1.922	6	103	47.26
1.901	6	212+	47.80
1.869	10	220	48.68
1.772	1	113	51.52
1.721	8	311	53.18
1.710	1	023	53.56
1.589	3	222	57.98
1.563	1	041+	59.04
1.555	4	213	59.40
1.543	3	132+	59.88
1.510	1	004	61.36
1.442	4	231+	64.56
1.427	2	042+	65.36
1.413	2	410	66.08
1.400	2	114	66.78
1.340	2	133+	70.18
1.333	2	322+	70.62
1.266	1	501	74.94
1.237	1	304+	77.02
1.195	1	323+	80.26
1.187	1	015	80.90
1.174	2	224	81.98
1.142	1	151	84.84
1.134	1	422+	85.58
1.083	1	125	90.68
1.079	1	600	91.10
1.032	1	144+	96.62
1.002	1	315	100.46
0.9143	1	531+	114.82
.8779	1	064+	122.66

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
6.47	2	100	13.67
6.04	4	001	14.66
4.42	14	101	20.09
4.42	100	011	20.09
3.74	34	110	23.78
3.24	3	200	27.53
3.18	8	111	28.05
3.02	8	002	29.56
2.853	5	201	31.33
2.853	2	021	31.33
2.737	6	012	32.70
2.737	9	102	32.70
2.268	3	211	39.71
2.268	26	121	39.71
2.208	10	202	40.83
2.208	9	022	40.83
2.158	7	300	41.82
2.032	1	301	44.55
1.922	7	103	47.25
1.922	7	013	47.25
1.901	5	212	47.80
1.901	3	122	47.80
1.869	13	220	48.68
1.785	1	221	51.12
1.772	1	113	51.52
1.721	10	311	53.17
1.721	1	131	53.17
1.709	1	023	53.57
1.599	4	222	57.99
1.563	1	041	59.04
1.555	6	213	59.41
1.543	2	312	59.88
1.543	2	132	59.88
1.510	2	004	61.36
1.442	5	231	64.56

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.427	2	042	65.36
1.427	2	402	65.36
1.413	3	410	66.08
1.400	2	114	66.77
1.370	1	223	68.44
1.340	3	133	70.18
1.333	1	322	70.61
1.333	1	232	70.61
1.266	1	501	74.95
1.246	1	330	76.37
1.237	1	304	77.02
1.195	2	323	80.26
1.187	1	015	80.90
1.174	3	224	81.97
1.142	1	151	84.85
1.134	1	422	85.58
1.134	1	242	85.58
1.083	1	125	90.67
1.079	1	600	91.10
1.048	1	341	94.59
1.007	1	513	99.82
1.002	1	315	100.46
0.9744	1	611	104.47
.9409	1	433	109.90
.9371	1	235	110.57
.9345	1	440	111.03
.9143	1	531	114.82
.8865	1	163	120.68
.8377	1	155	133.72
.8213	1	451	139.42
.8136	1	217	142.43
.7985	1	345	149.43
.7946	2	444	151.59
.7843	1	721	158.33

Chlorpromazine, $C_{17}H_{19}ClN_2S$

Synonym
3-chloro-10-(3'-dimethylamino-n-propyl)-phenothiazine

Stability
The material was unstable in light, air, and x-rays [McDowell, 1969].

Structure
Orthorhombic, Pbca (61), Z = 8. The structure was determined by McDowell [ibid.].

Atom positions
All the atoms were in general positions [ibid.].

Lattice constants [ibid.]
a = 23.50(4) A
b = 15.20(2)
c = 9.23(1)

CD cell: a = 15.20, b = 23.50, c = 9.23, space group Pcab; a/b = 0.6468, c/b = 0.3928

Volume
3297. $Å^3$

Density
(measured) 1.289 g/cm^3
(calculated) 1.285 g/cm^3

Thermal parameters
Isotropic: overall B = 5.0

Scattering factors
C^0, Cl^0, N^0, S^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.545 \times 10^{-3}$
I/I_c (calculated) = 0.88

References
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), p. 202.
McDowell, J. J. H. (1969). Acta Crystallogr. B25 2175.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
11.75	100	2 0 0	7.52
9.28	2	2 1 0	9.52
7.60	13	0 2 0	11.64
7.48	10	1 1 1	11.82
6.54	5	2 1 1	13.52
6.38	1	2 2 0	13.88
5.86	36	0 2 1	15.10
5.69	7	1 2 1	15.56
5.47	7	4 1 0	16.18
5.25	35	2 2 1	16.88
4.69	4	3 2 1	18.92
4.61	41	0 0 2	19.22
4.36	19	1 3 1	20.34
4.30	5	2 0 2	20.66
4.15	75	2 3 1	21.38

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.04	6	5 1 1	22.00
3.97	36	3 0 2	22.36
3.89	22	1 2 2	22.86
3.84	9	4 3 0+	23.16
3.79	4	6 1 0+	23.44
3.74	4	2 2 2	23.78
3.67	5	5 2 1	24.26
3.63	5	4 0 2	24.52
3.52	16	3 2 2+	25.26
3.47	8	1 4 1	25.62
3.38	11	1 3 2	26.38
3.27	11	4 2 2	27.22
3.20	5	3 4 1	27.82
3.13	6	3 3 2	28.52
3.09	2	7 1 1+	28.86
3.02	2	5 2 2	29.54
2.990	2	1 1 3	29.86
2.934	3	8 0 0+	30.44
2.845	1	2 4 2	31.42
2.813	2	3 1 3	31.78
2.748	3	8 1 1+	32.56
2.701	4	4 5 0+	33.14
2.677	6	7 3 1+	33.44
2.614	3	1 3 3	34.28
2.592	2	4 5 1	34.58
2.556	1	7 2 2	35.08
2.538	1	5 1 3+	35.34
2.524	1	1 5 2	35.54
2.493	2	3 3 3	36.00
2.477	2	2 6 0+	36.24
2.400	1	4 3 3	37.44
2.393	1	0 4 3	37.56
2.355	1	8 2 2	38.18
2.342	2	2 4 3	38.40
2.332	3	3 6 1	38.58
2.295	1	5 3 3+	39.22
2.264	1	2 0 4	39.78
2.255	1	4 6 1+	39.94
2.244	1	7 1 3+	40.16
2.234	1	5 5 2	40.34
2.227	1	8 3 2	40.48
2.214	2	4 4 3	40.72
2.209	3	7 4 2+	40.82
2.177	2	9 2 2+	41.44
2.130	3	6 5 2+	42.40
2.127	3	6 6 0+	42.46
2.105	2	8 1 3+	42.94
2.084	1	3 5 3	43.38
2.067	4	4 2 4+	43.76
2.040	1	6 4 3	44.36
2.037	1	4 7 0	44.44

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
11.75	100	2	0	0	7.52
9.30	2	2	1	0	9.51
7.60	13	0	2	0	11.63
7.48	9	1	1	1	11.82
6.55	5	2	1	1	13.51
6.38	1	2	2	0	13.87
5.87	2	4	0	0	15.07
5.87	36	0	2	1	15.09
5.69	6	1	2	1	15.55
5.48	7	4	1	0	16.16
5.25	38	2	2	1	16.88
4.70	2	3	2	1	18.88
4.65	1	4	2	0	19.08
4.62	45	0	0	2	19.22
4.36	20	1	3	1	20.33
4.34	2	1	1	2	20.45
4.30	4	2	0	2	20.66
4.15	81	2	3	1	21.37
4.15	2	4	2	1	21.39
4.13	4	2	1	2	21.48
4.04	4	5	1	1	22.00
3.98	40	3	0	2	22.34
3.94	4	0	2	2	22.52
3.89	23	1	2	2	22.84
3.86	1	3	3	1	23.00
3.85	2	3	1	2	23.10
3.84	7	4	3	0	23.16
3.80	1	0	4	0	23.39
3.79	3	6	1	0	23.44
3.74	4	2	2	2	23.77
3.67	5	5	2	1	24.24
3.63	6	4	0	2	24.51
3.54	5	4	3	1	25.11
3.53	3	4	1	2	25.21
3.52	14	3	2	2	25.26
3.51	3	0	4	1	25.33
3.51	2	6	1	1	25.37
3.48	1	6	2	0	25.57
3.48	7	1	4	1	25.61
3.38	12	1	3	2	26.38
3.37	2	2	4	1	26.45
3.29	4	5	0	2	27.06
3.27	11	4	2	2	27.21
3.21	5	3	4	1	27.80
3.19	4	4	4	0	27.94
3.13	7	3	3	2	28.51
3.10	1	6	3	0	28.79
3.09	1	7	1	1	28.88
3.02	2	5	2	2	29.54
2.991	2	1	1	3	29.85

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.950	1	4	3	2	30.27
2.937	2	8	0	0	30.40
2.934	1	0	4	2	30.45
2.930	1	6	1	2	30.48
2.846	1	2	4	2	31.41
2.814	2	3	1	3	31.77
2.753	2	8	1	1	32.50
2.747	1	3	4	2	32.57
2.709	3	3	5	1	33.04
2.700	3	4	5	0	33.15
2.683	3	4	1	3	33.37
2.678	4	7	3	1	33.43
2.673	1	7	1	2	33.50
2.625	1	4	4	2	34.14
2.613	3	1	3	3	34.28
2.591	2	4	5	1	34.59
2.557	1	7	2	2	35.07
2.538	1	5	1	3	35.34
2.524	1	1	5	2	35.54
2.493	3	3	3	3	36.00
2.476	1	2	6	0	36.25
2.400	1	4	3	3	37.44
2.391	1	0	4	3	37.59
2.356	1	8	2	2	38.17
2.343	2	2	4	3	38.39
2.332	3	3	6	1	38.57
2.295	1	5	3	3	39.22
2.264	1	2	0	4	39.78
2.256	1	4	6	1	39.93
2.243	1	7	1	3	40.16
2.234	1	5	5	2	40.35
2.226	1	8	3	2	40.49
2.215	2	4	4	3	40.71
2.209	1	7	4	2	40.82
2.177	2	9	2	2	41.44
2.137	1	3	6	2	42.27
2.130	2	6	5	2	42.40
2.127	1	6	6	0	42.46
2.104	2	8	1	3	42.95
2.084	1	3	5	3	43.37
2.073	2	6	6	1	43.63
2.070	1	7	3	3	43.69
2.067	3	4	2	4	43.76
2.062	2	11	1	1	43.87
2.041	1	6	4	3	44.35
2.037	1	4	7	0	44.44

Chromium cobalt silicide, $Co_9Cr_{15}Si_6$

Structure
Tetragonal, $P4_2/mnm(136)$, Z = 1, σ-phase, isostructural with σ-(Cr, Fe), from powder data, [Stüwe, 1959]. Much work has been done on the σ-phase structure which has multiple atoms in 5 sites, called A through E [Bergman and Shoemaker, 1954]. The ordering arrangement of the atoms is dependent on a complex combination of electronic and size factors [Spooner, 1968].

Atom positions
The positions used were those for σ-(Cr, Fe) [Spooner and Wilson, 1964], and for σ-(X, Y, Si) [Aronsson and Lundström, 1957]. Site occupancy shared by multiple atoms was assumed to be random and in the following proportions:

Site A:	2(a)	2.0 cobalt
Site B:	4(f)	4.0 chromium
Site C:	8(i)	5.5 chromium and 2.5 cobalt
Site D:	8(i)	6.0 silicon and 2 cobalt
Site E:	8(j)	5.5 chromium and 2.5 cobalt

Lattice constants [Stüwe, 1959]
a = 8.736 Å
c = 4.561

Volume
348.12 $Å^3$

Density
(calculated) 7.054 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Cr^0, Si^0 [Cromer and Mann, 1968].

Scale factor (integrated intensitites)
$\gamma = 0.146 \times 10^{-3}$

References
Aronsson, B. and Lundström, T. (1957). Acta Chem. Scand. 11, 365.
Bergman, G. and Shoemaker, D.P.(1954). Acta Crystallogr. 7, 857.
Cromer, D. T. and Mann, J. B.(1968). Acta Crystallogr. A24, 321.
Spooner, F. J. (1968). Acta Crystallogr. A24, 605.
Spooner, F.J. and Wilson, C.G. (1964). Acta Crystallogr. 17, 1533.
Stüwe, H. P. (1959). Trans. AIME 215, 408.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.904	4	2 1 0	22.76
3.089	3	2 2 0	28.88
2.967	7	2 1 1	30.10
2.455	1	3 0 1	36.58
2.423	2	3 2 0	37.08
2.362	14	3 1 1	38.06
2.281	19	0 0 2	39.48
2.139	5	1 1 2	42.22
2.119	90	4 1 0	42.64
2.059	50	3 3 0	43.94
2.021	50	2 0 2	44.80
1.970	65	2 1 2	46.04
1.922	100	4 1 1	47.26
1.877	35	3 3 1	48.46
1.834	7	2 2 2	49.66
1.758	15	3 1 2	51.96
1.713	1	5 1 0	53.44
1.660	2	3 2 2	55.28
1.632	3	4 3 1	56.34
1.604	1	5 1 1	57.40
1.529	1	5 2 1	60.52
1.387	4	4 3 2	67.48
1.370	2	5 1 2+	68.44
1.332	1	3 1 3	70.66
1.322	8	5 2 2+	71.28
1.2523	15	5 3 2	75.92
1.2352	19	4 1 3+	77.16
1.2272	5	6 0 2	77.76
1.2232	7	3 3 3	78.06
1.2154	5	6 1 2	78.66
1.2036	2	7 0 1	79.58
1.2001	11	7 2 0	79.86
1.1924	5	5 5 1	80.48
1.1815	4	6 2 2	81.38
1.1708	3	5 4 2+	82.28
1.1604	6	7 2 1	83.18
1.1470	1	4 3 3	84.38
1.1402	6	0 0 4	85.00
1.0619	1	7 2 2	93.00
1.0595	6	8 2 0	93.28
1.0320	4	8 2 1	96.56
1.0295	4	6 6 0	96.88
1.0041	10	4 1 4+	100.20
.9976	5	3 3 4	101.10
.9850	4	8 0 2	102.90
.9787	7	7 4 2	103.82
.9609	1	8 2 2	106.58
.9587	2	5 5 3	106.92
.9420	3	7 2 3	109.72
.9277	1	9 2 1+	112.26

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.8886	1	9 1 2	120.20
.8750	3	7 6 2+	123.36
.8692	3	8 2 3+	124.80
.8581	1	8 5 2+	127.72
.8539	2	9 3 2+	128.86
.8525	2	6 6 3	129.26
.8379	7	4 1 5+	133.66
.8340	2	3 3 5	134.92
.8267	9	7 2 4+	137.44
.8231	1	10 3 1	138.74

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.907	3	2 1 0	22.74
3.089	2	2 2 0	28.88
2.967	6	2 1 1	30.09
2.455	1	3 0 1	36.58
2.423	2	3 2 0	37.07
2.363	13	3 1 1	38.05
2.280	18	0 0 2	39.48
2.139	3	1 1 2	42.21
2.119	85	4 1 0	42.63
2.059	45	3 3 0	43.93
2.022	45	2 0 2	44.80
1.970	65	2 1 2	46.05
1.922	100	4 1 1	47.26
1.877	35	3 3 1	48.46
1.835	7	2 2 2	49.65
1.759	15	3 1 2	51.95
1.713	1	5 1 0	53.43
1.661	2	3 2 2	55.27
1.632	3	4 3 1	56.34
1.604	1	5 1 1	57.40
1.529	1	5 2 1	60.52
1.387	4	4 3 2	67.47
1.370	2	5 1 2	68.43
1.364	1	5 4 0	68.74
1.332	1	3 1 3	70.66
1.322	2	6 2 1	71.27
1.322	7	5 2 2	71.28
1.2522	17	5 3 2	75.93
1.2355	5	5 5 0	77.14
1.2353	17	4 1 3	77.16
1.2273	5	6 0 2	77.76
1.2231	7	3 3 3	78.07
1.2153	6	6 1 2	78.67
1.2038	1	7 0 1	79.57
1.2001	12	7 2 0	79.87

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.1925	5	5 5 1	80.47
1.1815	4	6 2 2	81.38
1.1709	1	6 4 1	82.27
1.1709	2	5 4 2	82.28
1.1606	7	7 2 1	83.17
1.1469	1	4 3 3	84.38
1.1402	7	0 0 4	84.99
1.0699	1	6 4 2	92.10
1.0620	1	7 2 2	92.99
1.0595	7	8 2 0	93.28
1.0320	4	8 2 1	96.56
1.0296	3	6 6 0	96.86
1.0043	3	6 6 1	100.17
1.0041	10	4 1 4	100.20
.9975	6	3 3 4	101.10
.9850	4	8 0 2	102.90
.9788	8	7 4 2	103.82
.9608	1	8 2 2	106.59
.9588	3	5 5 3	106.91
.9420	4	7 2 3	109.72
.8885	1	9 1 2	120.21
.8751	2	9 2 2	123.35
.8751	2	7 6 2	123.35
.8692	3	8 2 3	124.80
.8580	1	8 5 2	127.73
.8539	3	9 3 2	128.87
.8525	3	6 6 3	129.26
.8379	5	5 5 4	133.64
.8379	8	4 1 5	133.67
.8340	3	3 3 5	134.91
.8267	5	9 4 2	137.42
.8266	13	7 2 4	137.46
.8231	2	10 3 1	138.74
.8218	1	8 4 3	139.22

Cobalt copper tin, $CoCu_2Sn$

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy isostructural with Cu_2AlMn, from powder data [Dwight 1967].

Atom positions [ibid.]
4(b) 4 cobalt
8(c) 8 copper
4(a) 4 tin

Lattice constant [ibid.]
a = 5.982 A

Volume
214.1 A^3

Density
(calculated) 9.454 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Cu^0, Sn^0 [Cromer and Mann, 1968].

Scale factor (integrated intensities)
$\gamma = 1.42 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Dwight, A.E. (1967). Intermetallic Compounds (Wiley and Sons Inc., New York), Westbrook, J. H. (ed.) p. 174.

Calculated Pattern (Peak heights)

d(A)	I	hkℓ	2θ(°) λ = 1.540598A
3.453	10	1 1 1	25.78
2.990	3	2 0 0	29.86
2.115	100	2 2 0	42.72
1.804	4	3 1 1	50.56
1.496	13	4 0 0	62.00
1.372	1	3 3 1	68.30
1.221	20	4 2 2	78.22
1.151	1	5 1 1+	84.00
1.057	6	4 4 0	93.52
1.011	1	5 3 1	99.24
.9458	8	6 2 0	109.06
.8635	2	4 4 4	126.28
.7994	13	6 4 2	149.00
.7788	1	7 3 1+	163.06

Calculated Pattern (Integrated)

d(A)	I	hkℓ	2θ(°) λ = 1.540598A
3.454	9	1 1 1	25.77
2.991	2	2 0 0	29.85
2.115	100	2 2 0	42.72
1.804	4	3 1 1	50.56
1.495	14	4 0 0	62.01
1.372	1	3 3 1	68.29
1.338	1	4 2 0	70.32
1.221	25	4 2 2	78.22
1.151	1	5 1 1	84.00
1.057	7	4 4 0	93.51
1.011	1	5 3 1	99.25
.9458	11	6 2 0	109.06
.8634	4	4 4 4	126.29
.7994	30	6 4 2	149.00
.7788	1	5 5 3	163.06
.7788	3	7 3 1	163.06

Cobalt gallium hafnium, Co_2GaHf

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy isostructural with Cu_2AlMn, from powder data (x-ray and neutron) [Ziebeck and Webster, 1974].

Atom positions [ibid.]
8(c) 8 cobalt
4(a) 4 gallium
4(b) 4 hafnium

Lattice constant [ibid.]
a = 6.032 A

Volume
219.5 A^3

Density
(measured) 11.10 g/cm^3 [ibid.]
(calculated) 11.08 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ga^0, Hf^0 [Cromer and Mann, 1968] corrected for anomalous dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)
$\gamma = 1.287 \times 10^{-3}$

References

Cromer, D.T. and Liberman, D.(1970). J. Chem. Phys. 53, 1891.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Ziebeck, K. R. A. and Webster, P. J. (1974). J. Phys. Chem. Solids 35, 1.

Calculated Pattern (Peak heights)

d(A)	I	hkℓ	2θ(°) λ = 1.540598A
3.482	20	1 1 1	25.56
3.016	18	2 0 0	29.60
2.132	100	2 2 0	42.36
1.819	9	3 1 1	50.12
1.741	4	2 2 2	52.52
1.508	13	4 0 0	61.44
1.384	3	3 3 1	67.64
1.349	5	4 2 0	69.66
1.231	20	4 2 2	77.46
1.161	2	5 1 1+	83.14
1.066	6	4 4 0	92.50
1.020	2	5 3 1	98.14
1.005	2	4 4 2+	100.04
.9537	8	6 2 0	107.74
.9198	1	5 3 3	113.74
.9093	1	6 2 2	115.80
.8706	2	4 4 4	124.44
.8446	1	5 5 1+	131.56
.8365	1	6 4 0	134.10
.8061	12	6 4 2	145.74
.7853	2	7 3 1+	157.56

Calculated Pattern (Integrated)

d(A)	I	hkℓ	2θ(°) λ = 1.540598A
3.483	19	1 1 1	25.56
3.016	17	2 0 0	29.60
2.133	100	2 2 0	42.35
1.819	9	3 1 1	50.12
1.741	5	2 2 2	52.51
1.508	14	4 0 0	61.44
1.384	3	3 3 1	67.65
1.349	6	4 2 0	69.65
1.231	25	4 2 2	77.45
1.161	2	5 1 1	83.14
1.066	7	4 4 0	92.50
1.020	2	5 3 1	98.14
1.005	2	4 4 2	100.03
.9537	11	6 2 0	107.74
.9199	1	5 3 3	113.73
.9094	2	6 2 2	115.79
.8706	3	4 4 4	124.44
.8446	1	7 1 1	131.56
.8446	1	5 5 1	131.56
.8365	2	6 4 0	134.11
.8061	30	6 4 2	145.74
.7853	2	5 5 3	157.57
.7853	5	7 3 1	157.57

Cobalt gallium niobium, Co_2GaNb

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy isostructural with Cu_2AlMn, from powder data [Markiv et al., 1965].

Atom positions [ibid.]
8(c) 8 cobalt
4(a) 4 gallium
4(b) 4 niobium

Lattice constant [ibid.]
a = 5.954 A

Volume
211.1 A^3

Density
(calculated) 8.826 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ga^0, Nb^0 [Cromer and Mann, 1968]

Scale factors (integrated intensities)
$\gamma = 1.18 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Markiv, V.Ya., Voroshilov, Yu.V., Kripyakevich, P.I. and Cherkashin, E.E. (1965). Sov. Phys.-Crystallogr. 9, 619.

Calculated Pattern (Peak heights)

d(A)	I	hkl	2θ(°) λ = 1.540598A
3.437	2	1 1 1	25.90
2.976	4	2 0 0	30.00
2.105	100	2 2 0	42.94
1.719	1	2 2 2	53.26
1.488	13	4 0 0	62.34
1.331	1	4 2 0	70.70
1.2154	20	4 2 2	78.66
1.0526	6	4 4 0	94.08
.9414	9	6 2 0	109.82
.8594	2	4 4 4	127.36
.7956	14	6 4 2	151.00

Calculated Pattern (Integrated)

d(A)	I	hkl	2θ(°) λ = 1.540598A
3.438	2	1 1 1	25.90
2.977	3	2 0 0	29.99
2.105	100	2 2 0	42.93
1.719	1	2 2 2	53.25
1.488	14	4 0 0	62.33
1.331	1	4 2 0	70.70
1.2154	25	4 2 2	78.66
1.0525	7	4 4 0	94.08
.9414	12	6 2 0	109.82
.8594	4	4 4 4	127.36
.7956	35	6 4 2	151.00

Cobalt germanium, Co_3Ge_2

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 1, isostructural with Ni_2In and Ni_3Sn_2, from powder data [Lecocq and Michel, 1964].

Atom positions
The structure prototype, $2(Ni_2In)$, has 2 Ni atoms in positions 2(a) and also in 2(d); the indium are in 2(c). Studies on two isostructural compounds, Ni_3In_2 and Co_3Sn_2, indicated that in their structures the site 2(d) is only partially occupied [Kanematsu, 1962; Rajeswari and Manohar, 1970].

The positions used here for Co_3Ge_2 were:
2(a) 2 cobalt
2(d) 1 cobalt
2(c) 2 germanium

Lattice constants [Lecocq and Michel, 1964]
A composition range exists from 36 to 44 atomic percent Ge and the constants vary accordingly. For 40 atomic percent Ge:
a = 3.964 A
c = 4.992

Volume
67.93 A^3

Density
(calculated) 7.870 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ge^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.418 \times 10^{-3}$

References

Cromer, D. T. and Mann, J. B. (1968) Acta Crystallogr. A24, 321.
Kanematsu, K. (1962). J. Phys. Soc. Jap. 17, 85.
Lecocq, P. and Michel, A. (1964). Bull. Soc. Chim. Fr. 1964, 1911.
Rajeswari, H. and Manohar, H. (1970). Indian J. Pure Appl. Phys. 8, 363.

Calculated Pattern (Peak heights)

d(A)	I	hkℓ	2θ(°) λ = 1.540598A
3.432	2	1 0 0	25.94
2.827	35	1 0 1	31.62
2.495	5	0 0 2	35.96
2.019	100	1 0 2	44.86
1.982	100	1 1 0	45.74
1.623	5	2 0 1	56.66
1.552	6	1 1 2	59.50
1.497	4	1 0 3	61.92
1.414	25	2 0 2	66.00
1.256	4	2 1 1	75.68
1.248	5	0 0 4	76.22
1.195	1	2 0 3	80.30
1.151	19	2 1 2	84.00
1.144	10	3 0 0	84.62
1.056	15	1 1 4	93.68
1.040	1	3 0 2	95.56
1.023	2	2 1 3	97.68
.991	6	2 2 0	102.02
.935	1	3 1 1	110.90
.921	1	2 2 2	113.50
.890	8	3 1 2	119.98
.843	8	3 0 4	131.92
.826	1	3 1 3	137.54
.812	3	4 0 2	143.28
.809	4	1 0 6	144.60
.7913	1	2 1 5	153.56
.7779	1	3 2 1	163.92

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
3.433	2	1	0	0	25.93
2.829	30	1	0	1	31.61
2.496	5	0	0	2	35.95
2.019	100	1	0	2	44.86
1.982	100	1	1	0	45.74
1.623	5	2	0	1	56.66
1.552	6	1	1	2	59.51
1.497	4	1	0	3	61.92
1.414	25	2	0	2	66.00
1.256	4	2	1	1	75.67
1.248	5	0	0	4	76.23
1.195	2	2	0	3	80.29
1.151	20	2	1	2	83.99
1.144	12	3	0	0	84.62
1.056	18	1	1	4	93.67
1.040	1	3	0	2	95.55
1.023	2	2	1	3	97.67
.991	7	2	2	0	102.03
.959	1	1	0	5	106.93
.935	2	3	1	1	110.90
.921	1	2	2	2	113.51
.890	12	3	1	2	119.97
.863	1	2	0	5	126.39
.846	1	4	0	1	131.21
.843	14	3	0	4	131.93
.826	2	3	1	3	137.53
.812	8	4	0	2	143.29
.809	8	1	0	6	144.59
.7913	3	2	1	5	153.56
.7779	5	3	2	1	163.92

Cobalt germanium hafnium, $Co_{16}Ge_7Hf_6$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Gladyshevs'kii et al., 1962].

Atom positions
The positions are those determined by Bergman and Waugh [1956] for $Cu_{16}Mg_6Si_7$.

32(f)	32 cobalt(1)
32(f)	32 cobalt(2)
24(e)	24 hafnium
4(b)	4 germanium(1)
24(d)	24 germanium(2)

Lattice constant
a = 11.567 Å
(published value, a = 11.566 [Gladyshevs'kii et al., 1962])

Volume
1547.6 $Å^3$

Density
(calculated) 10.824 g/cm^3

Thermal parameters
Isotropic: cobalt, B = 1.0; germanium, B = 1.0; hafnium, B = 0.8

Scattering factors
Co^0, Ge^0, Hf^0 [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.370 \times 10^{-3}$

References

Bergman, G. and Waugh, J. L. T. (1956). Acta Crystallogr. 9, 214.

Gladyshevs'kii, E. I., Markiv, V. Ya., and Kuz'ma, Yu.B.(1962). Dopov. Akad. Nauk. Ukr. RSR, No. 4, p. 481.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 204, 212.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
6.672	30	1 1 1	13.26
5.779	6	2 0 0	15.32
3.488	1	3 1 1	25.52
3.339	5	2 2 2	26.68
2.892	9	4 0 0	30.90
2.653	40	3 3 1	33.76
2.586	2	4 2 0	34.66
2.361	40	4 2 2	38.08
2.226	100	3 3 3+	40.50
2.045	55	4 4 0	44.26
1.955	8	5 3 1	46.40
1.928	30	6 0 0+	47.10
1.743	7	6 2 2	52.44
1.620	8	5 5 1	56.80
1.604	3	6 4 0	57.40
1.506	4	7 3 1+	61.54
1.446	5	8 0 0	64.38
1.413	8	7 3 3	66.06
1.403	1	6 4 4+	66.62
1.363	25	8 2 2+	68.82
1.336	11	7 5 1+	70.44
1.327	5	6 6 2	70.98
1.270	4	7 5 3+	74.70
1.262	11	8 4 2	75.24
1.181	1	8 4 4	81.46
1.163	18	9 3 3	83.00
1.157	2	10 0 0	83.50
1.134	1	8 6 2+	85.56
1.118	2	7 7 3+	87.08
1.113	7	6 6 6	87.58
1.079	1	9 5 3	91.14
1.074	1	10 4 0	91.66
1.043	3	11 1 1+	95.22
1.022	1	8 8 0	97.78
1.011	2	9 7 1	99.32
1.007	5	8 8 2	99.84
.992	1	10 6 0	101.90
.981	1	9 7 3	103.46
.978	5	10 6 2	103.98
.964	4	8 8 4+	106.10
.954	4	11 5 1	107.68
.938	2	10 6 4+	110.38
.914	5	12 4 0	114.78
.903	1	8 8 6+	117.04
.8924	2	10 8 2	119.34
.8845	11	11 5 5+	121.12
.8823	8	10 6 6	121.64
.8645	6	13 3 1+	126.00
.8622	7	12 6 0+	126.60
.8458	2	13 3 3	131.20

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
6.678	40	1	1	1	13.25
5.783	8	2	0	0	15.31
4.090	1	2	2	0	21.71
3.488	2	3	1	1	25.52
3.339	8	2	2	2	26.68
2.892	15	4	0	0	30.90
2.654	65	3	3	1	33.75
2.586	2	4	2	0	34.65
2.361	70	4	2	2	38.08
2.226	80	5	1	1	40.49
2.226	95	3	3	3	40.49
2.045	100	4	4	0	44.26
1.955	14	5	3	1	46.40
1.928	40	6	0	0	47.10
1.928	17	4	4	2	47.10
1.744	14	6	2	2	52.43
1.620	15	5	5	1	56.79
1.604	6	6	4	0	57.40
1.506	6	7	3	1	61.53
1.506	2	5	5	3	61.53
1.446	9	8	0	0	64.38
1.413	16	7	3	3	66.06
1.403	1	6	4	4	66.62
1.363	20	6	6	0	68.81
1.363	25	8	2	2	68.81
1.336	13	7	5	1	70.44
1.336	9	5	5	5	70.44
1.327	9	6	6	2	70.98
1.270	2	9	1	1	74.70
1.270	7	7	5	3	74.70
1.262	20	8	4	2	75.23
1.233	1	6	6	4	77.32
1.181	3	8	4	4	81.46
1.163	35	9	3	3	83.00
1.163	2	7	5	5	83.00
1.157	2	10	0	0	83.51
1.134	1	8	6	2	85.55
1.134	1	10	2	0	85.55
1.118	3	7	7	3	87.08
1.118	1	9	5	1	87.08
1.113	13	6	6	6	87.59
1.079	2	9	5	3	91.15
1.074	2	10	4	0	91.66
1.056	1	10	4	2	93.69
1.043	6	11	1	1	95.22
1.043	1	7	7	5	95.22
1.022	2	8	8	0	97.78
1.011	4	9	7	1	99.32
1.007	11	8	8	2	99.83
.992	3	10	6	0	101.90

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.981	3	9	7	3	103.47
.978	11	10	6	2	103.99
.964	5	8	8	4	106.10
.964	4	12	0	0	106.10
.954	8	11	5	1	107.69
.938	1	12	2	2	110.38
.938	3	10	6	4	110.38
.929	1	11	5	3	112.01
.914	11	12	4	0	114.78
.906	1	9	9	1	116.47
.903	1	8	8	6	117.04
.8924	5	10	8	2	119.35
.8846	11	11	5	5	121.11
.8846	5	11	7	1	121.11
.8846	11	9	9	3	121.11
.8820	10	10	6	6	121.71
.8646	10	13	3	1	125.99
.8646	2	11	7	3	125.99
.8646	3	9	7	7	125.99
.8622	12	12	6	0	126.62
.8622	3	10	8	4	126.62
.8459	5	13	3	3	131.20

Cobalt germanium niobium, $Co_{16}Ge_7Nb_6$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Spiegel et al., 1963]. Kuz'ma et al. [1964] determined positions for $Co_{16}Nb_6Si_7$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions of $Co_{16}Nb_6Si_7$ were preferred.

32(f)	32 cobalt (1)
32(f)	32 cobalt (2)
4(b)	4 germanium (1)
24(d)	24 germanium (2)
24(e)	24 niobium

Lattice constant
a = 11.477 Å
(published value, 11.478 Å [Spiegel et al., 1963])

Volume
1511.8 $Å^3$

Density
(calculated) 8.825 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ge^0, Nb^0 [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.425 \times 10^{-3}$

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), pp. 204, 211.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I., and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.

Spiegel, F. X., Bardos, D., and Beck, P. A. (1963). Trans. AIME 227, 575.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.734	4	2 0 0	15.44
3.458	2	3 1 1	25.74
2.868	3	4 0 0	31.16
2.633	19	3 3 1	34.02
2.566	3	4 2 0	34.94
2.342	30	4 2 2	38.40
2.209	80	3 3 3+	40.82
2.029	100	4 4 0	44.62
1.940	17	5 3 1	46.80
1.913	20	6 0 0+	47.50
1.815	2	6 2 0	50.24
1.750	3	5 3 3	52.22
1.730	14	6 2 2	52.88
1.607	4	5 5 1+	57.28
1.494	5	7 3 1+	62.06
1.434	6	8 0 0	64.96
1.402	5	7 3 3	66.64
1.352	15	8 2 2+	69.44
1.325	7	5 5 5+	71.08
1.317	3	6 6 2	71.62
1.283	1	8 4 0	73.78
1.260	7	7 5 3+	75.40
1.252	7	8 4 2	75.92
1.203	1	9 3 1	79.62
1.171	7	8 4 4	82.24
1.153	14	9 3 3	83.80
1.148	2	8 6 0+	84.30
1.125	1	10 2 0+	86.38
1.109	3	7 7 3+	87.94
1.104	7	6 6 6+	88.46
1.066	1	10 4 0	92.58
1.035	1	11 1 1	96.20
1.014	3	8 8 0	98.82
1.003	4	9 7 1+	100.38
.9990	3	8 8 2	100.90
.9841	1	8 6 6+	103.02
.9700	7	10 6 2	105.14
.9564	2	12 0 0+	107.30
.9467	1	11 5 1+	108.92
.9435	1	12 2 0	109.46

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.738	3	2	0	0	15.43
3.460	2	3	1	1	25.72
2.869	3	4	0	0	31.15
2.633	17	3	3	1	34.02
2.566	2	4	2	0	34.93
2.343	30	4	2	2	38.39
2.209	35	5	1	1	40.82
2.209	40	3	3	3	40.82
2.029	100	4	4	0	44.63
1.940	17	5	3	1	46.79
1.913	17	6	0	0	47.49
1.913	4	4	4	2	47.49
1.815	2	6	2	0	50.24
1.750	3	5	3	3	52.22
1.730	14	6	2	2	52.87
1.607	1	7	1	1	57.28
1.607	3	5	5	1	57.28
1.494	4	7	3	1	62.07
1.494	1	5	5	3	62.07
1.435	7	8	0	0	64.95
1.402	6	7	3	3	66.65
1.353	9	8	2	2	69.43
1.353	8	6	6	0	69.43
1.325	4	7	5	1	71.08
1.325	4	5	5	5	71.08
1.317	3	6	6	2	71.62
1.283	1	8	4	0	73.78
1.260	1	9	1	1	75.39
1.260	7	7	5	3	75.39
1.252	7	8	4	2	75.92
1.203	1	9	3	1	79.62
1.171	8	8	4	4	82.24
1.153	15	9	3	3	83.80
1.153	1	7	7	1	83.80
1.148	1	8	6	0	84.31
1.125	1	10	2	0	86.39
1.110	1	9	5	1	87.94
1.110	2	7	7	3	87.94
1.104	1	10	2	2	88.45
1.104	6	6	6	6	88.45
1.066	1	10	4	0	92.58
1.035	2	11	1	1	96.21
1.014	4	8	8	0	98.81
1.003	3	9	7	1	100.38
1.003	1	11	3	1	100.38
.9989	4	8	8	2	100.91
.9700	9	10	6	2	105.15
.9564	1	8	8	4	107.30
.9564	1	12	0	0	107.30
.9466	1	11	5	1	108.93
.9434	1	12	2	0	109.47

Cobalt germanium tantalum, $Co_{16}Ge_7Ta_6$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Gladyshevs'kii et al., 1962]. Kuz'ma et al. [1964] determined positions for $Co_{16}Nb_6Si_7$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions of $Co_{16}Nb_6Si_7$ were preferred.

32(f)	32 cobalt(1)
32(f)	32 cobalt(2)
4(b)	4 germanium(1)
24(d)	24 germanium(2)
24(e)	24 tantalum

Lattice constant
a = 11.421 A
(published value, 11.420 Å [Gladyshevs'kii et al., 1962]).

Volume
1489.8 $Å^3$

Density
(calculated) 11.310 g/cm^3

Thermal parameters
Isotropic: cobalt B = 1.0; germanium B = 1.0; tantalum B = 0.8.

Scattering factors
Co^0, Ge^0, Ta^0 [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.463 \times 10^{-3}$

References

Gladyshevs'kii, E. I., Markiv, V. Ya., and Kuz'ma, Yu. B. (1962). Dopov. Akad. Nauk. Ukr. RSR, No. 4, p. 481.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 204, 212.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I. and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
6.593	17	1 1 1	13.42
5.705	4	2 0 0	15.52
4.037	3	2 2 0	22.00
3.443	2	3 1 1	25.86
3.295	11	2 2 2	27.04
2.855	14	4 0 0	31.30
2.620	35	3 3 1	34.20
2.553	4	4 2 0	35.12
2.331	40	4 2 2	38.60
2.198	100	3 3 3+	41.04
2.019	75	4 4 0	44.86
1.930	5	5 3 1	47.04
1.904	25	6 0 0+	47.74
1.722	3	6 2 2	53.16
1.599	10	5 5 1	57.58
1.584	3	6 4 0	58.20
1.487	9	7 3 1+	62.40
1.428	5	8 0 0	65.30
1.395	11	7 3 3	67.02
1.385	2	6 4 4+	67.58
1.346	25	8 2 2+	69.82
1.319	10	5 5 5+	71.48
1.310	2	6 6 2	72.02
1.254	5	7 5 3	75.82
1.246	10	8 4 2	76.36
1.166	3	8 4 4	82.72
1.148	15	9 3 3+	84.30
1.142	2	10 0 0	84.82
1.120	3	8 6 2+	86.92
1.104	6	7 7 3+	88.48
1.099	5	6 6 6	89.00
1.060	3	10 4 0	93.18
1.030	2	11 1 1	96.84
1.009	1	8 8 0	99.48
.998	3	9 7 1+	101.06
.994	6	8 8 2	101.60
.979	2	10 6 0	103.72
.969	1	9 7 3	105.34
.965	6	10 6 2	105.88
.952	3	8 8 4+	108.06
.942	4	11 5 1+	109.72

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
6.594	19	1	1	1	13.42
5.711	5	2	0	0	15.50
4.038	4	2	2	0	21.99
3.444	3	3	1	1	25.85
3.297	13	2	2	2	27.02
2.855	17	4	0	0	31.30
2.620	45	3	3	1	34.19
2.554	5	4	2	0	35.11
2.331	50	4	2	2	38.59
2.198	65	5	1	1	41.03
2.198	70	3	3	3	41.03
2.019	100	4	4	0	44.86
1.931	7	5	3	1	47.03
1.904	30	6	0	0	47.74
1.904	6	4	4	2	47.74
1.722	5	6	2	2	53.15
1.599	15	5	5	1	57.59
1.584	4	6	4	0	58.20
1.487	10	7	3	1	62.40
1.487	3	5	5	3	62.40
1.428	7	8	0	0	65.31
1.395	16	7	3	3	67.02
1.385	1	8	2	0	67.58
1.385	2	6	4	4	67.58
1.346	13	6	6	0	69.82
1.346	20	8	2	2	69.82
1.319	6	7	5	1	71.48
1.319	9	5	5	5	71.48
1.310	3	6	6	2	72.03
1.277	1	8	4	0	74.21
1.254	7	7	5	3	75.83
1.246	16	8	4	2	76.36
1.166	4	8	4	4	82.73
1.148	20	9	3	3	84.30
1.148	2	7	7	1	84.30
1.148	1	7	5	5	84.30
1.142	2	10	0	0	84.82
1.120	3	8	6	2	86.91
1.120	2	10	2	0	86.91
1.104	6	7	7	3	88.48
1.104	4	9	5	1	88.48
1.099	8	6	6	6	89.00
1.060	4	10	4	0	93.17
1.030	4	11	1	1	96.84
1.009	2	8	8	0	99.47
.998	1	11	3	1	101.06
.998	3	9	7	1	101.06
.994	1	10	4	4	101.59
.994	9	8	8	2	101.59
.979	3	10	6	0	103.73

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.969	2	9	7	3	105.34
.965	10	10	6	2	105.88
.952	2	12	0	0	108.07
.952	3	8	8	4	108.07
.942	6	11	5	1	109.72
.942	1	7	7	7	109.72

Cobalt hafnium tin, Co_2HfSn

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy isostructural with $AlCu_2Mn$, from powder data (x-ray and neutron) [Ziebeck and Webster, 1974].

Atom positions
8(c) 8 cobalt
4(b) 4 hafnium
4(a) 4 tin

Lattice constant
a = 6.218 Å [Table 1, Ziebeck and Webster, 1974].

Volume
240.41 $Å^3$

Density
(calculated) 11.466 g/cm^3
(measured) 11.400 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0 Sn^0 [Cromer and Mann, 1968]
Hf^0 [International Tables, 1974]
All factors were corrected for anomalous dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)
$\gamma = 1.253 \times 10^{-3}$

References
Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Cromer, D.T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.
Ziebeck, K.R.A. and Webster, P.J. (1974). J. Phys. Chem. Solids 35, 1.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.590	5	1 1 1	24.78
3.108	25	2 0 0	28.70
2.199	100	2 2 0	41.02
1.875	1	3 1 1	48.52
1.795	5	2 2 2	50.82
1.554	15	4 0 0	59.42
1.390	5	4 2 0	67.28
1.269	20	4 2 2	74.74
1.099	5	4 4 0	88.98
1.036	5	4 4 2+	96.02
.9832	10	6 2 0	103.16
.9374	1	6 2 2	110.52
.8975	1	4 4 4	118.24
.8623	1	6 4 0	126.58
.8309	10	6 4 2	135.96

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.590	5	1 1 1	24.78
3.109	25	2 0 0	28.69
2.198	100	2 2 0	41.02
1.875	1	3 1 1	48.52
1.795	5	2 2 2	50.83
1.554	15	4 0 0	59.41
1.390	10	4 2 0	67.29
1.269	25	4 2 2	74.73
1.099	5	4 4 0	88.98
1.036	5	4 4 2	96.03
1.036	1	6 0 0	96.03
.9832	10	6 2 0	103.16
.9374	5	6 2 2	110.52
.8975	5	4 4 4	118.25
.8623	5	6 4 0	126.59
.8309	25	6 4 2	135.96

Cobalt holmium, Co_2Ho

Structure
Cubic, Fd3m (227), Z = 8, isostructural with Cu_2Mg, from powder data [Harris et al., 1965].

Atom positions [ibid.]
8(a) 8 holmium
16(d) 16 cobalt

Lattice constant [ibid.]
a = 7.1734 Å
(published value, 7.1585 kX)

Volume
369.1 $Å^3$

Density
(calculated) 10.177 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ho^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 1.07 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Harris, I. R., Mansey, R. C., and Raynor, G. V. (1965). J. Less-Common Metals 9, 270.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.141	20	1 1 1	21.44
2.536	70	2 2 0	35.36
2.162	100	3 1 1	41.74
2.071	14	2 2 2	43.68
1.7932	1	4 0 0	50.88
1.6456	4	3 3 1	55.82
1.4643	20	4 2 2	63.48
1.3804	25	5 1 1+	67.84
1.2680	16	4 4 0	74.82
1.2126	3	5 3 1	78.88
1.1342	7	6 2 0	85.56
1.0940	7	5 3 3	89.52
1.0815	3	6 2 2	90.84
1.0045	1	7 1 1+	100.14
.9586	9	6 4 2	106.94
.9339	13	7 3 1+	111.14
.8967	3	8 0 0	118.42
.8454	5	8 2 2+	131.34
.8283	8	7 5 1+	136.86
.8229	1	6 6 2	138.82
.7874	2	7 5 3+	156.08

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.142	17	1 1 1	21.44
2.536	70	2 2 0	35.36
2.163	100	3 1 1	41.73
2.071	14	2 2 2	43.68
1.7934	1	4 0 0	50.88
1.6457	4	3 3 1	55.82
1.4643	20	4 2 2	63.48
1.3805	20	5 1 1	67.83
1.3805	7	3 3 3	67.83
1.2681	18	4 4 0	74.81
1.2125	3	5 3 1	78.88
1.1342	8	6 2 0	85.55
1.0939	8	5 3 3	89.52
1.0814	3	6 2 2	90.84
1.0045	1	7 1 1	100.15
1.0045	1	5 5 1	100.15
.9586	11	6 4 2	106.95
.9339	12	7 3 1	111.14
.9339	6	5 5 3	111.14
.8967	4	8 0 0	118.42
.8764	1	7 3 3	123.04
.8454	3	6 6 0	131.34
.8454	6	8 2 2	131.34
.8283	13	7 5 1	136.86
.8283	2	5 5 5	136.86
.8228	3	6 6 2	138.83
.8020	1	8 4 0	147.67
.7874	4	7 5 3	156.09
.7874	2	9 1 1	156.09

Cobalt iron sulfide, Co_8FeS_8

Structure
Cubic, Fm3m (225), Z = 4, π phase, isostructural with Co_9S_8, from powder data (neutron and x-ray) [Knop, 1962].

Atom positions [Pearson, 1967]

4(b)	3.6 cobalt	32(f)	3.6 iron
4(b)	0.4 iron	24(e)	8.0 sulfur
32(f)	28.4 cobalt	24(e)	24.0 sulfur

Lattice constant
a = 9.944(2) Å
(published value, a = 9.943(2) Å, [Knop, 1962])

Volume
983.3 $Å^3$

Density
(calculated) 5.295 g/cm^3

Thermal parameters
Isotropic: cobalt, B = 0.5; iron, B = 0.5; sulfur, B = 0.7

Scattering factors
Co^0, Fe^0, S^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.319 \times 10^{-3}$

References

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England). pp. 202, 204.

Knop, D. (1962). Chem. Ind. London, April 21, p. 739.

Pearson, W.B. (1967). Handbook of Lattice Spacings and Structures of Metals and Alloys, v.2, (Pergamon, Press, N.Y.) pp. 197, 788.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.734	35	1 1 1	15.44
4.968	6	2 0 0	17.84
3.515	6	2 2 0	25.32
2.998	100	3 1 1	29.78
2.870	25	2 2 2	31.14
2.486	8	4 0 0	36.10
2.281	14	3 3 1	39.48
2.223	3	4 2 0	40.54
2.030	2	4 2 2	44.60
1.913	35	5 1 1+	47.48
1.758	95	4 4 0	51.98
1.681	5	5 3 1	54.56
1.657	1	4 4 2+	55.40
1.572	1	6 2 0	58.68
1.516	9	5 3 3	61.06
1.499	5	6 2 2	61.84
1.435	2	4 4 4	64.92
1.392	3	7 1 1+	67.18
1.329	1	6 4 2	70.86
1.2947	13	7 3 1+	73.02
1.2429	11	8 0 0	76.60
1.2149	2	7 3 3	78.70
1.1483	7	7 5 1+	84.26
1.1406	2	6 6 2	84.96
1.1117	1	8 4 0	87.72
1.0915	2	7 5 3	89.78
1.0425	5	9 3 1	95.28
1.0148	20	8 4 4	98.76
.9994	2	7 7 1+	100.84
.9614	6	9 5 1+	106.50
.9569	2	10 2 2+	107.22
.8966	2	11 1 1+	118.44
.8789	8	8 8 0	122.42
.8688	2	11 3 1+	124.90
.8435	3	9 7 3+	131.92
.8404	2	10 6 2	132.86
.8286	1	8 8 4+	136.74
.8202	1	11 5 1+	139.84
.7987	5	9 7 5+	149.34
.7861	17	12 4 0	156.96

Cobalt iron sulfide, Co_8FeS_8- (continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.741	25	1	1	1	15.42
4.972	5	2	0	0	17.83
3.516	5	2	2	0	25.31
2.998	90	3	1	1	29.77
2.871	20	2	2	2	31.13
2.486	7	4	0	0	36.10
2.281	14	3	3	1	39.47
2.224	3	4	2	0	40.54
2.030	2	4	2	2	44.60
1.914	30	5	1	1	47.47
1.914	6	3	3	3	47.47
1.758	100	4	4	0	51.98
1.681	5	5	3	1	54.55
1.657	1	4	4	2	55.39
1.572	1	6	2	0	58.67
1.516	10	5	3	3	61.06
1.499	6	6	2	2	61.84
1.435	2	4	4	4	64.92
1.392	2	7	1	1	67.17
1.329	1	6	4	2	70.86
1.2946	8	7	3	1	73.03
1.2946	6	5	5	3	73.03
1.2430	13	8	0	0	76.59
1.2149	2	7	3	3	78.70
1.1482	7	7	5	1	84.27
1.1482	2	5	5	5	84.27
1.1407	2	6	6	2	84.96
1.1118	2	8	4	0	87.71
1.0915	2	7	5	3	89.78
1.0424	6	9	3	1	95.29
1.0149	30	8	4	4	98.75
.9994	1	7	7	1	100.84
.9613	1	7	7	3	106.51
.9613	6	9	5	1	106.51
.9569	2	10	2	2	107.23
.8966	2	11	1	1	118.43
.8966	2	7	7	5	118.43
.8789	13	8	8	0	122.42
.8688	2	11	3	1	124.90
.8688	1	9	7	1	124.90
.8434	4	9	7	3	131.93
.8434	1	11	3	3	131.93
.8404	3	10	6	2	132.86
.8287	1	8	8	4	136.73
.8202	2	11	5	1	139.83
.8202	1	7	7	7	139.83
.7987	8	9	7	5	149.34
.7987	5	11	5	3	149.34
.7861	50	12	4	0	156.96

Cobalt iron vanadium, $Co_{4.35}Fe_{13.47}V_{12.18}$

Structure
Tetragonal, $P4_2/mnm(136)$, Z = 1, σ-phase, isostructural with σ-(Cr,Fe), from powder data [Stüwe, 1959]. Much work has been done on the σ-phase structure which has multiple atoms in 5 sites, called A through E [Bergman and Shoemaker, 1954]. The ordering arrangement of the atoms is dependent on a complex combination of electronic and size factors [Spooner, 1968].

Atom positions
The positions used were those for σ-(Cr,Fe) [Spooner and Wilson, 1964]. Site occupancy shared by multiple atoms was assumed to be random and in the following proportions:

Site A:	2(a)	0.49 cobalt and 1.51 iron
Site B:	4(f)	4.0 vanadium
Site C:	8(i)	7.0 vanadium, 0.24 cobalt, and 0.76 iron
Site D:	8(i)	1.95 cobalt and 6.05 iron
Site E:	8(j)	1.66 cobalt, 5.16 iron, and 1.18 vanadium

Lattice constants [Stüwe, 1959]
a = 8.884 A
c = 4.600

Volume
363.1 $Å^3$

Density
(calculated) 7.45 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Fe^0, V^0 [Cromer and Mann, 1968].

Scale factor (integrated intensities)
$\gamma = 0.136 \times 10^{-3}$

References
Bergman, G. and Shoemaker, D.P.(1954). Acta Crystallogr. 7, 857.
Cromer, D.T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Spooner, F. J. (1968). Acta Crystallogr. A24, 605.
Spooner, F. J. and Wilson, C. G. (1964). Acta Crystallogr. 17, 1533.
Stüwe, H. P. (1959). Trans. AIME 215, 408.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.085	8	1 0 1	21.74
3.711	2	1 1 1	23.96
2.398	4	3 1 1	37.48
2.300	20	0 0 2	39.14
2.154	100	4 1 0	41.90
2.094	40	3 3 0	43.16
2.042	35	2 0 2	44.32
1.990	70	2 1 2	45.54
1.951	95	4 1 1	46.50
1.906	50	3 3 1	47.68
1.855	13	2 2 2	49.06
1.780	15	3 1 2	51.30
1.681	4	3 2 2	54.54
1.658	4	4 3 1	55.38
1.630	4	5 1 1	56.42
1.598	1	4 0 2	57.64
1.553	1	5 2 1	59.48
1.406	2	4 3 2	66.44
1.389	2	5 1 2	67.38
1.341	4	5 2 2	70.14
1.2703	12	5 3 2	74.66
1.2565	5	5 5 0	75.62
1.2492	14	4 1 3	76.14
1.2459	11	6 0 2	76.38
1.2371	8	3 3 3	77.02
1.2331	7	6 1 2	77.32
1.2203	11	7 2 0	78.28
1.2120	6	5 5 1	78.92
1.1989	4	6 2 2	79.96
1.1880	4	5 4 2	80.84
1.1796	7	7 2 1	81.54
1.1609	1	4 3 3	83.14
1.1501	7	0 0 4	84.10
1.0774	7	8 2 0	91.28
1.0490	3	8 2 1	94.50
1.0470	4	6 6 0	94.74
1.0210	2	6 6 1	97.96
1.0145	9	4 1 4	98.80
1.0081	4	3 3 4	99.66
1.0000	3	8 0 2	100.76
.9939	7	7 4 2	101.62
.9757	2	8 2 2	104.28
.9719	3	5 5 3	104.86
.9548	3	7 2 3	107.56
.9431	1	7 6 1+	109.52
.8887	2	7 6 2+	120.16
.8816	2	8 2 3	121.80
.8674	2	9 3 2	125.26
.8647	2	6 6 3	125.96
.8483	3	5 5 4	130.48

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.8461	5	4 1 5	131.12
.8423	2	3 3 5	132.28
.8398	3	9 4 2	133.04
.8369	7	7 2 4	133.96
.8337	1	8 4 3	135.02
.8288	2	8 6 2+	136.70
.8252	2	10 1 2	137.98
.8214	2	9 6 0	139.38

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.085	7	1 0 1	21.74
3.711	2	1 1 1	23.96
2.398	4	3 1 1	37.48
2.300	20	0 0 2	39.13
2.160	2	1 1 2	41.79
2.155	100	4 1 0	41.89
2.094	45	3 3 0	43.17
2.042	35	2 0 2	44.31
1.991	75	2 1 2	45.53
1.987	1	4 2 0	45.63
1.951	100	4 1 1	46.50
1.906	50	3 3 1	47.68
1.856	13	2 2 2	49.05
1.780	15	3 1 2	51.29
1.681	4	3 2 2	54.53
1.658	4	4 3 1	55.38
1.629	4	5 1 1	56.43
1.598	1	4 0 2	57.65
1.553	1	5 2 1	59.47
1.406	2	4 3 2	66.43
1.389	2	5 1 2	67.37
1.344	1	6 2 1	69.97
1.341	4	5 2 2	70.14
1.2702	14	5 3 2	74.66
1.2565	5	5 5 0	75.62
1.2493	16	4 1 3	76.13
1.2450	8	6 0 2	76.44
1.2371	9	3 3 3	77.02
1.2330	6	6 1 2	77.33
1.2235	1	7 0 1	78.04
1.2204	12	7 2 0	78.28
1.2121	7	5 5 1	78.92
1.1988	4	6 2 2	79.96
1.1901	1	6 4 1	80.67
1.1881	4	5 4 2	80.84

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.1796	9	7 2 1	81.54
1.1609	1	4 3 3	83.14
1.1511	1	5 1 3	84.01
1.1500	7	0 0 4	84.11
1.1477	1	6 3 2	84.31
1.0780	1	7 2 2	91.21
1.0774	8	8 2 0	91.28
1.0490	4	8 2 1	94.50
1.0470	3	6 6 0	94.73
1.0209	3	6 6 1	97.96
1.0146	11	4 1 4	98.80
1.0080	5	3 3 4	99.67
1.0001	4	8 0 2	100.75
.9938	8	7 4 2	101.63
.9757	2	8 2 2	104.28
.9719	3	5 5 3	104.86
.9709	1	8 4 1	105.00
.9549	4	7 2 3	107.55
.8888	1	9 2 2	120.15
.8888	1	7 6 2	120.15
.8815	3	8 2 3	121.81
.8674	3	9 3 2	125.27
.8647	2	6 6 3	125.96
.8483	4	5 5 4	130.47
.8461	7	4 1 5	131.12
.8423	4	3 3 5	132.28
.8398	5	9 4 2	133.05
.8369	11	7 2 4	133.96
.8368	1	10 3 1	134.01
.8337	1	8 4 3	135.03
.8288	4	8 6 2	136.70
.8288	1	10 0 2	136.70
.8252	4	10 1 2	137.97
.8214	4	9 6 0	139.38

Cobalt manganese silicide, Co_2MnSi

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy, isostructural with $AlCu_2Mn$, from powder data [Gladyshevs'kii et al., 1962].

Atom positions
8(c) 8 cobalt
4(b) 4 manganese
4(a) 4 silicon

Lattice constant
a = 5.670 Å [Gladyshevs'kii et al., 1962]

Volume
182.3 $Å^3$

Density
(calculated) 7.320 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Mn^0, Si^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.599 \times 10^{-3}$

References
Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Gladyshevs'kii, E.I., Kripyakevich, P.I., Teslyuk, M.Yu., Zarechnyuk, O. S. and Kuz'ma, Yu.B. (1962). Sov. Phys. Crystallogr. 6, 207.

Calculated Pattern (Peak Heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.274	5	1 1 1	27.22
2.834	5	2 0 0	31.54
2.004	100	2 2 0	45.20
1.710	1	3 1 1	53.56
1.636	1	2 2 2	56.16
1.417	10	4 0 0	65.84
1.268	1	4 2 0	74.82
1.157	20	4 2 2	83.44
1.002	5	4 4 0	100.44
.8965	10	6 2 0	118.46
.8184	1	4 4 4	140.52

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.274	5	1 1 1	27.22
2.835	5	2 0 0	31.53
2.005	100	2 2 0	45.20
1.710	1	3 1 1	53.56
1.637	1	2 2 2	56.15
1.418	15	4 0 0	65.83
1.268	1	4 2 0	74.83
1.157	20	4 2 2	83.45
1.002	5	4 4 0	100.44
.8965	10	6 2 0	118.46
.8184	5	4 4 4	140.52

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 2, isostructural with Ni_3Sn. The structure was determined by Alte da Veiga [1965].

Atom positions
6(h) 6 cobalt
2(c) 2 molybdenum

Lattice constants
a = 5.125 A
c = 4.113
(published values: a = 5.1245 [±.0015] and c = 4.1125 [±.0020]) [Alte da Veiga, 1965].

c/a = 0.8025

Volume
93.56 $Å^3$

Density
(calculated) 9.682 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^{2+}, Mo^{+} [Forsyth and Wells, 1959]; corrected for dispersion using Δf' values from Dauben and Templeton [1955].

Scale factors (integrated intensities)
$\gamma = 0.468 \times 10^{-3}$
I/I_c (calculated) = 7.6

References
Alte da Veiga, L.H. (1965). Acta Crystallogr. 18, 857.
Dauben, C. H., and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
Forsyth, J.B. and Wells, M. (1959). Acta Crystallogr. 12, 412.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.436	3	1 0 0	20.00
3.016	12	1 0 1	29.60
2.562	4	1 1 0	35.00
2.219	27	2 0 0	40.62
2.056	27	0 0 2	44.00
1.953	100	2 0 1	46.46
1.677	1	2 1 0	54.68
1.604	2	1 1 2	57.40
1.553	2	2 1 1	59.46
1.508	11	2 0 2	61.42
1.310	1	1 0 3	72.04
1.300	1	2 1 2	72.68
1.281	11	2 2 0	73.92
1.179	1	3 1 1	81.56
1.166	11	2 0 3	82.66
1.109	1	4 0 0	87.94
1.087	11	2 2 2	90.20
1.071	7	4 0 1	91.96
1.028	1	0 0 4	97.04
.988	1	3 2 1	102.40
.976	2	4 0 2	104.16
.933	2	2 0 4	111.30
.876	1	4 1 2+	123.06
.863	4	4 0 3	126.52
.8388	1	4 2 0	133.38
.8218	7	4 2 1	139.20
.8174	1	3 2 3	140.90
.8019	5	2 2 4	147.70

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.438	3	1 0 0	19.99
3.017	11	1 0 1	29.59
2.563	4	1 1 0	34.99
2.219	26	2 0 0	40.62
2.056	27	0 0 2	44.00
1.953	100	2 0 1	46.46
1.678	1	2 1 0	54.67
1.604	2	1 1 2	57.41
1.553	2	2 1 1	59.46
1.508	12	2 0 2	61.42
1.310	1	1 0 3	72.04
1.300	1	2 1 2	72.68
1.281	12	2 2 0	73.91
1.201	1	3 0 2	79.79
1.179	1	3 1 1	81.56
1.166	12	2 0 3	82.66
1.110	2	4 0 0	87.93
1.087	12	2 2 2	90.20
1.071	9	4 0 1	91.95
1.028	2	0 0 4	97.03
.988	1	3 2 1	102.40
.977	2	4 0 2	104.15
.933	2	2 0 4	111.31
.916	1	3 1 3	114.49
.876	1	4 1 2	123.07
.863	6	4 0 3	126.53
.8388	2	4 2 0	133.38
.8219	15	4 2 1	139.19
.8174	1	3 2 3	140.89
.8019	12	2 2 4	147.71

Structure
Orthorhombic, Pnma (62), Z = 4, isostructural with MnP. The structure was refined by Rundqvist [1962].

Atom positions
All atoms were located in positions 4(c).

Lattice constants
a = 5.077 A
b = 3.281
c = 5.587
[Rundqvist, 1962].

CD cell: a = 5.077, b = 5.587, c = 3.281, space group Pnam, a/b = 0.9087, c/b = 0.5873.

Volume
93.07 $Å^3$

Density
(calculated) 6.417 g/cm^3

Thermal parameters
Isotropic: overall B = 0.29

Scattering factors
Co^0, P^0 [International Tables, 1962]. The cobalt factors were corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.158 \times 10^{-3}$
I/I_c (calculated) = 2.28

References
Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 210.
Rundqvist, S. (1962). Acta Chem. Scand. 16, 287.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.757	7	1 0 1	23.66
2.829	68	0 1 1	31.60
2.793	20	0 0 2	32.02
2.538	18	2 0 0	35.34
2.472	41	1 1 1	36.32
2.447	20	1 0 2	36.70
2.311	2	2 0 1	38.94
2.008	7	2 1 0	45.12
1.962	51	1 1 2	46.24
1.889	100	2 1 1	48.12
1.879	46	2 0 2	48.40
1.748	19	1 0 3	52.28
1.640	26	0 2 0	56.02
1.631	4	2 1 2	56.38
1.620	38	0 1 3+	56.80
1.502	3	2 0 3	61.72
1.452	1	3 1 1	64.06
1.415	3	0 2 2	65.98
1.378	3	2 2 0	67.98
1.363	5	1 2 2	68.84
1.347	2	1 0 4	69.78
1.338	1	2 2 1	70.32
1.269	4	4 0 0	74.74
1.253	5	3 0 3	75.90
1.246	9	1 1 4	76.38
1.236	14	2 2 2	77.12
1.224	2	2 0 4	78.02
1.196	8	1 2 3	80.16
1.184	2	4 1 0	81.20
1.158	9	4 1 1	83.40
1.155	8	4 0 2	83.64
1.153	9	3 2 1	83.88
1.108	2	2 2 3	88.12
1.091	6	1 0 5	89.80
1.073	2	0 3 1	91.72
1.050	2	1 3 1	94.38
1.049	2	4 0 3	94.52
1.041	2	1 2 4	95.46
1.036	2	1 1 5	96.12
1.023	15	3 1 4	97.64
1.004	4	4 2 0	100.22
.999	6	1 3 2+	100.96
.996	6	3 2 3	101.38
.989	9	2 3 1	102.38
.981	2	2 2 4	103.50
.945	4	4 2 2	109.24
.943	5	0 3 3	109.54
.932	1	3 0 5	111.40
.916	7	5 1 2	114.42
.909	8	1 2 5	115.94
.892	2	5 0 3	119.54
.884	3	4 2 3	121.32
.882	5	1 1 6	121.66
.874	2	2 0 6	123.56
.8490	3	1 3 4	130.28
.8462	3	6 0 0	131.10
.8447	1	2 1 6	131.54
.8285	1	4 3 0	136.78
.8202	4	0 4 0	139.82
.8195	5	4 3 1+	140.08
.8107	4	6 1 1+	143.68
.8098	2	6 0 2+	144.04
.7967	1	5 1 4	150.40
.7943	1	4 3 2	151.74
.7917	4	3 1 6	153.28

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
3.757	6	1	0	1	23.66
2.829	62	0	1	1	31.60
2.794	17	0	0	2	32.01
2.539	17	2	0	0	35.33
2.471	38	1	1	1	36.32
2.447	18	1	0	2	36.69
2.311	2	2	0	1	38.94
2.008	7	2	1	0	45.12
1.962	52	1	1	2	46.24
1.889	100	2	1	1	48.12
1.879	38	2	0	2	48.41
1.748	20	1	0	3	52.28
1.640	28	0	2	0	56.01
1.630	2	2	1	2	56.39
1.620	12	3	0	1	56.80
1.620	28	0	1	3	56.80
1.502	2	2	0	3	61.73
1.452	2	3	1	1	64.06
1.415	3	0	2	2	65.99
1.378	4	2	2	0	67.98
1.363	5	1	2	2	68.84
1.347	3	1	0	4	69.78
1.338	1	2	2	1	70.31
1.269	5	4	0	0	74.73
1.252	5	3	0	3	75.91
1.246	9	1	1	4	76.38
1.238	1	4	0	1	76.98
1.236	16	2	2	2	77.13
1.224	2	2	0	4	78.02
1.196	9	1	2	3	80.16
1.184	2	4	1	0	81.19
1.158	10	4	1	1	83.39
1.156	4	4	0	2	83.61
1.153	8	3	2	1	83.88
1.108	2	2	2	3	88.12
1.091	7	1	0	5	89.80
1.090	1	4	1	2	89.94
1.073	2	0	3	1	91.73
1.058	1	0	1	5	93.48
1.050	2	1	3	1	94.37
1.049	2	4	0	3	94.52
1.041	2	1	2	4	95.47
1.036	2	1	1	5	96.13
1.023	18	3	1	4	97.64
1.004	1	2	3	0	100.16
1.004	5	4	2	0	100.23
.999	3	4	1	3	100.90
.999	5	1	3	2	100.97
.995	5	3	2	3	101.39
.989	11	2	3	1	102.38

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.988	1	4	2	1	102.45
.981	2	2	2	4	103.50
.945	4	4	2	2	109.25
.943	6	0	3	3	109.53
.932	1	3	0	5	111.40
.916	10	5	1	2	114.41
.909	11	1	2	5	115.94
.891	3	5	0	3	119.55
.884	3	4	2	3	121.32
.882	7	1	1	6	121.66
.874	3	2	0	6	123.56
.8490	5	1	3	4	130.28
.8462	4	6	0	0	131.10
.8447	2	2	1	6	131.53
.8285	2	4	3	0	136.79
.8202	7	0	4	0	139.80
.8196	8	4	3	1	140.07
.8194	2	6	1	0	140.15
.8107	6	6	1	1	143.68
.8107	3	3	2	5	143.68
.8098	2	6	0	2	144.05
.7967	2	5	1	4	150.40
.7943	2	4	3	2	151.75
.7917	11	3	1	6	153.28
.7885	2	1	0	7	155.36
.7870	2	0	4	2	156.33
.7862	1	6	1	2	156.89
.7833	13	5	2	3	159.09

Cobalt phosphide, CoP_3

Structure
Cubic, Im3 (204), Z = 8, isostructural with $CoAs_3$, from powder data [Rundqvist and Ersson, 1968]. Munson and Kasper [1968] reported a high pressure phase deficient in cobalt, with a similar cell.

Atom positions [Rundqvist and Ersson, 1968]
8(c) 8 cobalt
24(g) 24 phosphorus

Lattice constant
a = 7.7078 A
(published value, 7.7073 Å [Rundqvist and Ersson, 1968]).

Volume
457.92 $Å^3$

Density
(calculated) 4.404 g/cm^3

Thermal parameters
Isotropic [Rundqvist and Ersson, 1968].

Scattering factors
Co^0, P^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.196 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Munson, R. A. and Kasper, J. S.(1968). Inorg. Chem. 7, 390.
Rundqvist, S. and Ersson, N. (1968). Ark. Kemi 30, 103.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.447	25	1 1 0	16.26
3.8538	100	2 0 0	23.06
3.1467	15	2 1 1	28.34
2.7250	65	2 2 0	32.84
2.4365	100	0 1 3	36.86
2.2245	30	2 2 2	40.52
2.0598	25	1 2 3	43.92
1.9271	8	4 0 0	47.12
1.8166	6	3 3 0+	50.18
1.7233	90	4 2 0+	53.10
1.6435	6	3 3 2	55.90
1.5735	50	4 2 2	58.62
1.5115	25	4 3 1+	61.28
1.3624	2	4 4 0	68.86
1.3220	7	4 3 3+	71.28
1.2847	2	4 4 2	73.68
1.2188	13	0 2 6+	78.40
1.1892	1	1 4 5+	80.74
1.1620	11	6 2 2	83.04
1.1365	7	1 3 6	85.34
1.1125	10	4 4 4	87.64
1.0901	2	3 4 5+	89.92
1.0689	11	6 4 0+	92.22
1.0488	3	6 3 3+	94.52
1.0299	5	2 4 6+	96.82
1.0121	6	7 3 0	99.12
.9789	4	2 3 7+	103.80
.9635	4	8 0 0	106.16
.9488	1	1 4 7+	108.56
.9347	11	6 4 4+	111.00
.9213	1	3 5 6+	113.46
.9084	12	6 6 0+	115.98
.8960	11	7 4 3+	118.56
.8842	3	6 6 2	121.20
.8618	1	8 4 0+	126.72
.8512	2	0 1 9+	129.64
.8410	7	2 4 8+	132.68
.8311	1	7 6 1+	135.88
.8216	1	6 6 4	139.28
.8125	1	4 5 7+	142.92
.7950	6	3 6 7+	151.36
.7867	4	8 4 4	156.58

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.450	20	1	1	0	16.25
3.8539	100	2	0	0	23.06
3.1467	16	2	1	1	28.34
2.7251	70	2	2	0	32.84
2.4374	18	3	1	0	36.85
2.4374	95	0	1	3	36.85
2.2251	35	2	2	2	40.51
2.0600	25	1	2	3	43.92
1.9270	10	4	0	0	47.13
1.8167	5	3	3	0	50.17
1.8167	2	4	1	1	50.17
1.7235	60	4	2	0	53.09
1.7235	50	0	2	4	53.09
1.6433	7	3	3	2	55.91
1.5733	60	4	2	2	58.63
1.5116	25	4	3	1	61.27
1.5116	2	5	1	0	61.27
1.5116	2	0	1	5	61.27
1.5116	5	1	3	4	61.27
1.3626	3	4	4	0	68.85
1.3219	2	5	3	0	71.29
1.3219	5	4	3	3	71.29
1.3219	3	0	3	5	71.29
1.2846	3	4	4	2	73.69
1.2187	8	6	2	0	78.40
1.2187	9	0	2	6	78.40
1.1893	1	1	4	5	80.73
1.1620	15	6	2	2	83.04
1.1365	1	6	3	1	85.35
1.1365	8	1	3	6	85.35
1.1125	13	4	4	4	87.64
1.0900	1	5	4	3	89.93
1.0900	1	0	1	7	89.93
1.0900	1	3	4	5	89.93
1.0689	8	6	4	0	92.22
1.0689	7	0	4	6	92.22
1.0489	2	6	3	3	94.51
1.0489	1	1	2	7	94.51
1.0300	2	6	4	2	96.81
1.0300	4	2	4	6	96.81
1.0121	8	7	3	0	99.12
1.0121	1	0	3	7	99.12
.9789	4	2	3	7	103.80
.9635	6	8	0	0	106.16
.9488	1	1	4	7	108.56
.9347	2	8	2	0	111.00
.9347	4	0	2	8	111.00
.9347	10	6	4	4	111.00
.9213	2	3	5	6	113.47
.9084	14	6	6	0	115.99

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.9084	5	8	2	2	115.99
.8960	1	0	5	7	118.56
.8960	1	7	5	0	118.56
.8960	2	1	3	8	118.56
.8960	11	7	4	3	118.56
.8960	1	3	4	7	118.56
.8841	5	6	6	2	121.21
.8618	2	8	4	0	126.73
.8512	2	0	1	9	129.64
.8410	8	8	4	2	132.68
.8410	8	2	4	8	132.68
.8312	1	7	6	1	135.88
.8312	1	1	2	9	135.88
.8217	3	6	6	4	139.27
.8125	1	7	5	4	142.92
.8125	2	4	5	7	142.92
.7950	2	9	3	2	151.36
.7950	16	3	6	7	151.36
.7867	12	8	4	4	156.58

Cobalt plutonium, $CoPu_2$

Structure
Hexagonal, $P\bar{6}2m$ (189), Z = 3, cobalt-rich end member, isostructural with Fe_2P, from powder data [Ellinger, 1961].

Atom positions
The positions were assigned by comparisons of cell edge and atomic radii ratios; the positions for Ni_6Si_2P [Rundqvist and Jellinek, 1959] were preferred to those for Fe_2P, for this cobalt-rich end member.

3(f)	3 pluto ium	2(c)	2 cobalt
3(g)	3 plutonium	1(b)	1 cobalt

Lattice constants [Ellinger, 1961]
a = 7.763 A
c = 3.648

Volume
190.4 A^3

Density
(calculated) 14.21 g/cm^3

Thermal parameters
Isotropic: plutonium, B = 0.4
cobalt, B = 0.52, the value for nickel, used by Rundqvist and Jellinek [1959].

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

Scale factor (integrated intensities)
$\gamma = 0.707 \times 10^{-3}$

References

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

Ellinger, F. H. (1961). The Metal Plutonium. World Metallurgical Congress, 1957 (Univ. of Chicago Press, Chicago) p. 288.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, England) pp. 204, 212.

Rundqvist, S. and Jellinek, F. (1959). Acta Chem. Scand. 13, 425.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
6.72	7	1 0 0	13.16
3.880	16	1 1 0	22.90
3.361	1	2 0 0	26.50
3.207	9	1 0 1	27.80
2.657	100	1 1 1	33.70
2.541	60	2 1 0	35.30
2.472	40	2 0 1	36.32
2.240	20	3 0 0	40.22
2.085	15	2 1 1	43.36
1.940	3	2 2 0	46.78
1.910	1	3 0 1	47.58
1.865	6	3 1 0	48.80
1.824	12	0 0 2	49.96
1.713	2	2 2 1	53.44
1.681	3	4 0 0	54.56
1.660	15	3 1 1	55.28
1.651	3	1 1 2	55.62
1.542	4	3 2 0	59.92
1.526	8	4 0 1	60.62
1.482	17	2 1 2	62.64
1.467	2	4 1 0	63.34
1.420	16	3 2 1	65.68
1.415	10	3 0 2	65.98
1.361	5	4 1 1	68.94
1.345	4	5 0 0	69.90
1.329	2	2 2 2	70.84
1.304	3	3 1 2	72.42
1.294	2	3 3 0	73.08
1.271	4	4 2 0	74.64
1.262	2	5 0 1	75.26
1.236	2	4 0 2	77.10
1.219	1	3 3 1	78.36
1.207	2	5 1 0	79.28
1.200	4	4 2 1	79.88
1.178	3	3 2 2	81.70
1.160	5	1 1 3	83.18
1.146	2	5 1 1	84.44
1.143	4	2 0 3+	84.70
1.097	1	2 1 3	89.22
1.082	4	5 0 2	90.76
1.076	1	5 2 0	91.38
1.058	1	4 3 1	93.48
1.055	3	3 3 2	93.76
1.042	4	4 2 2	95.28
1.032	3	5 2 1	96.50
1.025	1	6 1 0	97.42
1.018	3	3 1 3	98.28
1.007	3	5 1 2	99.82
.987	8	6 1 1	102.60
.985	5	4 0 3	102.96

Calculated Pattern (Peak heights)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.970	1	4	4	0	105.08
.960	2	5	3	0	106.66
.955	5	3	2	3	107.54
.945	1	4	3	2	109.16
.938	4	4	4	1	110.46
.936	2	4	1	3	110.74
.929	1	5	3	1	112.08
.927	2	5	2	2	112.38
.912	1	0	0	4	115.26
.903	1	6	2	1	117.04
.902	1	5	0	3	117.32
.894	2	6	1	2	119.06
.891	1	7	1	0	119.76

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
6.72	6	1	0	0	13.16
3.882	15	1	1	0	22.89
3.361	1	2	0	0	26.49
3.206	9	1	0	1	27.80
2.658	100	1	1	1	33.69
2.541	60	2	1	0	35.29
2.472	40	2	0	1	36.31
2.241	25	3	0	0	40.21
2.085	16	2	1	1	43.36
1.941	3	2	2	0	46.77
1.909	1	3	0	1	47.58
1.865	7	3	1	0	48.80
1.824	14	0	0	2	49.96
1.713	3	2	2	1	53.43
1.681	3	4	0	0	54.56
1.660	17	3	1	1	55.28
1.651	3	1	1	2	55.63
1.542	5	3	2	0	59.92
1.527	10	4	0	1	60.61
1.482	20	2	1	2	62.64
1.467	1	4	1	0	63.34
1.421	19	3	2	1	65.67
1.415	9	3	0	2	65.98
1.361	6	4	1	1	68.93
1.345	5	5	0	0	69.90
1.329	2	2	2	2	70.84
1.304	4	3	1	2	72.42
1.294	2	3	3	0	73.08
1.271	5	4	2	0	74.64
1.262	2	5	0	1	75.26

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.236	2	4	0	2	77.10
1.219	1	3	3	1	78.35
1.207	3	5	1	0	79.28
1.200	4	4	2	1	79.88
1.178	4	3	2	2	81.70
1.160	6	1	1	3	83.18
1.146	2	5	1	1	84.44
1.143	3	2	0	3	84.70
1.143	1	4	1	2	84.73
1.105	1	4	3	0	88.37
1.097	2	2	1	3	89.22
1.082	5	5	0	2	90.75
1.077	2	5	2	0	91.37
1.058	1	4	3	1	93.48
1.055	3	3	3	2	93.76
1.043	5	4	2	2	95.27
1.033	4	5	2	1	96.50
1.025	2	6	1	0	97.41
1.019	4	3	1	3	98.27
1.007	4	5	1	2	99.82
.987	10	6	1	1	102.60
.985	3	4	0	3	102.87
.970	1	4	4	0	105.09
.960	2	5	3	0	106.65
.955	6	3	2	3	107.54
.945	1	4	3	2	109.16
.938	5	4	4	1	110.45
.936	2	4	1	3	110.73
.929	1	5	3	1	112.07
.927	3	5	2	2	112.38
.912	2	0	0	4	115.26
.903	2	6	2	1	117.03
.902	1	5	0	3	117.32
.894	3	6	1	2	119.06
.890	1	7	1	0	119.77

Cobalt plutonium, $CoPu_6$

Structure
Tetragonal, I4/mcm (140), Z = 4, isostructural with MnU_6, from powder data [Ellinger, 1961].

Atom positions
The positions and distributions of MnU_6 were used [Baenziger et al., 1950]

Lattice constants
[Poole et al., 1961, Table 6.1]
a = 10.476 A
c = 5.340
(published values: a = 10.475, c = 5.340 Å)

Volume
586.1 $Å^3$

Density
(calculated) 17.12 g/cm^3

Thermal parameters
Isotropic: cobalt, B = 1.0; plutonium, B = 0.75

Scattering factors
Co^0, Pu^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 2.67 \times 10^{-3}$

References

Baenziger, N. C., Rundle, R. E., Snow, A. I., and Wilson, A. S. (1950). Acta Crystallogr. 3, 34.

Ellinger, F. H. (1961). The Metal Plutonium. World Metallurgical Conference, 1957, (Univ. of Chicago Press, Chicago) p. 288

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Poole, D.M., Bale, M. G., Mardon, P. G., Marples, J. A. C., and Nichols, J. C. (1961). Plutonium 1960. International Conference on Plutonium Metallurgy, (2nd) Cleaver Hume Press, London). p. 276.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
7.41	4	1 1 0	11.94
3.70	1	2 2 0	24.02
3.52	2	2 1 1	25.28
3.31	2	3 1 0	26.90
2.670	30	0 0 2	33.54
2.618	5	4 0 0	34.22
2.552	100	3 2 1	35.14
2.512	4	1 1 2	35.72
2.469	2	3 3 0	36.36
2.378	1	2 0 2	37.80
2.342	6	4 2 0	38.40
2.294	6	4 1 1	39.24
2.166	2	2 2 2	41.66
2.079	4	3 1 2	43.50
2.055	12	5 1 0	44.04
1.951	2	4 3 1	46.52
1.870	5	4 0 2	48.66
1.761	2	4 2 2	51.88
1.746	5	6 0 0	52.36
1.639	6	6 1 1	56.06
1.628	7	5 1 2	56.48
1.518	17	3 2 3	61.00
1.481	6	5 5 0	62.66
1.461	7	6 0 2	63.62
1.458	5	4 1 3	63.80
1.389	4	7 2 1	67.34
1.335	3	0 0 4	70.48
1.295	9	5 5 2	72.98
1.238	2	6 1 3	76.98
1.235	2	6 6 0	77.20
1.195	11	8 3 1	80.28
1.160	1	4 2 4	83.24
1.119	4	5 1 4+	86.98
1.111	1	7 6 1+	87.76
1.061	2	6 0 4	93.16
1.048	2	10 0 0	94.66
1.021	1	9 3 2	98.02
1.010	7	8 3 3	99.44
1.002	4	3 2 5	100.42
.992	3	5 5 4	101.92
.975	3	10 0 2	104.34
.969	3	8 7 1	105.28
.958	1	7 6 3+	107.08

Cobalt plutonium, $CoPu_6$ - (continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
7.41	3	1	1	0	11.94
3.70	1	2	2	0	24.01
3.52	2	2	1	1	25.27
3.31	2	3	1	0	26.89
2.670	25	0	0	2	33.54
2.619	4	4	0	0	34.21
2.552	100	3	2	1	35.13
2.512	2	1	1	2	35.72
2.469	2	3	3	0	36.35
2.379	1	2	0	2	37.79
2.343	6	4	2	0	38.40
2.294	6	4	1	1	39.24
2.166	2	2	2	2	41.67
2.079	4	3	1	2	43.50
2.055	13	5	1	0	44.04
1.950	2	4	3	1	46.52
1.870	5	4	0	2	48.66
1.761	2	4	2	2	51.88
1.746	6	6	0	0	52.36
1.639	6	6	1	1	56.06
1.628	8	5	1	2	56.47
1.522	1	4	4	2	60.82
1.518	19	3	2	3	61.00
1.482	7	5	5	0	62.66
1.461	8	6	0	2	63.62
1.458	1	4	1	3	63.79
1.389	5	7	2	1	67.34
1.335	3	0	0	4	70.48
1.295	10	5	5	2	72.97
1.238	2	6	1	3	76.98
1.235	1	6	6	0	77.21
1.195	13	8	3	1	80.27
1.160	1	4	2	4	83.23
1.121	1	6	6	2	86.85
1.119	3	5	1	4	86.96
1.119	2	7	2	3	87.00
1.061	2	6	0	4	93.16
1.048	2	10	0	0	94.66
1.020	1	9	3	2	98.03
1.010	8	8	3	3	99.43
1.002	5	3	2	5	100.43
.992	4	5	5	4	101.92
.975	3	10	0	2	104.35
.969	4	8	7	1	105.28

Cobalt plutonium, Co_2Pu

Structure
Cubic, Fd3m (227), Z = 8, isostructural with Cu_2Mg, from powder data [Ellinger, 1961]. Their sample was described as plutonium-rich.

Atom positions
8(a) 8 plutonium
16(d) 16 cobalt
The origin was taken at $\bar{4}3m$.

Lattice constant
a = 7.081 A [Ellinger, 1961].

Volume
355.1 $Å^3$

Density
(calculated) 13.462 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0 [Cromer and Mann, 1968]
Pu^0 [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 1.370 \times 10^{-3}$

References
Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Ellinger, F. H. (1961). In The Metal Plutonium, (Univ. of Chicago Press, Chicago). World Metallurgical Conference, 1957 (edited by Coffinberry, A. S. and Miner, W. N.) p. 288.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.08	45	1 1 1	21.74
2.504	90	2 2 0	35.84
2.135	100	3 1 1	42.30
2.044	10	2 2 2	44.28
1.771	5	4 0 0	51.58
1.624	10	3 3 1	56.62
1.446	25	4 2 2	64.40
1.363	25	5 1 1+	68.84
1.252	15	4 4 0	75.96
1.197	5	5 3 1	80.12
1.120	10	6 2 0	86.94
1.080	5	5 3 3	91.02
1.067	1	6 2 2	92.38
1.022	1	4 4 4	97.82
.991	5	7 1 1+	101.96
.946	10	6 4 2	109.00
.922	15	7 3 1+	113.36
.885	5	8 0 0	120.98
.865	1	7 3 3	125.86
.834	5	8 2 2+	134.76

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.09	40	1 1 1	21.72
2.504	85	2 2 0	35.84
2.135	100	3 1 1	42.30
2.044	10	2 2 2	44.28
1.770	5	4 0 0	51.59
1.624	10	3 3 1	56.61
1.445	30	4 2 2	64.41
1.363	20	5 1 1	68.84
1.363	5	3 3 3	68.84
1.252	20	4 4 0	75.96
1.197	5	5 3 1	80.12
1.120	10	6 2 0	86.95
1.080	10	5 3 3	91.02
1.068	1	6 2 2	92.37
1.022	1	4 4 4	97.82
.992	1	7 1 1	101.95
.992	1	5 5 1	101.95
.946	15	6 4 2	108.99
.922	15	7 3 1	113.35
.922	5	5 5 3	113.35
.885	5	8 0 0	120.98
.865	1	7 3 3	125.86
.835	10	8 2 2	134.76
.835	5	6 6 0	134.76
.818	15	7 5 1	140.81

Cobalt plutonium, Co_3Pu

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 9, isostructural with Ni_3Pu, from powder data [Poole et al., 1961].

Atom positions
The positions assumed were those refined for Ni_3Pu [Cromer and Olsen, 1959].

Lattice constants [Poole et al., 1961]
a = 5.003 Å
c = 24.42

Volume
529.3 $Å^3$

Density
(calculated) 11.82 g/cm^3

Thermal parameters
Isotropic values were used from Cromer and Olsen [1959], with their data for nickel applied to the cobalt atoms here.

Scattering factors
Co^0, Pu^0 [International Tables, 1962], corrected for anomalous dispersion [Cromer and Olsen, 1959].

Scale factor (integrated intensities)
$\gamma = 0.369 \times 10^{-3}$

References
Cromer, D. T. and Olsen, C. E. (1959). Acta Crystallogr. 12, 689.
International Tables for X-ray Crystallography, III, (The Kynoch Press, Birmingham, England), pp. 202,204.
Poole, D. M., Bale, M. G., Marden, P. G., Marples, J. A. C., and Nichols, J. L. (1961). In Plutonium, 1960 (Cleaver Hume Press, London). International Conference on Plutonium Metallurgy, (2nd). Edited by Grison, E., Lord, W. B. H., and Fowler, R. D., p. 267.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
8.14	8	0 0 3	10.86
4.26	35	1 0 1	20.82
4.07	14	0 0 6	21.82
3.531	5	1 0 4	25.20
3.241	2	0 1 5	27.50
2.717	65	1 0 7	32.94
2.501	80	1 1 0	35.88
2.495	85	0 1 8	35.96
2.391	2	1 1 3	37.58
2.157	35	0 2 1	41.84
2.131	100	1 1 6	42.38
2.041	10	0 2 4	44.34
2.035	13	0 0 12	44.48
1.975	14	0 1 11+	45.90
1.839	6	1 1 9+	49.52
1.767	4	2 0 8	51.70
1.723	2	1 0 13	53.10
1.634	4	2 1 1	56.26
1.628	5	0 0 15	56.48
1.618	10	0 1 14	56.86
1.581	1	2 1 4	58.30
1.578	2	1 1 12	58.42
1.482	15	2 1 7	62.62
1.444	17	1 2 8+	64.50
1.419	7	0 2 13	65.74
1.364	12	1 1 15	68.74
1.361	25	3 0 6+	68.94
1.359	18	2 0 14	69.08
1.318	4	1 2 11	71.54
1.2749	1	0 3 9+	74.34
1.2506	13	2 2 0	76.04
1.2344	1	2 1 13	77.22
1.2001	2	1 3 1	79.86
1.1971	4	2 0 17	80.10
1.1939	8	1 2 14	80.36
1.1753	2	0 1 20	81.90
1.1630	1	0 0 21	82.96
1.1361	6	1 3 7	85.38
1.1182	4	3 1 8	87.08
1.1154	3	2 1 16	87.36
1.1053	1	0 2 19	88.36
1.0820	3	4 0 1	90.78
1.0804	5	3 0 15+	90.96
1.0754	2	1 0 22	91.50
1.0656	4	2 2 12	92.58
1.0569	2	3 1 11	93.58
1.0545	7	1 1 21	93.86
1.0208	1	0 4 8	97.98

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
8.14	7	0	0	3	10.86
4.27	30	1	0	1	20.81
4.08	2	0	1	2	21.75
4.07	12	0	0	6	21.82
3.533	4	1	0	4	25.18
3.241	2	0	1	5	27.50
2.717	65	1	0	7	32.94
2.713	3	0	0	9	32.99
2.502	70	1	1	0	35.87
2.495	45	0	1	8	35.96
2.391	2	1	1	3	37.59
2.158	40	0	2	1	41.83
2.133	8	2	0	2	42.34
2.131	100	1	1	6	42.38
2.127	4	1	0	10	42.46
2.042	9	0	2	4	44.33
2.035	10	0	0	12	44.48
1.980	8	2	0	5	45.78
1.976	11	0	1	11	45.89
1.840	2	0	2	7	49.49
1.839	5	1	1	9	49.52
1.767	4	2	0	8	51.70
1.723	2	1	0	13	53.10
1.634	4	2	1	1	56.25
1.628	4	0	0	15	56.48
1.618	11	0	1	14	56.86
1.582	1	2	1	4	58.29
1.579	1	1	1	12	58.41
1.482	18	2	1	7	62.61
1.444	11	3	0	0	64.47
1.443	14	1	2	8	64.52
1.440	1	1	0	16	64.70
1.419	8	0	2	13	65.74
1.364	12	1	1	15	68.74
1.361	10	0	3	6	68.94
1.361	10	3	0	6	68.94
1.360	1	2	1	10	68.99
1.359	12	2	0	14	69.08
1.318	5	1	2	11	71.54
1.2508	17	2	2	0	76.03
1.2344	1	2	1	13	77.22
1.2002	2	1	3	1	79.85
1.1972	3	2	0	17	80.09
1.1956	2	2	2	6	80.23
1.1939	7	1	2	14	80.36
1.1752	2	0	1	20	81.91
1.1629	2	0	0	21	82.97
1.1362	7	1	3	7	85.37
1.1359	1	2	2	9	85.40
1.1182	6	3	1	8	87.09

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.1165	1	2	1	16	87.25
1.1054	1	0	2	19	88.35
1.0821	3	4	0	1	90.77
1.0804	3	3	0	15	90.96
1.0804	3	0	3	15	90.96
1.0753	2	1	0	22	91.51
1.0665	1	4	0	4	92.48
1.0656	5	2	2	12	92.59
1.0568	2	3	1	11	93.59
1.0545	8	1	1	21	93.86
1.0208	1	0	4	8	97.98
1.0123	1	1	3	13	99.10

Cobalt plutonium, $Co_{17}Pu_2$

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 2, isostructural with $Ni_{17}Th_2$, from powder data [Ellinger, 1961]. Bouchet et al. [1966] determined positions for $Co_{17}Ho_2$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions for $Co_{17}Ho_2$ were used.

6(g)	6 cobalt(1)
12(j)	12 cobalt(2)
12(k)	12 cobalt(3)
4(f)	4 cobalt(4)
2(b)	2 plutonium(1)
2(d)	2 plutonium(2)

Lattice constants
a = 8.325 A
c = 8.104 [Ellinger, 1961]

Volume
486.4 A^3

Density
(calculated) 10.145 g/cm^3

Thermal parameters
Isotropic: cobalt B = 0.6; plutonium B = 0.5.

Scattering factors
Co^0 [International Tables, 1962]
Pu^0 [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 0.399 \times 10^{-3}$

References

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Ellinger, F. H. (1961). In The Metal Plutonium (Univ. of Chicago Press, Chicago). World Metallurgical Conference, 1957 (edited by Coffinberry, A. S. and Miner, W. N.) p. 288.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 204.

International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
7.202	1	1 0 0	12.28
5.381	16	1 0 1	16.46
4.160	19	1 1 0	21.34
4.052	8	0 0 2	21.92
3.604	2	2 0 0	24.68
3.531	6	1 0 2	25.20
3.293	12	2 0 1	27.06
2.903	60	1 1 2	30.78
2.725	2	2 1 0	32.84
2.693	7	2 0 2	33.24
2.583	13	2 1 1	34.70
2.529	11	1 0 3	35.46
2.403	45	3 0 0	37.40
2.261	6	2 1 2	39.84
2.161	25	2 0 3	41.76
2.081	55	2 2 0	43.44
2.067	100	3 0 2	43.76
2.026	25	0 0 4	44.70
1.951	2	1 0 4	46.52
1.942	1	3 1 1	46.74
1.919	14	2 1 3	47.34
1.851	4	2 2 2	49.18
1.793	1	3 1 2	50.88
1.766	3	2 0 4	51.72
1.626	4	2 1 4	56.56
1.621	7	3 2 1	56.76
1.607	3	3 1 3	57.28
1.581	3	1 0 5	58.30
1.573	4	4 1 0	58.64
1.549	10	3 0 4	59.64
1.531	3	3 2 2	60.40
1.499	2	4 0 3	61.84
1.478	1	2 0 5	62.82
1.467	15	4 1 2	63.36
1.452	15	2 2 4	64.10
1.423	1	3 1 4	65.54
1.420	2	5 0 1	65.72
1.411	7	3 2 3	66.20
1.393	5	2 1 5	67.14
1.388	6	3 3 0	67.44
1.359	1	5 0 2	69.08
1.351	1	0 0 6	69.54
1.344	1	4 2 1	69.96
1.313	15	3 3 2	71.86
1.291	1	4 2 2	73.24
1.285	6	1 1 6	73.68
1.281	5	3 2 4	73.90
1.278	3	5 1 1	74.10
1.272	3	5 0 3	74.54
1.259	1	3 1 5	75.44

Calculated Pattern (Peak heights)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.233	1	5	1	2	77.30
1.216	5	4	2	3	78.58
1.202	12	6	0	0	79.74
1.177	13	3	0	6	81.72
1.168	3	5	1	3	82.56
1.158	4	3	2	5	83.42
1.155	3	5	2	0	83.70
1.145	3	3	3	4	84.58
1.131	1	4	2	4	85.90
1.110	6	5	2	2	87.86
1.102	1	2	0	7	88.66
1.091	1	5	1	4	89.82
1.077	1	5	0	5	91.30
1.041	5	4	4	0	95.50
1.033	10	6	0	4	96.38
1.025	6	4	1	6	97.46
1.018	1	6	1	3	98.28
1.013	3	0	0	8	99.00
1.012	3	5	1	5	99.18
.992	1	6	2	1	101.84
.984	1	1	1	8	103.00
.971	1	6	2	2	105.04
.968	7	3	3	6	105.48
.962	2	5	3	3	106.34
.955	1	7	1	0	107.54
.938	4	6	2	3	110.48
.933	4	3	0	8	111.22
.929	5	7	1	2	111.94
.926	5	4	4	4	112.64
.918	1	5	3	4	114.08
.917	1	5	4	1	114.24
.911	5	2	2	8	115.50
.908	4	6	3	0	115.98
.898	1	6	0	6	118.20
.897	1	6	2	4	118.44
.894	1	1	0	9	119.10
.886	8	6	3	2	120.70
.882	2	4	2	7	121.64
.878	5	5	2	6	122.74
.873	2	5	4	3	123.74
.869	2	5	3	5	124.78

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
7.210	1	1	0	0	12.27
5.387	13	1	0	1	16.44
4.163	17	1	1	0	21.33
4.052	7	0	0	2	21.92
3.605	2	2	0	0	24.68
3.532	6	1	0	2	25.19
3.294	11	2	0	1	27.05
2.903	60	1	1	2	30.77
2.725	1	2	1	0	32.84
2.693	6	2	0	2	33.24
2.583	13	2	1	1	34.70
2.530	11	1	0	3	35.46
2.403	45	3	0	0	37.39
2.261	6	2	1	2	39.83
2.162	25	2	0	3	41.75
2.081	55	2	2	0	43.45
2.067	100	3	0	2	43.76
2.026	25	0	0	4	44.69
1.950	2	1	0	4	46.52
1.941	1	3	1	1	46.75
1.918	15	2	1	3	47.35
1.851	5	2	2	2	49.17
1.793	1	3	1	2	50.88
1.766	3	2	0	4	51.72
1.654	1	3	2	0	55.51
1.626	3	2	1	4	56.56
1.621	6	3	2	1	56.76
1.607	3	3	1	3	57.28
1.581	3	1	0	5	58.30
1.573	4	4	1	0	58.63
1.549	11	3	0	4	59.64
1.531	3	3	2	2	60.40
1.499	2	4	0	3	61.83
1.478	1	2	0	5	62.81
1.467	17	4	1	2	63.37
1.452	17	2	2	4	64.09
1.423	1	3	1	4	65.54
1.420	2	5	0	1	65.72
1.411	8	3	2	3	66.20
1.393	5	2	1	5	67.14
1.388	6	3	3	0	67.44
1.358	1	5	0	2	69.09
1.351	1	0	0	6	69.54
1.344	1	4	2	1	69.96
1.313	17	3	3	2	71.86
1.291	1	4	2	2	73.23
1.285	6	1	1	6	73.68
1.281	2	3	2	4	73.91
1.279	3	5	1	1	74.09
1.272	3	5	0	3	74.54

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.259	2	3	1	5	75.44
1.233	1	5	1	2	77.29
1.217	5	4	2	3	78.57
1.202	14	6	0	0	79.74
1.177	16	3	0	6	81.72
1.175	1	5	0	4	81.95
1.168	4	5	1	3	82.55
1.158	4	3	2	5	83.43
1.154	2	5	2	0	83.71
1.145	3	3	3	4	84.58
1.131	1	4	2	4	85.89
1.110	7	5	2	2	87.86
1.102	2	2	0	7	88.67
1.091	1	5	1	4	89.82
1.077	2	5	0	5	91.29
1.041	6	4	4	0	95.50
1.034	12	6	0	4	96.37
1.025	8	4	1	6	97.47
1.022	1	5	3	1	97.86
1.018	1	6	1	3	98.30
1.013	3	0	0	8	99.00
1.012	3	5	1	5	99.18
.998	1	5	3	2	101.01
.992	1	6	2	1	101.85
.984	1	1	1	8	103.00
.971	1	6	2	2	105.04
.968	8	3	3	6	105.48
.962	3	5	3	3	106.34
.955	2	7	1	0	107.54
.938	5	6	2	3	110.48
.933	5	3	0	8	111.22
.929	7	7	1	2	111.94
.926	7	4	4	4	112.64
.918	1	5	3	4	114.07
.917	1	5	4	1	114.25
.911	7	2	2	8	115.49
.910	1	6	1	5	115.69
.908	3	6	3	0	116.00
.898	1	6	0	6	118.19
.897	1	6	2	4	118.44
.894	1	1	0	9	119.11
.886	11	6	3	2	120.70
.882	2	4	2	7	121.65
.878	7	5	2	6	122.75
.876	1	7	2	1	123.21
.874	3	5	4	3	123.73
.869	3	5	3	5	124.78

Cobalt praseodymium, Co_2Pr

Structure
Cubic, Fd3m (227), Z = 8, isostructural with Cu_2Mg, from powder data [Harris et al., 1965].

Atom positions
8(a) 8 praseodymium
16(d) 16 cobalt

Lattice constant
a = 7.3063 A
(published value, 7.2911 kX [Harris et al., 1965]).

Volume
390.0 A^3

Density
(calculated) 8.814 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0 [Cromer and Mann, 1968]
Pr^0 [International Tables, 1974]

Scale factor (integrated intnesities)
$\gamma = 0.575 \times 10^{-3}$

References

Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.

Harris, I. R., Mansey, R. C., and Raynor, G. V. (1965). J. Less-Common Metals 9, 270.

International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 100.

Calculated Pattern (Peak heights)

d(A)	I	hkl	2θ(°) λ = 1.540598A
4.215	10	1 1 1	21.06
2.583	65	2 2 0	34.70
2.203	100	3 1 1	40.94
2.109	15	2 2 2	42.84
1.676	1	3 3 1	54.72
1.4913	15	4 2 2	62.20
1.4060	25	5 1 1+	66.44
1.2917	15	4 4 0	73.22
1.2350	1	5 3 1	77.18
1.1552	5	6 2 0	83.64
1.1141	5	5 3 3	87.48
1.1015	5	6 2 2	88.74
1.0231	1	7 1 1+	97.68
.9763	5	6 4 2	104.18
.9512	10	7 3 1+	108.16
.9133	1	8 0 0	115.00
.8610	5	8 2 2+	126.92
.8437	10	7 5 1+	131.86
.8381	1	6 6 2	133.60
.8020	1	7 5 3+	147.68

Calculated Pattern (Integrated)

d(A)	I	hkl	2θ(°) λ = 1.540598A
4.218	10	1 1 1	21.04
2.583	60	2 2 0	34.70
2.203	100	3 1 1	40.93
2.109	15	2 2 2	42.84
1.676	1	3 3 1	54.72
1.4914	20	4 2 2	62.20
1.4061	20	5 1 1	66.44
1.4061	5	3 3 3	66.44
1.2916	20	4 4 0	73.22
1.2350	1	5 3 1	77.18
1.1552	5	6 2 0	83.64
1.1142	10	5 3 3	87.47
1.1015	5	6 2 2	88.75
.9763	10	6 4 2	104.18
.9512	10	7 3 1	108.16
.9512	5	5 5 3	108.16
.9133	5	8 0 0	115.01
.8611	1	6 6 0	126.91
.8611	5	8 2 2	126.91
.8437	10	7 5 1	131.86
.8437	1	5 5 5	131.86
.8381	5	6 6 2	133.59
.8020	1	7 5 3	147.69
.8020	1	9 1 1	147.69

Cobalt rhodium sulfide, Co_8RhS_8

Structure
Cubic, Fm3m (225), Z = 4, π phase, isostructural with Co_9S_8, from powder data [Knop, 1962].

Atom positions [Pearson, 1967]
32(f) 32 cobalt 8(c) 8 sulfur
4(b) 4 rhodium 24(e) 24 sulfur

Lattice constant
a = 9.978(2) Å
(published value, a = 9.977(2) Å, [Knop, 1962])

Volume
993.4 $Å^3$

Density
(calculated) 5.555 g/cm^3

Thermal parameters
Isotropic: cobalt, B = 0.5; rhodium, B = 0.4; sulfur, B = 0.7

Scattering factors
Co^0, Rh^0, S^0 [International tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.413 \times 10^{-3}$

References

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England). pp. 202, 204, 210.

Knop, D. (1962). Chem. Ind. London, April 21, p. 739.

Pearson, W. B. (1967). Handbook of Lattice Spacings and Structures of Metals and Alloys, v.2, (Pergamon Press, N.Y.), pp. 204, 807.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.757	7	1	1	1	15.38
4.985	12	2	0	0	17.78
3.526	12	2	2	0	25.24
3.008	100	3	1	1	29.68
2.881	10	2	2	2	31.02
2.494	3	4	0	0	35.98
2.288	5	3	3	1	39.34
2.231	7	4	2	0	40.40
2.037	4	4	2	2	44.44
1.920	30	5	1	1+	47.30
1.763	75	4	4	0	51.80
1.686	1	5	3	1	54.36
1.663	2	4	4	2+	55.18
1.577	2	6	2	0	58.46
1.522	9	5	3	3	60.82
1.504	2	6	2	2	61.60
1.3334	2	6	4	2	70.58
1.2990	14	7	3	1+	72.74
1.2473	9	8	0	0	76.28
1.2190	1	7	3	3	78.38
1.2100	1	6	4	4+	79.08
1.1760	1	8	2	2+	81.84
1.1521	7	7	5	1+	83.92
1.1446	1	6	6	2	84.60
1.0886	1	8	4	2	90.08
1.0460	5	9	3	1	94.86
1.0183	18	8	4	4	98.30
.9785	1	8	6	2+	103.86
.9646	6	9	5	1+	105.98
.9601	1	10	2	2+	106.70
.9264	1	10	4	0+	112.50
.8997	3	11	1	1+	117.78
.8819	7	8	8	0	121.72
.8463	4	9	7	3+	131.06
.8433	1	10	6	2	131.96
.8093	1	10	6	4+	144.28
.8015	6	9	7	5+	147.94
.7888	14	12	4	0	155.12
.7792	1	8	8	6+	162.70

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.761	6	1	1	1	15.37
4.989	11	2	0	0	17.76
3.528	11	2	2	0	25.22
3.008	100	3	1	1	29.67
2.880	10	2	2	2	31.02
2.494	3	4	0	0	35.97
2.289	5	3	3	1	39.33
2.231	7	4	2	0	40.39
2.037	4	4	2	2	44.44
1.920	30	5	1	1	47.30
1.920	8	3	3	3	47.30
1.764	85	4	4	0	51.79
1.687	1	5	3	1	54.35
1.663	1	6	0	0	55.19
1.663	2	4	4	2	55.19
1.578	2	6	2	0	58.45
1.522	11	5	3	3	60.83
1.504	2	6	2	2	61.61
1.4402	1	4	4	4	64.67
1.3972	1	7	1	1	66.91
1.3837	1	6	4	0	67.66
1.3334	2	6	4	2	70.58
1.2990	11	7	3	1	72.74
1.2990	7	5	5	3	72.74
1.2472	11	8	0	0	76.28
1.2190	1	7	3	3	78.38
1.2100	1	6	4	4	79.08
1.1522	8	7	5	1	83.91
1.1522	2	5	5	5	83.91
1.1446	1	6	6	2	84.60
1.0887	1	8	4	2	90.07
1.0460	7	9	3	1	94.86
1.0184	25	8	4	4	98.30
.9784	1	8	6	2	103.87
.9646	6	9	5	1	105.99
.9646	2	7	7	3	105.99
.9264	1	10	4	0	112.50
.9109	1	10	4	2	115.49
.8997	2	11	1	1	117.78
.8997	2	7	7	5	117.78
.8819	11	8	8	0	121.72
.8718	1	11	3	1	124.16
.8463	2	11	3	3	131.06
.8463	5	9	7	3	131.06
.8433	1	10	6	2	131.97
.8093	2	10	6	4	144.27
.8015	7	11	5	3	147.94
.8015	9	9	7	5	147.94
.7888	45	12	4	0	155.11
.7792	2	8	8	6	162.71
.7792	2	12	4	2	162.71

Cobalt ruthenium sulfide, Co_8RuS_8

Structure
Cubic, Fm3m (225), Z = 4, π phase, isostructural with Co_9S_8, from powder data [Knop, 1962].

Atom positions [Pearson, 1967].

32(f)	32 cobalt	8(c)	8 sulfur
4(b)	4 ruthenium	24(e)	24 sulfur

Lattice constant [Knop, 1962]
a = 9.945(2)A
(published value, a = 9.944(2) Å)

Volume
983.6 $Å^3$

Density
(calculated) 5.599 g/cm^3

Thermal parameters
Isotropic: cobalt, B = 0.5; ruthenium, B = 0.4; sulfur, B = 0.7

Scattering factors
Co^0, Ru^0, S^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.409 \times 10^{-3}$

References

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England) pp. 202, 204, 210.

Knop, O. (1962). Chem. Ind. London, April 21, p. 739.

Pearson, W.B. (1967). Handbook of Lattice Spacings and Structures of Metals and Alloys, V.2, (Pergamon Press, N.Y.). pp. 204, 808.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
5.734	8	1 1 1	15.44
4.968	12	2 0 0	17.84
3.515	11	2 2 0	25.32
2.998	100	3 1 1	29.78
2.870	10	2 2 2	31.14
2.486	3	4 0 0	36.10
2.282	5	3 3 1	39.46
2.223	6	4 2 0	40.54
2.030	4	4 2 2	44.60
1.9141	30	5 1 1+	47.46
1.7578	75	4 4 0	51.98
1.6812	1	5 3 1	54.54
1.6577	2	4 4 2+	55.38
1.5726	2	6 2 0	58.66
1.5164	9	5 3 3	61.06
1.4991	2	6 2 2	61.84
1.3291	2	6 4 2	70.84
1.2947	14	7 3 1+	73.02
1.2431	9	8 0 0	76.58
1.2149	1	7 3 3	78.70
1.2059	1	6 4 4+	79.40
1.1720	1	8 2 2+	82.18
1.1483	7	7 5 1+	84.26
1.1408	1	6 6 2	84.94
1.0850	1	8 4 2	90.46
1.0425	5	9 3 1	95.28
1.0150	19	8 4 4	98.74
.9751	1	8 6 2+	104.36
.9614	6	9 5 1+	106.50
.9570	1	10 2 2+	107.20
.9233	1	10 4 0+	113.08
.8967	3	11 1 1+	118.42
.8790	7	8 8 0	122.40
.8435	4	9 7 3+	131.90
.8405	1	10 6 2	132.82
.8067	1	10 6 4+	145.46
.7988	6	9 7 5+	149.30
.7862	14	12 4 0	156.90

Cobalt ruthenium sulfide, Co_8RuS_8 - (continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.742	7	1	1	1	15.42
4.973	10	2	0	0	17.82
3.516	11	2	2	0	25.31
2.999	100	3	1	1	29.77
2.871	10	2	2	2	31.13
2.486	3	4	0	0	36.10
2.282	6	3	3	1	39.46
2.224	7	4	2	0	40.53
2.030	4	4	2	2	44.60
1.9139	30	5	1	1	47.47
1.9139	8	3	3	3	47.47
1.7580	85	4	4	0	51.97
1.6810	1	5	3	1	54.55
1.6575	1	6	0	0	55.39
1.6575	2	4	4	2	55.39
1.5724	2	6	2	0	58.66
1.5166	11	5	3	3	61.05
1.4993	2	6	2	2	61.83
1.4354	1	4	4	4	64.91
1.3926	1	7	1	1	67.17
1.3290	2	6	4	2	70.85
1.2947	11	7	3	1	73.02
1.2947	7	5	5	3	73.02
1.2431	12	8	0	0	76.58
1.2150	1	7	3	3	78.69
1.2060	1	6	4	4	79.39
1.1483	8	7	5	1	84.26
1.1483	2	5	5	5	84.26
1.1408	1	6	6	2	84.95
1.0851	1	8	4	2	90.45
1.0425	6	9	3	1	95.27
1.0150	25	8	4	4	98.74
.9752	1	8	6	2	104.35
.9614	2	7	7	3	106.49
.9614	6	9	5	1	106.49
.9234	1	10	4	0	113.07
.9079	1	10	4	2	116.10
.8967	2	11	1	1	118.42
.8967	2	7	7	5	118.42
.8790	11	8	8	0	122.40
.8689	1	11	3	1	124.88
.8435	6	9	7	3	131.90
.8435	2	11	3	3	131.90
.8405	1	10	6	2	132.83
.8066	2	10	6	4	145.47
.7988	9	9	7	5	149.30
.7988	7	11	5	3	149.30
.7862	47	12	4	0	156.90

Cobalt tantalum silicide, $Co_{16}Ta_6Si_7$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Spiegel et al., 1963]. Kuz'ma et al. [1964] determined positions for $Co_{16}Nb_6Si_7$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions of $Co_{16}Nb_6Si_7$ were preferred.

32(f)	32 cobalt (1)
32(f)	32 cobalt (2)
4(b)	4 silicon (1)
24(d)	24 silicon (2)
24(e)	24 tantalum

Lattice constant
a = 11.199 Å
(published value, 11.198 Å [Spiegel et al., 1963]).

Volume
1404.6 $Å^3$

Density
(calculated) 10.523 g/cm^3

Thermal parameters
Isotropic: cobalt B = 1.0; silicon B = 1.0; tantalum B = 0.8.

Scattering factors
Co^0, Si^0, Ta^0 [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.361 \times 10^{-3}$

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), pp. 202, 204, 212.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I., and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.

Spiegel, F. X., Bardos, D., and Beck, P. A. (1963). Trans. AIME 227, 575.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
6.458	25	1 1 1	13.70
5.597	8	2 0 0	15.82
3.959	1	2 2 0	22.44
3.232	40	2 2 2	27.58
2.800	2	4 0 0	31.94
2.569	30	3 3 1	34.90
2.504	6	4 2 0	35.84
2.286	35	4 2 2	39.38
2.155	100	5 1 1+	41.88
1.980	45	4 4 0	45.80
1.893	3	5 3 1	48.02
1.866	25	6 0 0	48.76
1.568	12	5 5 1	58.84
1.553	4	6 4 0	59.48
1.458	8	7 3 1+	63.78
1.400	2	8 0 0	66.78
1.368	9	7 3 3	68.52
1.358	2	6 4 4+	69.10
1.320	20	8 2 2+	71.42
1.293	11	5 5 5+	73.12
1.229	4	7 5 3	77.60
1.222	9	8 4 2	78.16
1.125	14	9 3 3+	86.38
1.120	2	10 0 0	86.92
1.098	3	10 2 0+	89.08
1.083	6	7 7 3+	90.72
1.078	3	6 6 6	91.26
1.040	3	10 4 0	95.60
1.010	2	11 1 1	99.44
.9785	2	9 7 1+	103.86
.9747	6	8 8 2+	104.42
.9604	2	10 6 0	106.66
.9499	1	9 7 3	108.38
.9465	2	10 6 2	108.94
.9332	4	8 8 4+	111.26
.9236	4	11 5 1+	113.02
.9083	5	10 6 4+	116.00
.8995	1	11 5 3+	117.82
.8854	2	12 4 0	120.92
.8745	2	10 8 0+	123.50
.8640	1	10 8 2	126.14
.8564	8	11 5 5+	128.18
.8542	5	10 6 6	128.78
.8371	8	13 3 1+	133.92
.8349	6	12 6 0	134.62
.8256	1	12 6 2	137.82
.8190	3	13 3 3+	140.30

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
6.466	40	1	1	1	13.68
5.599	12	2	0	0	15.81
3.959	2	2	2	0	22.44
3.377	1	3	1	1	26.37
3.233	70	2	2	2	27.57
2.800	4	4	0	0	31.94
2.569	50	3	3	1	34.89
2.504	10	4	2	0	35.83
2.286	60	4	2	2	39.38
2.155	100	5	1	1	41.88
2.155	85	3	3	3	41.88
1.980	85	4	4	0	45.80
1.893	6	5	3	1	48.02
1.866	40	6	0	0	48.75
1.866	6	4	4	2	48.75
1.616	1	4	4	4	56.92
1.568	25	5	5	1	58.84
1.553	8	6	4	0	59.47
1.458	11	7	3	1	63.79
1.458	6	5	5	3	63.79
1.400	5	8	0	0	66.77
1.368	19	7	3	3	68.53
1.358	3	6	4	4	69.11
1.320	19	6	6	0	71.41
1.320	25	8	2	2	71.41
1.293	10	7	5	1	73.12
1.293	13	5	5	5	73.12
1.229	8	7	5	3	77.61
1.222	18	8	4	2	78.16
1.194	1	6	6	4	80.37
1.143	1	8	4	4	84.74
1.126	25	9	3	3	86.37
1.126	2	7	7	1	86.37
1.126	2	7	5	5	86.37
1.120	3	10	0	0	86.92
1.098	3	8	6	2	89.09
1.098	3	10	2	0	89.09
1.083	7	7	7	3	90.71
1.083	6	9	5	1	90.71
1.078	7	6	6	6	91.26
1.040	6	10	4	0	95.60
1.010	5	11	1	1	99.43
.9899	1	8	8	0	102.19
.9785	3	9	7	1	103.86
.9785	1	9	5	5	103.86
.9747	12	8	8	2	104.42
.9747	2	10	4	4	104.42
.9603	5	10	6	0	106.67
.9499	2	9	7	3	108.38
.9465	6	10	6	2	108.95

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.9332	9	8	8	4	111.26
.9332	2	12	0	0	111.26
.9237	9	11	5	1	113.01
.9237	2	7	7	7	113.01
.9206	1	12	2	0	113.60
.9084	4	12	2	2	115.99
.9084	8	10	6	4	115.99
.8995	2	11	5	3	117.82
.8854	5	12	4	0	120.93
.8745	2	12	4	2	123.49
.8745	2	10	8	0	123.49
.8745	2	8	8	6	123.49
.8640	3	10	8	2	126.13
.8564	15	11	5	5	128.17
.8564	3	11	7	1	128.17
.8564	5	9	9	3	128.17
.8539	7	10	6	6	128.87
.8371	16	13	3	1	133.93
.8371	5	11	7	3	133.93
.8371	6	9	7	7	133.93
.8347	9	12	6	0	134.68
.8256	4	12	6	2	137.82
.8190	8	13	3	3	140.30
.8190	5	9	9	5	140.30
.8082	2	8	8	8	144.76

Cobalt titanium silicide, $Co_{16}Ti_6Si_7$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Spiegel et al., 1963]. Kuz'ma et al. [1964] determined positions for $Co_{16}Nb_6Si_7$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions for $Co_{16}Nb_6Si_7$ were preferred.

32(f)	32 cobalt (1)
32(f)	32 cobalt (2)
4(b)	4 silicon (1)
24(d)	24 silicon (2)
24(e)	24 titanium

Lattice constant
a = 11.202 Å
(published value, 11.201 Å [Spiegel et al., 1963])

Volume
1405.7 $Å^3$

Density
(calculated) 6.743 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Si^0, Ti^0 [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.215 \times 10^{-3}$

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I., and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.

Spiegel, F. X., Bardos, D., and Beck, P. A. (1963). Trans. AIME 227, 575.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
6.458	6	1 1 1	13.70
5.597	30	2 0 0	15.82
3.959	3	2 2 0	22.44
3.234	2	2 2 2	27.56
2.800	20	4 0 0	31.94
2.570	4	3 3 1	34.88
2.505	7	4 2 0	35.82
2.286	20	4 2 2	39.38
2.155	90	5 1 1+	41.88
1.980	100	4 4 0	45.78
1.893	35	5 3 1	48.02
1.867	25	6 0 0	48.74
1.771	7	6 2 0	51.56
1.708	15	5 3 3	53.60
1.689	8	6 2 2	54.28
1.617	3	4 4 4	56.90
1.569	2	7 1 1+	58.82
1.497	1	6 4 2	61.94
1.459	2	7 3 1+	63.76
1.400	4	8 0 0	66.76
1.369	1	7 3 3	68.50
1.359	1	6 4 4+	69.08
1.320	14	6 6 0+	71.40
1.293	9	7 5 1+	73.10
1.230	11	7 5 3+	77.58
1.222	4	8 4 2	78.14
1.174	6	9 3 1	81.98
1.143	8	8 4 4	84.72
1.126	17	9 3 3	86.34
1.120	3	8 6 0	86.88
1.083	2	9 5 1+	90.68
1.078	5	6 6 6	91.22
1.040	1	10 4 0+	95.56
1.010	2	11 1 1+	99.40
.9901	4	8 8 0	102.16
.9787	6	9 7 1+	103.82
.9750	2	8 8 2	104.38
.9606	1	8 6 6	106.62
.9501	2	9 7 3+	108.34
.9468	4	10 6 2	108.90
.9335	3	8 8 4	111.22
.9208	1	12 2 0	113.56
.9086	1	10 6 4	115.94
.8856	3	12 4 0	120.88
.8567	5	11 5 5+	128.10
.8373	8	13 3 1+	133.86
.8351	7	12 6 0	134.56
.8258	2	12 6 2	137.74
.8192	2	9 9 5	140.22

Calculated Pattern (Integrated)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
6.467	5	1	1	1	13.68
5.601	25	2	0	0	15.81
3.961	3	2	2	0	22.43
3.234	2	2	2	2	27.56
2.800	19	4	0	0	31.93
2.570	4	3	3	1	34.88
2.505	7	4	2	0	35.82
2.287	19	4	2	2	39.37
2.156	45	5	1	1	41.87
2.156	40	3	3	3	41.87
1.980	100	4	4	0	45.78
1.893	35	5	3	1	48.01
1.867	20	6	0	0	48.73
1.867	3	4	4	2	48.73
1.771	7	6	2	0	51.56
1.708	15	5	3	3	53.61
1.689	8	6	2	2	54.28
1.617	4	4	4	4	56.90
1.569	2	7	1	1	58.82
1.497	1	6	4	2	61.94
1.458	1	7	3	1	63.77
1.458	1	5	5	3	63.77
1.400	4	8	0	0	66.75
1.369	2	7	3	3	68.51
1.358	1	6	4	4	69.09
1.320	10	6	6	0	71.39
1.320	5	8	2	2	71.39
1.293	6	7	5	1	73.10
1.293	4	5	5	5	73.10
1.252	1	8	4	0	75.91
1.230	3	9	1	1	77.58
1.230	9	7	5	3	77.58
1.222	5	8	4	2	78.14
1.194	1	6	6	4	80.34
1.174	7	9	3	1	81.99
1.143	9	8	4	4	84.71
1.126	19	9	3	3	86.35
1.126	1	7	7	1	86.35
1.120	2	8	6	0	86.89
1.098	1	10	2	0	89.06
1.083	1	9	5	1	90.68
1.078	5	6	6	6	91.22
1.010	2	11	1	1	99.39
.9901	5	8	8	0	102.15
.9787	4	9	7	1	103.82
.9787	3	11	3	1	103.82
.9787	1	9	5	5	103.82
.9750	2	8	8	2	104.38
.9606	1	8	6	6	106.63
.9501	1	9	7	3	108.33

Calculated Pattern (Integrated)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
.9501	1	11	3	3	108.33
.9467	5	10	6	2	108.90
.9335	4	8	8	4	111.21
.9208	1	12	2	0	113.56
.9086	1	10	6	4	115.94
.8856	4	12	4	0	120.87
.8747	1	10	8	0	123.43
.8643	1	10	8	2	126.07
.8566	3	11	5	5	128.11
.8566	1	11	7	1	128.11
.8566	3	9	9	3	128.11
.8373	7	13	3	1	133.85
.8373	4	11	7	3	133.85
.8373	3	9	7	7	133.85
.8349	6	12	6	0	134.61
.8258	4	12	6	2	137.74
.8192	5	9	9	5	140.22
.8084	1	8	8	8	144.66

Diazepam, $C_{16}H_{13}ClN_2O$

Synonym
7-chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one

Structure
Monoclinic, $P2_1/a$ (14), Z = 4. The structure was determined by Camerman and Camerman[1972].

Atom positions
All the atoms were in general positions. The value of 0.2274 was used for the x coordinate of carbon (5).

Lattice constants
a = 12.929(4) A
b = 13.355(7)
c = 7.976(2)
β = 90.01(3)°
(published values: a=12.9284(41), b=13.3537(68) c=7.9763(17), β=90.010(25)° [Camerman and Camerman, 1972]).

CD cell: a = 12.929, b = 13.355, c = 7.976, β = 90.01, space group $P2_1/a$; a/b = 0.9681, c/b = 0.5972

Volume
1377.2 A^3

Density
(measured) 1.39 g/cm^3
(calculated) 1.37 g/cm^3

Thermal parameters
Isotropic: overall B = 3.0

Scattering factors
C^0, H^0, N^0, O^0, Cl^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.575 \times 10^{-3}$
I/I_c (calculated) = 0.64

Additional pattern
1. MacDonald et al. [1972]

References

Camerman, A. and Camerman, C. (1972). J. Amer. Chem. Soc. 94, 268.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

MacDonald, A., Michaelis, A. F., and Senkowski, B. Z. (1972). In Analytical Profiles of Drug Substances I (1972). (Academic Press, N. Y.), p. 79.

Calculated Pattern (Peak heights)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
9.28	33	1	1	0	9.52
7.96	22	0	0	1	11.10
6.84	2	0	1	1	12.94
6.67	9	0	2	0	13.26
6.46	31	2	0	0	13.70
6.05	6	-1	1	1	14.64
5.93	1	1	2	0	14.92
5.12	11	0	2	1	17.32
5.02	20	2	0	1	17.66
4.70	100	-2	1	1	18.88
4.64	77	2	2	0	19.10
4.21	3	1	3	0	21.10
4.10	5	3	1	0	21.66
4.01	16	-2	2	1+	22.14
3.887	84	0	3	1	22.86
3.821	5	0	1	2	23.26
3.720	41	1	3	1+	23.90
3.645	12	-3	1	1	24.40
3.619	21	3	2	0	24.58
3.394	6	2	0	2	26.24
3.331	16	-2	3	1+	26.74
3.309	9	1	2	2	26.92
3.297	11	-3	2	1+	27.02
3.232	12	1	4	0	27.58
3.140	4	4	1	0	28.40
3.079	2	0	4	1	28.98
3.026	14	-2	2	2+	29.50
2.996	23	1	4	1+	29.80
2.967	4	2	4	0	30.10
2.923	11	-4	1	1+	30.56
2.886	15	-3	3	1+	30.96
2.779	6	-2	4	1	32.18
2.733	1	4	2	1	32.74
2.698	5	2	3	2+	33.18
2.681	8	-3	2	2	33.40
2.639	3	3	4	0	33.94
2.556	1	0	4	2+	35.08
2.538	1	5	1	0	35.34
2.510	5	1	4	2+	35.74
2.506	5	-3	4	1+	35.80
2.485	2	1	5	1+	36.12
2.458	1	2	0	3+	36.52
2.418	6	-2	1	3+	37.16
2.413	7	5	2	0	37.24
2.379	3	2	4	2+	37.78
2.358	4	2	5	1+	38.14
2.352	4	-4	2	2+	38.24
2.308	2	2	2	3+	39.00
2.270	1	3	5	0	39.68
2.248	2	-1	3	3+	40.08

Calculated Pattern (Peak heights)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
2.230	3	-3	1	3+	40.42
2.183	6	3	5	1+	41.32
2.152	4	-5	3	1+	41.94
2.144	3	3	2	3+	42.12
2.127	2	6	1	0	42.46
2.099	2	-2	5	2+	43.06
2.080	2	0	4	3+	43.48
2.063	4	-5	2	2+	43.84
2.059	3	4	5	0+	43.94
2.016	1	3	3	3+	44.92
2.007	4	-4	4	2+	45.14
1.986	2	6	2	1	45.64
1.980	2	-5	4	1+	45.78
1.972	5	0	1	4+	45.98
1.950	2	5	3	2+	46.54
1.922	1	1	6	2	47.26
1.910	1	0	2	4	47.56
1.895	1	-6	0	2	47.96
1.885	4	0	5	3+	48.24
1.873	2	3	4	3+	48.56
1.865	2	-4	3	3+	48.80
1.836	1	-5	1	3+	49.60
1.830	2	2	7	0+	49.80
1.819	1	5	4	2+	50.10
1.809	3	2	5	3	50.40
1.780	3	7	2	0+	51.28
1.748	1	-2	3	4+	52.28
1.721	1	0	7	2	53.18
1.706	1	7	3	0+	53.68
1.697	1	-4	0	4+	53.98
1.684	1	-5	5	2+	54.44
1.665	2	4	6	2+	55.10
1.650	1	-2	6	3+	55.66
1.621	1	-1	8	1+	56.74
1.598	1	-3	7	2+	57.64
1.584	1	2	8	1+	58.18
1.549	1	-2	0	5+	59.66

Calculated Pattern (Integrated)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
9.29	34	1	1	0	9.51
7.98	23	0	0	1	11.08
6.85	2	0	1	1	12.92
6.68	9	0	2	0	13.25
6.46	37	2	0	0	13.69
6.05	6	-1	1	1	14.63
5.93	1	1	2	0	14.92
5.12	12	0	2	1	17.31
5.02	21	2	0	1	17.65
4.76	1	-1	2	1	18.62
4.76	2	1	2	1	18.63
4.70	100	-2	1	1	18.86
4.70	8	2	1	1	18.86
4.64	79	2	2	0	19.09
4.21	3	1	3	0	21.09
4.10	5	3	1	0	21.65
4.01	13	-2	2	1	22.13
4.01	5	2	2	1	22.13
3.887	100	0	3	1	22.86
3.821	3	0	1	2	23.26
3.723	15	-1	3	1	23.88
3.722	32	1	3	1	23.89
3.666	3	2	3	0	24.26
3.664	1	1	1	2	24.27
3.648	9	-3	1	1	24.38
3.621	23	3	2	0	24.56
3.394	7	2	0	2	26.24
3.331	10	-2	3	1	26.74
3.331	8	2	3	1	26.74
3.310	5	1	2	2	26.92
3.297	5	-3	2	1	27.02
3.297	2	3	2	1	27.02
3.290	3	-2	1	2	27.08
3.289	1	2	1	2	27.09
3.233	13	1	4	0	27.57
3.142	4	4	1	0	28.39
3.096	1	3	3	0	28.81
3.080	2	0	4	1	28.97
3.026	11	-2	2	2	29.50
3.025	6	2	2	2	29.50
2.996	7	-1	4	1	29.80
2.996	12	1	4	1	29.80
2.995	8	4	0	1	29.80
2.966	3	2	4	0	30.10
2.923	7	-4	1	1	30.56
2.923	6	4	1	1	30.56
2.895	6	-1	3	2	30.86
2.887	8	-3	3	1	30.95
2.886	8	3	3	1	30.96
2.780	7	-2	4	1	32.17

Diazepam, $C_{16}H_{13}ClN_2O$ -(Continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.780	1	2	4	1	32.17
2.733	1	4	2	1	32.74
2.699	2	-2	3	2	33.16
2.699	3	2	3	2	33.17
2.681	9	-3	2	2	33.39
2.639	3	3	4	0	33.94
2.539	1	5	1	0	35.33
2.511	4	1	4	2	35.73
2.511	1	4	0	2	35.73
2.506	1	-3	4	1	35.81
2.506	1	3	4	1	35.81
2.485	2	1	5	1	36.11
2.459	1	2	0	3	36.52
2.419	3	5	1	1	37.14
2.418	4	-2	1	3	37.15
2.418	1	2	1	3	37.15
2.411	4	5	2	0	37.26
2.380	1	-2	4	2	37.76
2.380	2	2	4	2	37.77
2.358	2	-2	5	1	38.13
2.358	4	2	5	1	38.13
2.351	2	-4	2	2	38.26
2.307	1	2	2	3	39.01
2.270	2	3	5	0	39.67
2.248	1	-1	3	3	40.08
2.231	2	-3	1	3	40.39
2.230	1	-4	4	1	40.42
2.230	1	4	4	1	40.42
2.194	2	1	6	0	41.12
2.187	1	-1	5	2	41.24
2.187	1	4	3	2	41.25
2.184	1	-3	5	1	41.31
2.184	6	3	5	1	41.31
2.153	3	-5	3	1	41.93
2.153	1	5	3	1	41.93
2.152	1	2	3	3	41.94
2.143	1	-3	2	3	42.13
2.143	2	3	2	3	42.13
2.127	3	6	1	0	42.46
2.099	2	-2	5	2	43.06
2.099	1	2	5	2	43.06
2.080	1	0	4	3	43.48
2.064	3	-5	2	2	43.84
2.063	1	5	2	2	43.84
2.059	1	4	5	0	43.94
2.055	1	6	1	1	44.02
2.007	4	-4	4	2	45.14
2.007	1	4	4	2	45.15
1.986	2	6	2	1	45.64
1.973	2	-3	5	2	45.96

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.973	2	3	5	2	45.96
1.972	3	0	1	4	45.98
1.950	1	5	3	2	46.53
1.950	1	1	1	4	46.55
1.922	2	1	6	2	47.25
1.911	1	0	2	4	47.55
1.896	1	-6	0	2	47.94
1.890	1	-1	2	4	48.10
1.885	2	-6	3	1	48.25
1.884	2	0	5	3	48.26
1.873	2	3	4	3	48.57
1.865	1	-4	3	3	48.80
1.836	1	-5	1	3	49.61
1.830	1	2	7	0	49.79
1.829	1	4	5	2	49.80
1.819	1	5	4	2	50.10
1.809	3	2	5	3	50.41
1.787	1	-4	6	1	51.08
1.780	3	7	2	0	51.28
1.721	1	0	7	2	53.18
1.706	1	7	3	0	53.68
1.684	1	-5	5	2	54.44
1.666	1	4	6	2	55.09
1.650	1	-2	6	3	55.65
1.621	1	-1	8	1	56.74
1.584	1	2	8	1	58.19
1.549	1	-2	0	5	59.65

(N,N)-Dimethyltryptamine, $C_{12}H_{16}N_2$

Synonyms
DMT, 3-[2-(dimethylamino)-ethyl]indole

Structure
Monoclinic, $P2_1/c$ (14), Z = 8. The structure was determined by Falkenberg [1972].

Atom positions [ibid.]
All the atoms were in general positions, with 2 molecules in the asymmetric unit.

Polymorphism [ibid.]
The batch of the material described here also contained crystals of an entirely different polymorph. The latter could easily be distinguished by its optical properties and crystal shape, and had the monoclinic space group $P2_1/c$ with Z = 4.

Lattice constants [ibid.]
a = 12.99(1) A
b = 12.08(1)
c = 18.38(2)
β = 127.85(1)°

CD cell: a = 14.61, b = 12.08, c = 12.99, β = 96.73°, space group $P2_1/n$; a/b = 1.2098, c/b = 1.0753

Volume
2278. A^3

Density
(measured) 1.080 g/cm^3
(calculated) 1.098 g/cm^3

Thermal parameters
Isotropic: overall B = 5.0

Scattering factors
C^0, H^0, N^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.321 \times 10^{-3}$
I/I_c (calculated) = 0.39

Additional pattern
1. Folen [1975].

References

Falkenberg, G. (1972). Acta Crystallogr. B28, 3075.
Folen, V. A. (1975). J. Forens. Sci. 20, 348.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
9.28	47	0	1	1	9.52
8.80	14	-1	1	1	10.04
7.81	4	1	1	0	11.32
7.27	15	-1	1	2+	12.16
6.45	45	-2	0	2	13.72
6.21	100	0	1	2	14.24
6.04	49	0	2	0	14.66
5.68	7	-2	1	2	15.58
5.57	11	0	2	1	15.90
5.49	51	-2	1	1	16.14
5.40	7	-1	1	3	16.40
5.20	14	1	2	0	17.04
5.12	22	2	0	0+	17.30
5.04	8	-1	2	2	17.60
4.71	35	1	0	2	18.82
4.64	48	0	2	2	19.12
4.56	7	-2	0	4	19.46
4.48	68	1	2	1+	19.80
4.41	17	-2	2	2	20.14
4.36	31	-1	0	4	20.34
4.31	61	-2	2	1	20.58
4.26	99	-2	1	4+	20.82
4.13	73	-2	2	3	21.52
4.05	6	-3	1	3	21.92
4.00	22	-3	0	4	22.22
3.89	12	2	1	1	22.86
3.79	35	-3	1	4	23.44
3.71	12	1	2	2+	23.94
3.64	16	-2	2	4	24.44
3.53	11	-1	2	4	25.18
3.51	23	-2	1	5+	25.36
3.45	3	1	3	1	25.84
3.42	7	3	0	0	26.06
3.37	14	-2	3	1+	26.40
3.33	10	-3	2	4	26.72
3.28	12	-3	2	1+	27.18
3.22	11	-4	0	4+	27.72
3.17	2	2	3	0	28.16
3.11	14	-4	1	4	28.64
3.10	8	1	2	3+	28.82
3.06	3	1	3	2	29.14
3.02	6	-2	0	6+	29.60
2.976	3	-4	1	5+	30.00
2.951	5	-3	1	6+	30.26
2.919	2	2	2	2	30.60
2.864	6	3	1	1	31.20
2.845	3	-4	2	4+	31.42
2.826	3	-4	0	6+	31.64
2.746	4	-4	2	2+	32.58
2.712	10	-2	3	5+	33.00

Calculated Pattern (Peak heights)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.651	2	-3	3	5+	33.78
2.618	4	1	2	4	34.22
2.606	5	3	3	0+	34.38
2.560	6	-4	2	6+	35.02
2.483	1	-2	1	7	36.14
2.464	3	-3	4	2	36.44
2.448	3	-4	3	2	36.68
2.443	3	-4	3	5	36.76
2.413	3	-2	3	6	37.24
2.382	2	1	1	5+	37.74
2.360	2	4	2	0	38.10
2.348	2	3	2	2	38.30
2.303	5	-5	1	7	39.08
2.262	1	-2	5	2	39.82
2.255	1	-1	4	5+	39.94
2.241	3	-4	1	8+	40.20
2.239	3	2	4	2	40.24
2.221	1	-2	5	3	40.58
2.200	2	-3	3	7+	41.00
2.186	2	2	5	0+	41.26
2.173	1	-1	2	7+	41.52
2.153	2	-4	4	2+	41.92
2.139	2	-5	1	8+	42.22
2.134	2	-6	0	4+	42.32
2.114	1	-6	1	6+	42.74
2.098	1	-6	1	4+	43.08
2.063	1	-4	4	6+	43.84
2.055	1	1	1	6+	44.02
2.039	1	-1	4	6+	44.40
2.027	2	-5	3	7+	44.68
2.007	2	1	5	3+	45.14
1.984	2	-4	3	8+	45.70
1.967	1	-1	5	5+	46.10
1.959	2	3	0	4	46.30
1.943	1	5	2	0+	46.72
1.934	1	-4	2	9+	46.94
1.922	1	-2	6	2+	47.26
1.897	2	-2	6	3+	47.92
1.874	2	2	6	0+	48.54
1.856	2	-6	3	7+	49.04
1.852	2	1	6	2	49.16
1.843	1	0	3	7+	49.40
1.824	1	-5	0	10+	49.96
1.798	2	-3	3	9+	50.72
1.783	1	2	1	6+	51.20
1.761	1	-7	2	7+	51.88
1.727	1	-7	2	8+	52.98
1.678	1	0	7	2+	54.66
1.670	1	-4	3	10+	54.94
1.659	1	-7	0	10+	55.34
1.642	1	-4	1	11+	55.94

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
9.28	46	0	1	1	9.52
9.13	2	-1	0	2	9.68
8.82	14	-1	1	1	10.02
7.82	4	1	1	0	11.31
7.28	11	-1	1	2	12.15
7.26	5	0	0	2	12.19
6.45	45	-2	0	2	13.72
6.22	100	0	1	2	14.23
6.04	47	0	2	0	14.65
5.69	6	-2	1	2	15.56
5.58	7	0	2	1	15.88
5.49	49	-2	1	1	16.12
5.47	7	-1	2	1	16.19
5.40	4	-1	1	3	16.42
5.20	12	1	2	0	17.02
5.13	18	2	0	0	17.28
5.12	5	-2	1	3	17.30
5.04	7	-1	2	2	17.59
4.72	3	2	1	0	18.78
4.71	31	1	0	2	18.81
4.64	48	0	2	2	19.10
4.56	2	-2	0	4	19.44
4.49	40	0	1	3	19.75
4.48	43	1	2	1	19.82
4.41	10	-2	2	2	20.12
4.36	25	-1	0	4	20.33
4.32	55	-2	2	1	20.56
4.27	66	-2	1	4	20.79
4.27	22	-1	2	3	20.80
4.26	19	-3	0	2	20.83
4.13	77	-2	2	3	21.51
4.10	6	-1	1	4	21.63
4.05	3	-3	1	3	21.92
4.02	2	-3	1	2	22.10
4.00	22	-3	0	4	22.22
3.89	11	2	1	1	22.85
3.80	38	-3	1	4	23.42
3.78	2	0	2	3	23.54
3.72	8	1	2	2	23.92
3.72	4	-3	1	1	23.93
3.64	17	-2	2	4	24.43
3.63	1	0	0	4	24.51
3.54	9	-1	2	4	25.15
3.51	20	-2	1	5	25.35
3.50	7	-3	2	3	25.41
3.47	1	0	1	4	25.61
3.45	2	1	3	1	25.83
3.42	6	3	0	0	26.04
3.40	5	2	2	1	26.21
3.38	6	-3	1	5	26.33

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
3.37	11	-2	3	1	26.41
3.35	2	-1	3	3	26.60
3.33	10	-3	2	4	26.72
3.29	2	3	1	0	27.08
3.28	1	-2	3	3	27.17
3.28	10	-3	2	1	27.17
3.23	9	-4	0	4	27.64
3.21	7	2	1	2	27.74
3.17	1	2	3	0	28.15
3.12	14	-4	1	4	28.62
3.11	1	0	2	4	28.68
3.10	5	1	2	3	28.82
3.09	1	0	3	3	28.82
3.08	2	-4	0	2	28.92
3.06	3	1	3	2	29.14
3.02	2	0	4	0	29.55
3.02	3	-2	3	4	29.56
3.02	3	-2	0	6	29.61
2.978	2	-4	1	5	29.98
2.975	1	3	2	0	30.01
2.960	1	-1	3	4	30.17
2.957	2	-1	2	5	30.20
2.950	3	-3	1	6	30.27
2.939	2	-3	3	3	30.39
2.919	1	2	2	2	30.61
2.906	1	1	0	4	30.75
2.876	3	2	3	1	31.08
2.864	5	3	1	1	31.20
2.848	1	-4	2	3	31.39
2.845	2	-4	2	4	31.42
2.827	3	-4	0	6	31.63
2.822	1	0	1	5	31.68
2.752	1	-4	1	6	32.50
2.747	3	-4	2	2	32.57
2.735	1	-2	4	2	32.72
2.717	1	-3	2	6	32.94
2.712	2	-2	4	1	33.00
2.712	8	-2	3	5	33.00
2.698	3	-2	2	6	33.18
2.695	1	0	3	4	33.21
2.651	2	-3	3	5	33.78
2.618	4	1	2	4	34.22
2.606	4	3	3	0	34.38
2.602	1	2	4	0	34.44
2.566	4	-3	1	7	34.94
2.560	4	-4	2	6	35.02
2.543	1	1	4	2	35.26
2.484	1	-2	1	7	36.13
2.471	1	-3	4	3	36.32
2.464	3	-3	4	2	36.44

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.449	2	-4	3	2	36.67
2.443	1	-4	3	5	36.76
2.413	4	-2	3	6	37.23
2.382	1	1	1	5	37.74
2.360	2	4	2	0	38.09
2.348	1	3	2	2	38.31
2.303	5	-5	1	7	39.08
2.262	1	-2	5	2	39.81
2.243	1	-1	5	3	40.18
2.242	1	-4	1	8	40.19
2.238	2	2	4	2	40.26
2.222	1	-2	5	3	40.57
2.204	1	-4	4	4	40.91
2.199	2	-3	3	7	41.00
2.158	1	-4	4	2	41.83
2.139	1	-5	1	8	42.22
2.134	1	-4	2	8	42.31
2.131	1	-6	0	4	42.39
2.098	1	-6	1	4	43.08
2.039	1	-1	4	6	44.40
2.027	1	-5	3	7	44.67
2.007	1	1	5	3	45.14
1.985	1	-4	3	8	45.67
1.983	1	-1	1	8	45.71
1.960	2	3	0	4	46.30
1.934	1	-4	2	9	46.94
1.898	1	-6	2	8	47.90
1.897	2	-2	6	3	47.92
1.874	1	2	6	0	48.54
1.856	1	-6	3	7	49.04
1.852	1	1	6	2	49.17
1.799	1	-6	2	9	50.70
1.798	1	-3	3	9	50.72
1.783	1	2	1	6	51.21
1.763	1	-7	2	7	51.82
1.727	1	-7	2	8	52.98
1.679	1	0	7	2	54.62
1.670	1	-7	2	9	54.92
1.670	1	-4	3	10	54.95

Methapyrilene hydrochloride, $C_{14}H_{20}ClN_3S$

Synonyms
1. 2-[(2)-dimethylaminoethyl-2-thenylamino]-pyridine hydrochloride
2. thenylpyramine hydrochloride

Structure
Monoclinic, $P2_1/c$ (14), Z = 8. The structure was determined by Clark and Palenik [1972]. There were two molecules in the asymmetric unit and in one of them the thiophene ring was disordered; one sulfur and one carbon atom shared occupancy of each of 2 sites, on an approximately equal basis.

Atom positions
Three hydrogen atoms on the disordered thiophene ring were omitted from the refinement and their positions not determined. All other atoms were in general positions.

Lattice constants
a = 10.937(3) Å
b = 10.418(3)
c = 28.258(8)
β = 106.21(2)°
(published values: a = 10.936, b = 10.417
c = 28.256, β = 106.21° [Clark and Palenik, 1972]

CD cell: a = 27.305, b = 10.418, c = 10.937, β = 96.41°, space group $P2_1/n$, a/b = 2.6209, c/b = 1.0498

Volume
3091.8 Å^3

Density
(measured) 1.273 g/cm^3
(calculated) 1.280 g/cm^3

Thermal parameters
Isotropic: overall B = 5.0

Scattering factors
C^0, H^0, Cl^0, N^0, S^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.213 \times 10^{-3}$
I/I_c (calculated) = 0.35

Additional pattern
1. PDF 12-872 [Rose and Williams, 1959]

References

Clark, G. R. and Palenik, G. J. (1972). J. Amer. Chem. Soc. 94, 4005.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Rose, H. A. and Williams, J. G. (1959). J. Amer. Pharm. Ass. 48, 487.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
9.71	3	0 1 1	9.10
8.26	7	0 1 2	10.70
7.52	60	-1 1 1	11.76
7.10	10	-1 1 2	12.46
6.79	26	1 1 1*	13.02
6.59	3	-1 0 4	13.42
6.37	5	-1 1 3	13.90
6.01	1	1 1 2	14.72
5.68	13	0 1 4	15.58
5.58	2	-1 1 4	15.88
5.43	5	-2 0 2	16.30
5.21	40	0 2 0	17.02
4.85	93	-2 0 4*	18.26
4.69	20	2 1 0	18.92
4.59	8	-1 2 2	19.34
4.52	47	0 0 6	19.62
4.37	24	-1 2 3	20.30
4.25	7	-1 1 6	20.90
4.13	100	2 1 2*	21.52
4.02	37	-2 0 6*	22.10
3.757	67	-2 1 6*	23.66
3.684	53	2 0 4*	24.14
3.553	38	-2 2 4	25.04
3.469	10	-1 2 6	25.66
3.437	5	-2 1 7*	25.90
3.401	15	-3 1 1*	26.18
3.341	7	1 2 5*	26.66
3.300	4	-2 0 8*	27.00
3.269	2	-1 3 2	27.26
3.225	4	0 1 8	27.64
3.186	17	1 1 7*	27.98
3.144	23	-2 1 8	28.36
3.091	2	0 3 4	28.86
3.064	2	1 2 6*	29.12
3.008	20	2 2 4*	29.68
2.974	16	-3 2 3*	30.02
2.912	21	2 1 6	30.68
2.879	6	3 1 3*	31.04
2.850	2	-3 2 5	31.36
2.834	3	2 3 1	31.54
2.788	5	-2 2 8	32.08
2.746	3	0 3 6*	32.58
2.736	3	-2 3 5	32.70
2.715	9	-4 0 4*	32.96
2.688	2	-1 2 9	33.30
2.679	2	2 1 7	33.42
2.651	2	-2 1 10	33.78
2.626	6	-1 3 7*	34.12
2.623	6	1 1 9*	34.16
2.601	7	-2 2 9*	34.46

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.546	9	3 1 5*	35.22
2.527	6	2 3 4*	35.50
2.502	6	1 4 1*	35.86
2.475	7	-1 4 3*	36.26
2.449	3	4 0 2*	36.66
2.430	7	0 4 4*	36.96
2.409	3	1 3 7*	37.30
2.391	4	1 4 3*	37.58
2.388	4	-3 2 9*	37.64
2.367	2	-4 1 8	37.98
2.346	4	3 2 5*	38.34
2.332	4	-4 2 6*	38.58
2.301	1	-1 2 11*	39.12
2.285	2	2 3 6*	39.40
2.276	2	0 3 9	39.56
2.272	2	-1 4 6*	39.64
2.262	1	0 0 12*	39.82
2.246	1	3 1 7*	40.12
2.222	3	-4 0 10*	40.56
2.213	3	1 1 11*	40.74
2.194	1	2 4 3*	41.10
2.175	3	2 0 10	41.48
2.152	2	-2 3 10	41.94
2.138	4	-4 3 2*	42.24
2.133	4	1 3 9	42.34
2.128	4	2 1 10*	42.44
2.124	4	-2 2 12*	42.52
2.094	1	3 3 5*	43.16
2.069	2	-3 4 5	43.72
2.063	3	4 2 4*	43.86
2.044	2	1 5 0*	44.28
2.038	2	-1 5 2*	44.42
2.030	3	0 5 3*	44.60
2.010	2	-2 0 14*	45.08
1.999	5	4 1 6	45.32
1.982	1	-3 4 7	45.74
1.973	3	-2 1 14*	45.96
1.947	2	4 3 3*	46.62
1.939	3	0 0 14*	46.82
1.933	2	-2 3 12*	46.96
1.929	2	-3 4 8	47.08
1.917	2	3 3 7*	47.38
1.890	3	2 5 2	48.10
1.872	2	-5 2 9*	48.60
1.863	2	2 1 12	48.84
1.858	2	-3 3 12	48.98
1.850	1	4 4 0*	49.22
1.843	2	-1 1 15*	49.42
1.822	3	-5 3 1*	50.02
1.801	2	-3 1 15*	50.64

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.795	3	-4 1 14*	50.84
1.791	2	1 4 10*	50.96
1.775	3	-3 3 13*	51.44
1.770	3	-6 0 8*	51.60
1.750	1	6 0 0*	52.22
1.744	2	-3 4 11*	52.42
1.740	2	4 2 8*	52.56
1.720	1	3 4 7*	53.22
1.710	2	-6 2 6*	53.54
1.697	1	-1 6 3*	54.00
1.694	1	-3 3 14*	54.10
1.668	2	4 0 10*	55.00
1.659	1	-2 5 10*	55.34
1.655	2	-1 6 5*	55.48
1.619	1	-6 2 10*	56.84
1.612	1	2 5 8*	57.08
1.588	2	4 5 2*	58.02
1.559	1	1 4 13*	59.22
1.555	1	-4 1 17*	59.38
1.550	1	-4 3 15*	59.58
1.547	1	-7 1 5*	59.74

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
9.73	3	0 1 1	9.09
8.26	8	0 1 2	10.70
7.52	72	-1 1 1	11.76
7.40	5	1 1 0	11.96
7.11	11	-1 1 2	12.44
6.83	1	0 1 3	12.95
6.80	20	1 1 1	13.00
6.78	13	0 0 4	13.04
6.60	2	-1 0 4	13.41
6.37	6	-1 1 3	13.89
6.02	1	1 1 2	14.71
5.68	15	0 1 4	15.58
5.58	2	-1 1 4	15.88
5.43	6	-2 0 2	16.30
5.25	18	2 0 0	16.87
5.21	46	0 2 0	17.01
4.86	11	0 2 2	18.23
4.86	57	-2 0 4	18.24
4.85	53	-1 1 5	18.26
4.83	1	-2 1 1	18.37
4.82	5	-2 1 2	18.40
4.81	2	0 1 5	18.42
4.69	21	2 1 0	18.91
4.67	1	1 2 0	19.00
4.67	6	-2 1 3	19.01

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.59	6	-1	2	2	19.32
4.52	58	0	0	6	19.61
4.51	1	1	2	1	19.68
4.49	4	2	0	2	19.74
4.40	2	-2	1	4	20.14
4.37	29	-1	2	3	20.29
4.25	5	-1	1	6	20.90
4.15	90	0	1	6	21.40
4.13	1	0	2	4	21.49
4.13	100	2	1	2	21.52
4.09	2	-1	2	4	21.72
4.09	18	-2	1	5	21.72
4.03	33	-2	0	6	22.05
4.02	21	1	1	5	22.12
3.787	1	1	0	6	23.47
3.765	2	-2	2	1	23.61
3.760	42	-2	2	2	23.64
3.757	46	-2	1	6	23.67
3.750	3	-1	1	7	23.71
3.698	22	2	2	0	24.04
3.686	7	-2	2	3	24.12
3.684	52	2	0	4	24.14
3.640	1	1	2	4	24.44
3.571	2	2	2	1	24.91
3.559	1	1	1	6	25.00
3.554	50	-2	2	4	25.04
3.529	1	-1	0	8	25.22
3.470	12	-1	2	6	25.65
3.440	2	-3	1	2	25.88
3.438	2	-2	1	7	25.89
3.415	1	0	2	6	26.07
3.404	11	-3	1	1	26.16
3.402	7	2	2	2	26.17
3.392	1	0	0	8	26.25
3.364	3	0	3	2	26.47
3.351	2	-3	1	4	26.58
3.342	3	-1	1	8	26.65
3.339	4	1	2	5	26.67
3.300	4	-2	0	8	27.00
3.270	1	-1	3	2	27.25
3.242	1	0	3	3	27.49
3.239	1	1	3	1	27.51
3.225	3	0	1	8	27.64
3.194	11	3	1	1	27.91
3.186	2	-2	2	6	27.98
3.186	13	1	1	7	27.99
3.146	31	-2	1	8	28.35
3.091	1	0	3	4	28.86
3.073	1	-1	3	4	29.03
3.063	1	1	2	6	29.13

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
3.034	2	2	0	6	29.42
3.014	8	1	3	3	29.62
3.008	11	2	2	4	29.68
3.006	9	-1	1	9	29.69
2.985	12	-2	2	7	29.91
2.974	13	-3	2	3	30.02
2.963	9	-3	2	1	30.14
2.933	7	-3	1	7	30.45
2.926	2	-2	3	2	30.52
2.925	3	0	3	5	30.54
2.921	1	-1	2	8	30.58
2.913	26	2	1	6	30.67
2.884	1	-2	1	9	30.98
2.879	5	3	1	3	31.04
2.851	2	-3	2	5	31.35
2.834	4	2	3	1	31.54
2.788	7	-2	2	8	32.08
2.754	2	0	3	6	32.48
2.748	1	2	3	2	32.56
2.743	1	-2	0	10	32.62
2.736	1	-2	3	5	32.70
2.723	4	-4	0	2	32.86
2.717	7	-4	0	4	32.94
2.714	2	1	3	5	32.97
2.713	2	0	0	10	32.98
2.689	1	-1	2	9	33.29
2.678	1	2	1	7	33.44
2.653	2	-2	1	10	33.76
2.630	1	-2	3	6	34.06
2.629	2	-4	1	4	34.07
2.628	3	-1	3	7	34.09
2.626	2	4	0	0	34.12
2.621	1	2	2	6	34.18
2.618	3	1	1	9	34.23
2.609	1	0	2	9	34.34
2.601	5	-2	2	9	34.46
2.600	3	-3	1	9	34.47
2.593	2	0	4	1	34.57
2.558	2	0	4	2	35.05
2.547	6	3	1	5	35.21
2.546	5	4	1	0	35.22
2.544	1	2	0	8	35.25
2.533	1	-1	4	1	35.41
2.528	2	1	4	0	35.48
2.527	5	2	3	4	35.49
2.516	1	-1	4	2	35.66
2.507	2	-3	3	3	35.79
2.502	6	1	4	1	35.87
2.492	1	-1	1	11	36.02
2.478	5	-1	4	3	36.22

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.475	4	-1 3 8	36.27
2.471	1	2 1 8	36.32
2.453	2	4 0 2	36.60
2.449	1	-2 1 11	36.66
2.431	5	0 4 4	36.94
2.430	3	-4 0 8	36.96
2.426	2	0 3 8	37.02
2.409	2	1 3 7	37.29
2.393	3	1 4 3	37.55
2.392	1	-2 3 8	37.57
2.388	1	4 1 2	37.64
2.387	2	-3 2 9	37.66
2.367	2	-4 1 8	37.99
2.345	3	3 2 5	38.35
2.333	3	-4 2 6	38.57
2.330	2	-2 4 3	38.61
2.326	2	-2 0 12	38.68
2.285	1	2 3 6	39.41
2.277	2	0 3 9	39.55
2.244	1	3 1 7	40.14
2.222	3	-4 0 10	40.56
2.213	2	1 1 11	40.74
2.212	1	-3 3 8	40.76
2.210	1	0 1 12	40.80
2.194	1	2 4 3	41.10
2.176	3	2 0 10	41.47
2.153	3	-2 3 10	41.94
2.143	1	4 2 3	42.12
2.143	2	-4 3 2	42.13
2.138	2	-5 1 3	42.23
2.134	1	1 3 9	42.32
2.130	2	2 1 10	42.41
2.128	2	-5 1 5	42.45
2.125	1	-4 3 1	42.51
2.124	2	-2 2 12	42.53
2.121	1	-1 1 13	42.60
2.115	1	-3 4 3	42.72
2.069	1	-3 4 5	43.71
2.063	3	4 2 4	43.85
2.059	2	0 5 2	43.93
2.037	1	-1 5 2	44.43
2.030	2	0 5 3	44.59
2.030	1	-3 4 6	44.60
2.030	1	1 5 1	44.61
2.012	1	5 1 1	45.02
2.010	1	-2 0 14	45.08
1.999	6	4 1 6	45.32
1.983	1	-3 4 7	45.73
1.977	1	-4 1 12	45.86
1.973	3	-2 1 14	45.96

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.947	1	4 3 3	46.60
1.941	1	-3 0 14	46.77
1.938	2	0 0 14	46.84
1.933	1	-2 3 12	46.98
1.928	1	-3 4 8	47.09
1.919	1	-3 2 13	47.33
1.917	2	3 3 7	47.39
1.902	1	-1 5 6	47.79
1.890	3	2 5 2	48.10
1.886	1	4 3 4	48.21
1.882	1	-4 4 2	48.31
1.878	1	-4 2 12	48.42
1.872	1	-5 2 9	48.60
1.863	2	2 1 12	48.84
1.858	2	-3 3 12	48.98
1.844	1	2 3 10	49.39
1.843	1	-1 1 15	49.42
1.842	1	4 0 8	49.44
1.822	2	-5 3 1	50.01
1.801	1	-3 1 15	50.64
1.796	1	-3 5 4	50.81
1.794	1	-1 5 8	50.85
1.794	1	-4 1 14	50.86
1.791	1	1 4 10	50.96
1.780	1	2 2 12	51.29
1.777	1	-4 4 8	51.38
1.775	2	0 5 8	51.43
1.774	2	-3 3 13	51.46
1.770	2	-6 0 8	51.60
1.750	1	6 0 0	52.22
1.744	1	-3 4 11	52.42
1.740	1	-2 1 16	52.57
1.737	1	4 2 8	52.66
1.723	1	3 4 7	53.10
1.711	1	-6 2 6	53.52
1.709	1	-4 1 15	53.58
1.694	1	-3 3 14	54.09
1.671	1	-2 2 16	54.90
1.668	1	4 0 10	54.99
1.665	1	2 5 7	55.10
1.659	1	-2 5 10	55.32
1.655	1	-1 6 5	55.46
1.653	1	0 5 10	55.56
1.588	1	4 5 2	58.03
1.550	1	-4 3 15	59.58

Silicon nitride, β-Si_3N_4

Structure
Hexagonal, $P6_3/m$ (176), Z = 4. The structure was determined by Hardie and Jack [1957].

Atom positions [ibid.]
6(h) 6 silicon
6(h) 6 nitrogen
2(c) 2 nitrogen

Polymorphism [ibid.]
A polymorph, α-Si_3N_4 is also hexagonal, with space group P31c; its structure has the same tetrahedral units as the β form but their arrangement is different.

Lattice constants
a = 7.608 A
c = 2.9109
(published values a = 7.608, c = 2.9107 [Hardie and Jack, 1957]).

CD cell; a = 7.608, c = 2.9109, c/a = 0.3826

Volume
145.9 $Å^3$

Density
(measured) 3.19 g/cm^3
(calculated) 3.193 g/cm^3

Thermal parameters
Isotropic: overall B = 0.5

Scattering factors
Si^0, N^0 [International Tables, 1962].

Scale factors (integrated intensities)
$\gamma = 0.457 \times 10^{-3}$

Additional pattern
1. PDF card 9-259 [Decker, General Electric Co., Schenectady, N.Y.]

References
Hardie, D. and Jack, K. H. (1957). Nature, London, No. 4581, Aug. 17, p. 332.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkl	2θ(°) λ = 1.540598Å
6.58	40	1 0 0	13.44
3.80	40	1 1 0	23.38
3.29	100	2 0 0	27.06
2.66	95	1 0 1	33.64
2.49	95	2 1 0	36.04
2.31	6	1 1 1	38.94
2.20	5	3 0 0	41.08
2.18	35	2 0 1	41.36
1.902	8	2 2 0	47.78
1.892	5	2 1 1	48.04
1.827	12	1 3 0	49.86
1.753	35	3 0 1	52.14
1.592	11	2 2 1	57.86
1.548	6	1 3 1+	59.70
1.511	14	2 3 0+	61.28
1.455	14	0 0 2	63.92
1.438	7	1 4 0+	64.80
1.434	6	4 0 1	64.98
1.359	2	1 1 2	69.04
1.341	40	2 3 1	70.10
1.331	8	2 0 2	70.70
1.318	4	5 0 0	71.54
1.289	20	4 1 1	73.40
1.268	6	3 3 0	74.82
1.257	16	2 1 2	75.62
1.200	2	5 0 1	79.84
1.183	1	5 1 0+	81.22
1.156	2	2 2 2	83.58
1.145	3	2 4 1+	84.58
1.138	4	1 3 2	85.16
1.096	4	5 1 1	89.28
1.083	3	4 3 0	90.66
1.055	1	2 5 0	93.80
1.048	7	2 3 2+	94.58
1.023	4	1 4 2+	97.72
1.015	1	3 4 1	98.72
1.005	2	1 6 0	100.10
.9919	3	2 5 1+	101.90
.9769	3	5 0 2	104.10
.9599	3	1 0 3	106.74
.9560	5	3 3 2	107.36
.9497	10	1 6 1+	108.40
.9413	2	5 3 0	109.84
.9307	2	2 0 3	111.72
.9182	2	5 1 2+	114.06
.9137	2	2 6 0+	114.92
.9040	4	4 4 1	116.88
.8956	2	7 0 1+	118.66

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
6.59	35	1	0	0	13.43
3.80	41	1	1	0	23.37
3.29	100	2	0	0	27.04
2.66	100	1	0	1	33.63
2.49	100	2	1	0	36.04
2.31	6	1	1	1	38.93
2.20	3	3	0	0	41.06
2.18	35	2	0	1	41.36
1.902	9	2	2	0	47.78
1.892	5	2	1	1	48.04
1.827	13	1	3	0	49.86
1.753	40	3	0	1	52.13
1.592	13	2	2	1	57.87
1.548	2	3	1	1	59.70
1.548	5	1	3	1	59.70
1.512	7	3	2	0	61.28
1.512	9	2	3	0	61.28
1.455	17	0	0	2	63.91
1.438	4	4	1	0	64.79
1.438	5	1	4	0	64.79
1.434	3	4	0	1	65.00
1.359	3	1	1	2	69.04
1.341	6	3	2	1	70.09
1.341	45	2	3	1	70.09
1.331	9	2	0	2	70.71
1.318	5	5	0	0	71.54
1.289	25	4	1	1	73.39
1.268	7	3	3	0	74.82
1.257	19	2	1	2	75.62
1.200	2	5	0	1	79.83
1.183	2	5	1	0	81.22
1.156	3	2	2	2	83.59
1.145	4	2	4	1	84.58
1.138	4	1	3	2	85.16
1.096	5	5	1	1	89.28
1.083	4	4	3	0	90.66
1.055	1	2	5	0	93.79
1.048	4	3	2	2	94.57
1.048	5	2	3	2	94.57
1.023	3	1	4	2	97.72
1.023	3	4	1	2	97.72
1.015	1	3	4	1	98.72
1.005	3	1	6	0	100.11
.9919	1	5	2	1	101.90
.9919	4	2	5	1	101.90
.9768	5	5	0	2	104.11
.9599	3	1	0	3	106.74
.9560	6	3	3	2	107.36
.9510	1	4	4	0	108.19
.9498	10	1	6	1	108.39

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
.9498	4	6	1	1	108.39
.9412	2	5	3	0	109.85
.9307	3	2	0	3	111.72
.9182	2	5	1	2	114.06
.9137	3	2	6	0	114.93
.9040	5	4	4	1	116.89
.8956	1	5	3	1	118.66
.8956	2	7	0	1	118.66

Vanadium sulfide, α-V_3S

Structure
Tetragonal, $I\bar{4}2m$ (121), Z = 8. The structure was determined by Pedersen and Grønvold [1959], and is closely related to that of Ni_3P.

Atom positions [ibid.]

8(i)	8 vanadium(1)	8(f)	8 vanadium(3)
8(i)	8 vanadium(2)	8(g)	8 sulfur

Polymorphism [ibid.]
The material was stable above 950 °C, and appeared also in samples quenched from 1400 °C. A tetragonal polymorph, β-V_3S is stable below 825 °C, and has the space group $P4_2/nbc$. The structures are closely related.

Lattice constants [ibid.]
a = 9.470 A
c = 4.589

CD cell: a = 9.470, c = 4.589, c/a = 0.4846

Volume
411.6 $Å^3$

Density
(measured) 5.895 g/cm^3
(calculated) 5.968 g/cm^3

Thermal parameters
B = 0 since absorption and temperature effects nearly balance each other [Pedersen and Grønvold, 1959].

Scattering factors
S^0, V^0 [Cromer polynomial format: Cromer, 1972; Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.171 \times 10^{-3}$

References

Cromer, D. T. (1972). Private communication.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Pedersen, B. and Grønvold, F. (1959). Acta Crystallogr. 12, 1022.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.13	1	1 0 1	21.52
3.112	1	2 1 1	28.66
2.994	1	3 1 0	29.82
2.601	8	3 0 1	34.46
2.280	100	3 2 1	39.50
2.232	55	3 3 0	40.38
2.170	60	1 1 2	41.58
2.118	30	4 2 0	42.66
2.064	20	2 0 2	43.82
2.054	100	4 1 1	44.06

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.892	40	2 2 2	48.04
1.857	16	5 1 0	49.02
1.821	12	3 1 2	50.04
1.751	7	4 3 1+	52.20
1.648	9	4 0 2	55.74
1.643	9	5 2 1	55.92
1.600	3	3 3 2	57.56
1.578	1	6 0 0	58.42
1.497	4	6 2 0	61.92
1.474	14	6 1 1	63.00
1.408	1	5 4 1	66.36
1.376	1	3 0 3	68.06
1.352	5	4 4 2	69.44
1.349	6	6 3 1	69.62
1.339	11	7 1 0+	70.22
1.326	9	5 3 2	71.06
1.322	17	3 2 3	71.28
1.313	3	6 4 0	71.82
1.300	10	6 0 2	72.66
1.2732	15	4 1 3	74.46
1.2515	10	7 2 1	75.98
1.2434	5	7 3 0	76.56
1.1900	2	4 3 3+	80.68
1.1722	3	6 5 1	82.16
1.1566	13	5 5 2	83.52
1.1472	8	0 0 4	84.36
1.1378	10	7 4 1	85.22
1.1160	2	6 6 0	87.30
1.1010	1	7 5 0	88.80
1.0911	5	6 1 3	89.82
1.0774	7	8 3 1	91.28
1.0521	6	8 0 2	94.14
1.0374	2	6 3 3	95.90
1.0269	3	8 2 2	97.20
1.0257	1	9 0 1	97.36
1.0203	6	3 3 4	98.04
1.0133	1	7 0 3	98.96
1.0087	4	4 2 4	99.58
1.0023	2	9 2 1+	100.44
.9909	5	7 2 3	102.04
.9806	2	8 5 1	103.54
.9761	4	5 1 4	104.22
.9515	3	9 1 2	108.10
.9502	2	6 5 3	108.32
.9470	5	10 0 0	108.86
.9411	6	9 4 1	109.88
.9317	6	7 4 3	111.54

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.13	1	1	0	1	21.50
3.112	1	2	1	1	28.66
2.995	1	3	1	0	29.81
2.601	8	3	0	1	34.46
2.294	1	0	0	2	39.23
2.280	100	3	2	1	39.50
2.232	55	3	3	0	40.38
2.171	60	1	1	2	41.57
2.118	30	4	2	0	42.66
2.065	14	2	0	2	43.81
2.054	100	4	1	1	44.05
1.893	40	2	2	2	48.03
1.857	17	5	1	0	49.01
1.821	13	3	1	2	50.04
1.751	3	5	0	1	52.21
1.751	4	4	3	1	52.21
1.648	9	4	0	2	55.75
1.642	6	5	2	1	55.95
1.600	3	3	3	2	57.56
1.578	1	6	0	0	58.42
1.497	4	6	2	0	61.92
1.474	16	6	1	1	63.00
1.408	1	5	4	1	66.35
1.377	1	3	0	3	68.05
1.352	5	4	4	2	69.44
1.349	4	6	3	1	69.62
1.339	7	7	1	0	70.22
1.339	5	5	5	0	70.22
1.326	10	5	3	2	71.05
1.322	14	3	2	3	71.29
1.313	2	6	4	0	71.83
1.300	11	6	0	2	72.65
1.2976	2	7	0	1	72.83
1.2732	18	4	1	3	74.46
1.2540	1	6	2	2	75.80
1.2515	11	7	2	1	75.98
1.2435	5	7	3	0	76.56
1.1900	1	5	0	3	80.68
1.1900	1	4	3	3	80.68
1.1723	4	6	5	1	82.16
1.1566	15	5	5	2	83.51
1.1541	2	5	2	3	83.74
1.1472	9	0	0	4	84.36
1.1398	2	6	4	2	85.04
1.1379	11	7	4	1	85.21
1.1161	2	6	6	0	87.29
1.1009	1	7	5	0	88.81
1.0911	5	6	1	3	89.82
1.0774	9	8	3	1	91.28
1.0520	7	8	0	2	94.15

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.0374	2	6	3	3	95.89
1.0270	3	8	2	2	97.19
1.0256	1	9	0	1	97.37
1.0204	8	3	3	4	98.04
1.0134	1	7	0	3	98.95
1.0087	5	4	2	4	99.57
1.0024	2	9	2	1	100.44
1.0024	1	7	6	1	100.44
.9909	6	7	2	3	102.03
.9806	2	8	5	1	103.54
.9760	5	5	1	4	104.22
.9516	4	9	1	2	108.09
.9502	2	6	5	3	108.32
.9470	6	10	0	0	108.86
.9411	8	9	4	1	109.87
.9316	8	7	4	3	111.55

Vanadium sulfide, β-V_3S

Structure
Tetragonal, $P4_2/nbc$ (133), Z = 8. The structure was determined by Pedersen and Grønvold [1959] and shows relationship to the β-W structure type.

Atom positions [ibid.]

8(j)	8 vanadium(1)	8(i)	8 vanadium(3)
8(j)	8 vanadium(2)	8(h)	8 sulfur

Polymorphism [ibid.]
The material was stable below 825 °C. A tetragonal polymorph, α-V_3S has the space group $I\bar{4}2m$; it is stable above 950 °C and appears also in samples quenched from 1400 °C. The two structures are closely related.

Lattice constants [ibid.]
a = 9.381 A
c = 4.663

CD cell: a = 9.381, c = 4.663, c/a = 0.4971

Volume
410.4 $Å^3$

Density
(measured) 5.939 g/cm^3
(calculated) 5.985 g/cm^3

Thermal parameters
B = 0, since absorption and temperature effects nearly balance each other [Pedersen and Grønvold, 1959].

Scattering factors
V^0, S^0, [Cromer polynomial format: Cromer, 1972; Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.152 \times 10^{-3}$

References

Cromer, D. T. (1972). Private communication.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Pedersen, B. and Grønvold, F. (1959). Acta Crystallogr. 12, 1022.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.502	25	3 1 1	35.86
2.345	2	4 0 0	38.36
2.332	2	0 0 2	38.58
2.272	100	3 2 1	39.64
2.211	60	3 3 0	40.78
2.200	75	1 1 2	41.00
2.097	45	4 2 0+	43.10
2.045	75	4 1 1	44.26
1.913	30	4 2 1	47.50
1.907	60	2 2 2	47.64
1.840	20	5 1 0	49.50
1.834	19	3 1 2	49.68
1.711	6	5 1 1	53.50
1.653	9	4 0 2	55.54
1.605	4	3 3 2	57.38
1.483	4	6 2 0+	62.58
1.464	15	6 1 1	63.48
1.414	1	6 2 1	66.04
1.398	1	5 4 1	66.88
1.377	2	3 1 3	68.04
1.351	4	4 4 2	69.50
1.339	2	6 3 1	70.22
1.334	14	3 2 3	70.52
1.326	13	7 1 0+	71.00
1.324	14	5 3 2	71.16
1.2984	14	6 0 2	72.78
1.2953	10	4 0 3	72.98
1.2835	12	4 1 3	73.76
1.2761	3	7 1 1	74.26
1.2531	9	6 4 1	75.86
1.2498	7	4 2 3	76.10
1.2420	6	7 2 1	76.66
1.2317	5	7 3 0	77.42
1.1910	7	7 3 1	80.60
1.1878	5	5 1 3	80.86
1.1657	9	0 0 4	82.72
1.1530	15	5 5 2	83.84
1.1361	2	6 4 2	85.38
1.1055	2	6 6 0	88.34
1.0947	5	6 1 3	89.44
1.0907	1	7 5 0	89.86
1.0687	8	8 3 1	92.24
1.0619	5	7 5 1	93.00
1.0476	6	8 0 2	94.66
1.0312	7	3 3 4	96.66
1.0231	4	8 4 1	97.68
1.0225	4	8 2 2	97.76
1.0190	6	4 2 4	98.22
1.0114	2	9 1 1	99.22
1.0090	2	7 1 3	99.54

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.503	20	3	1	1	35.85
2.345	2	4	0	0	38.35
2.331	1	0	0	2	38.58
2.272	100	3	2	1	39.64
2.211	55	3	3	0	40.78
2.200	65	1	1	2	41.00
2.098	35	4	2	0	43.09
2.095	16	4	0	1	43.14
2.088	16	2	0	2	43.30
2.045	75	4	1	1	44.26
1.913	20	4	2	1	47.49
1.907	55	2	2	2	47.64
1.840	20	5	1	0	49.50
1.833	13	3	1	2	49.70
1.711	7	5	1	1	53.50
1.653	9	4	0	2	55.53
1.604	5	3	3	2	57.39
1.483	4	6	2	0	62.57
1.482	1	6	0	1	62.62
1.464	17	6	1	1	63.48
1.413	1	6	2	1	66.04
1.398	1	5	4	1	66.89
1.377	3	3	1	3	68.04
1.351	5	4	4	2	69.50
1.339	1	6	3	1	70.21
1.334	15	3	2	3	70.52
1.327	8	7	1	0	70.99
1.327	5	5	5	0	70.99
1.324	10	5	3	2	71.14
1.301	3	6	4	0	72.62
1.2985	15	6	0	2	72.77
1.2956	3	4	0	3	72.96
1.2834	14	4	1	3	73.77
1.2760	3	7	1	1	74.27
1.2531	10	6	4	1	75.87
1.2515	1	6	2	2	75.98
1.2488	5	4	2	3	76.17
1.2420	7	7	2	1	76.66
1.2318	6	7	3	0	77.42
1.1909	8	7	3	1	80.60
1.1873	2	5	1	3	80.90
1.1657	10	0	0	4	82.72
1.1531	18	5	5	2	83.83
1.1360	2	6	4	2	85.38
1.1056	3	6	6	0	88.33
1.0948	6	6	1	3	89.44
1.0905	1	7	5	0	89.88
1.0687	9	8	3	1	92.23
1.0619	6	7	5	1	93.01
1.0476	7	8	0	2	94.67

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.0312	9	3	3	4	96.66
1.0233	3	8	4	1	97.66
1.0224	3	8	2	2	97.78
1.0190	6	4	2	4	98.22
1.0113	3	9	1	1	99.23
1.0091	2	7	1	3	99.52

	Vol. or Sec.	Page
Aluminum, Al	1	11
Aluminum antimony, AlSb	4	72
Aluminum bismuth oxide, $Al_4Bi_2O_9$	11m	5
Aluminum chloride, $AlCl_3$	9m	61
Aluminum chloride hydrate (chloraluminite), $AlCl_3 \cdot 6H_2O$	7	3
Aluminum copper, Al_4Cu_9	11m	79
Aluminum fluoride hydroxide silicate, topaz, $Al_2(F,OH)_2SiO_4$	1m	4
Aluminum lithium, Al_4Li_9	10m	98
Aluminum nickel, AlNi	6m	82
Aluminum nitride, AlN	12m	5
Aluminum nitrate hydrate, $Al(NO_3)_3 \cdot 9H_2O$	11m	6
Aluminum oxide (corundum), α-Al_2O_3	9	3
Aluminum oxide hydrate (boehmite), α-$Al_2O_3 \cdot H_2O$	3	38
Aluminum oxide hydrate, diaspore, β-$Al_2O_3 \cdot H_2O$	3	41
Aluminum phosphate, $Al(PO_3)_3$	2m	3
Aluminum phosphate (berlinite), $AlPO_4$ (trigonal)	10	3
Aluminum phosphate, $AlPO_4$ (orthorhombic)	10	4
Aluminum silicate (mullite), $Al_6Si_2O_{13}$	3m	3
Aluminum tungsten oxide, $Al_2(WO_4)_3$	11m	7
Ammonium aluminum fluoride, $(NH_4)_3AlF_6$	9m	5
Ammonium aluminum selenate hydrate, $NH_4Al(SeO_4)_2 \cdot 12H_2O$	9m	6
Ammonium aluminum sulfate, $NH_4Al(SO_4)_2$	10m	5
Ammonium aluminum sulfate hydrate (tschermigite), $NH_4Al(SO_4)_2 \cdot 12H_2O$	6	3
Ammonium azide, NH_4N_3	9	4
Ammonium beryllium fluoride, $(NH_4)_2BeF_4$	3m	5
Ammonium boron fluoride, NH_4BF_4	3m	6
Ammonium bromide, NH_4Br	2	49
Ammonium cadmium chloride, NH_4CdCl_3	5m	6
Ammonium cadmium sulfate, $(NH_4)_2Cd_2(SO_4)_3$	7m	5
Ammonium cadmium sulfate hydrate, $(NH_4)_2Cd(SO_4)_2 \cdot 6H_2O$	8m	5
Ammonium calcium sulfate, $(NH_4)_2Ca_2(SO_4)_3$	8m	7
Ammonium chlorate, NH_4ClO_4 (orthorhombic)	7	6
Ammonium chloride (sal-ammoniac), NH_4Cl	1	59
Ammonium chromium sulfate hydrate, $NH_4Cr(SO_4)_2 \cdot 12H_2O$	6	7
Ammonium cobalt (II) chloride, NH_4CoCl_3	6m	5
Ammonium cobalt fluoride, NH_4CoF_3	8m	9
Ammonium copper bromide hydrate, $(NH_4)_2CuBr_4 \cdot 2H_2O$	10m	6
Ammonium copper chloride, NH_4CuCl_3	7m	7
Ammonium copper chloride hydrate, $(NH_4)_2CuCl_4 \cdot 2H_2O$	12m	6
Ammonium copper fluoride, NH_4CuF_3	11m	8
Ammonium gallium sulfate hydrate, $NH_4Ga(SO_4)_2 \cdot 12H_2O$	6	9
Ammonium germanium fluoride, $(NH_4)_2GeF_6$	6	8
Ammonium hydrogen carbonate (teschemacherite), $(NH_4)HCO_3$	9	5
Ammonium hydrogen phosphate, $NH_4H_2PO_4$	4	64
Ammonium iodate, NH_4IO_3	10m	7
Ammonium iodide, NH_4I	4	56
Ammonium iridium chloride, $(NH_4)_2IrCl_6$	8	6
Ammonium iron chloride hydrate, $(NH_4)_2FeCl_5 \cdot H_2O$	14m	7
Ammonium iron fluoride, $(NH_4)_3FeF_6$	9m	9
Ammonium iron sulfate, $NH_4Fe(SO_4)_2$	10m	8
Ammonium iron sulfate hydrate, $NH_4Fe(SO_4)_2 \cdot 12H_2O$	6	10
Ammonium lead chloride, $(NH_4)_2PbCl_6$	11m	10
Ammonium magnesium aluminum fluoride, NH_4MgAlF_6	10m	9
Ammonium magnesium chromium oxide hydrate, $(NH_4)_2Mg(CrO_4)_2 \cdot 6H_2O$	8m	10
Ammonium magnesium phosphate hydrate (struvite), $MgNH_4PO_4 \cdot 6H_2O$	3m	41
Ammonium manganese chloride hydrate, $(NH_4)_2MnCl_4 \cdot 2H_2O$	11m	11
Ammonium manganese(II) fluoride, NH_4MnF_3	5m	8
Ammonium manganese sulfate, $(NH_4)_2Mn_2(SO_4)_3$	7m	8
Ammonium manganese sulfate hydrate, $(NH_4)_2Mn(SO_4)_2 \cdot 6H_2O$	8m	12
Ammonium mercury chloride, NH_4HgCl_3	8m	14
Ammonium molybdenum oxide phosphate hydrate, $(NH_4)_3(MoO_3)_{12}PO_4 \cdot 4H_2O$	8	10
Ammonium nickel(II) chloride, NH_4NiCl_3	6m	6
Ammonium nickel chromium oxide hydrate, $(NH_4)_2Ni(CrO_4)_2 \cdot 6H_2O$	8m	16
Ammonium nitrate (nitrammite), NH_4NO_3	7	4
Ammonium osmium bromide, $(NH_4)_2OsBr_6$	3	71
Ammonium osmium chloride, $(NH_4)_2OsCl_6$	1m	6
Ammonium palladium chloride, $(NH_4)_2PdCl_4$	6	6
Ammonium palladium chloride, $(NH_4)_2PdCl_6$	8	7
Ammonium platinum bromide, $(NH_4)_2PtBr_6$	9	6
Ammonium platinum chloride, $(NH_4)_2PtCl_6$	5	3
Ammonium potassium iron chloride hydrate (kremersite), $(NH_4,K)_2FeCl_5 \cdot H_2O$	14m	8
Ammonium rhenium oxide, NH_4ReO_4	9	7
Ammonium selenium bromide, $(NH_4)_2SeBr_6$	8	4

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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Ammonium silicon fluoride (cryptohalite), $(NH_4)_2SiF_6$	5	5
Ammonium strontium chromium oxide, $(NH_4)_2Sr(CrO_4)_2$	14m	9
Ammonium sulfate (mascagnite), $(NH_4)_2SO_4$	9	8
Ammonium tellurium bromide, $(NH_4)_2TeBr_6$	8	5
Ammonium tellurium chloride, $(NH_4)_2TeCl_6$	8	8
Ammonium tin chloride, $(NH_4)_2SnCl_6$	5	4
Ammonium vanadium oxide, NH_4VO_3	8	9
Ammonium zinc fluoride, NH_4ZnF_3	8m	18
Ammonium zirconium fluoride, $(NH_4)_3ZrF_7$	6	14
Antimony, Sb	3	14
Antimony cerium, CeSb	4m	40
Antimony dysprosium, DySb	4m	41
Antimony erbium, ErSb	4m	41
Antimony(III) fluoride, SbF_3	2m	4
Antimony gadolinium, GdSb	4m	42
Antimony gallium, GaSb	6	30
Antimony gold (aurostibite), $AuSb_2$	7	18
Antimony indium, InSb	4	73
Antimony(III) iodide, SbI_3	6	16
Antimony lanthanum, LaSb	4m	42
Antimony neodymium, NdSb	4m	43
Antimony(III) oxide (senarmontite), Sb_2O_3 (cubic)	3	31
Antimony(III) oxide, valentinite, Sb_2O_3 (orthorhombic)	10	6
Antimony(IV) oxide (cervantite), Sb_2O_4	10	8
Antimony(V) oxide, Sb_2O_5	10	10
Antimony praseodymium, PrSb	4m	43
Antimony scandium, SbSc	4m	44
Antimony selenide, Sb_2Se_3	3m	7
Antimony silver sulfide, $AgSbS_2$ (cubic)	5m	48
Antimony silver sulfide (miargyrite), $AgSbS_2$ (monoclinic)	5m	49
Antimony silver sulfide (pyrargyrite), Ag_3SbS_3 (trigonal)	5m	51
Antimony silver telluride, $AgSbTe_2$	3m	47
Antimony(III) sulfide (stibnite), Sb_2S_3	5	6
Antimony telluride, Sb_2Te_3	3m	8
Antimony terbium, SbTb	5m	61
Antimony thorium, SbTh	4m	44
Antimony thulium, SbTm	4m	45
Antimony ytterbium, SbYb	4m	45
Antimony yttrium, SbY	4m	46
Arsenic, As	3	6
Arsenic cerium, AsCe	4m	51
Arsenic(III) iodide, AsI_3	13m	7
Arsenic oxide (arsenolite), As_2O_3 (cubic)	1	51
Arsenic oxide, claudetite, As_2O_3 (monoclinic)	3m	9
Barium, Ba	4	7
Barium aluminum oxide, $BaAl_2O_4$	5m	11
Barium aluminum oxide, $Ba_3Al_2O_6$	12m	7
Barium arsenate, $Ba_3(AsO_4)_2$	2m	6
Barium borate, BaB_4O_7	4m	6
Barium borate, high form, BaB_2O_4	4m	4
Barium borate, BaB_8O_{13}	7m	10
Barium bromate hydrate, $Ba(BrO_3)_2 \cdot H_2O$	8m	19
Barium bromide, $BaBr_2$	10m	63
Barium bromide fluoride, BaBrF	10m	10
Barium bromide hydrate, $BaBr_2 \cdot H_2O$	3m	10
Barium calcium nitrate, $Ba_{.25}Ca_{.75}(NO_3)_2$	12m	38
Barium calcium nitrate, $Ba_{.50}Ca_{.50}(NO_3)_2$	12m	38
Barium calcium nitrate, $Ba_{.75}Ca_{.25}(NO_3)_2$	12m	38
Barium calcium tungsten oxide, Ba_2CaWO_6	9m	10
Barium carbonate (witherite), $BaCO_3$ (orthorhombic)	2	54
Barium carbonate, $BaCO_3$ (cubic) at 1075 °C	10	11
Barium chlorate hydrate, $Ba(ClO_4)_2 \cdot 3H_2O$	2m	7
Barium chlorate hydrate, $Ba(ClO_3)_2 \cdot H_2O$	8m	21
Barium chloride, $BaCl_2$, (cubic)	9m	13
Barium chloride, $BaCl_2$, (orthorhombic)	9m	11
Barium chloride fluoride, BaClF	10m	11
Barium chloride hydrate, $BaCl_2 \cdot 2H_2O$	12m	9
Barium fluoride, BaF_2	1	70
Barium hydroxide phosphate, $Ba_5(OH)(PO_4)_3$	11m	12
Barium iodide, BaI_2	10m	66
Barium lead chloride, $BaPbCl_4$	11m	13
Barium lead nitrate, $Ba_{.67}Pb_{.33}(NO_3)_2$	12m	40
Barium lead nitrate, $Ba_{.67}Pb_{.33}(NO_3)_2$	12m	40
Barium molybdenum oxide, $BaMoO_4$	7	7
Barium molybdenum oxide, Ba_2MoO_5	12m	10
Barium nitrate (nitrobarite), $Ba(NO_3)_2$	11m	14
Barium oxide, BaO	9m	63
Barium oxide, BaO_2	6	18
Barium phosphate, $Ba_3(PO_4)_2$	12m	12
Barium selenide, BaSe	5m	61
Barium silicate, β-$BaSiO_3$	13m	8
Barium silicate (sanbornite), β-$BaSi_2O_5$	13m	10
Barium silicate, Ba_2SiO_4	13m	12
Barium silicate, $Ba_2Si_3O_8$	13m	13
Barium silicate, Ba_3SiO_5	13m	15
Barium silicate, $Ba_3Si_5O_{13}$	13m	17
Barium silicon fluoride, $BaSiF_6$	4m	7
Barium strontium nitrate, $Ba_{.25}Sr_{.75}(NO_3)_2$	12m	42
Barium strontium nitrate, $Ba_{.50}Sr_{.50}(NO_3)_2$	12m	42
Barium strontium nitrate, $Ba_{.75}Sr_{.25}(NO_3)_2$	12m	42
Barium sulfate (baryte), $BaSO_4$	10m	12
Barium sulfide, BaS	7	8
Barium tin oxide, $BaSnO_3$	3m	11
Barium titanium oxide, $BaTiO_3$	3	45
Barium titanium silicate (fresnoite), $Ba_2TiSi_2O_8$	9m	14
Barium tungsten oxide, $BaWO_4$	7	9
Barium tungsten oxide, Ba_2WO_5	12m	14

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Barium vanadium oxide, $Ba_3(VO_4)_2$	14m	10
Barium zirconium oxide, $BaZrO_3$	5	8
Beryllium, alpha, Be	9m	64
Beryllium aluminum oxide (chrysoberyl), $BeAl_2O_4$	9	10
Beryllium aluminum silicate, beryl, $Be_3Al_2(SiO_3)_6$	9	13
Beryllium calcium oxide, $Be_{17}Ca_{12}O_{29}$	7m	89
Beryllium chromium oxide, $BeCr_2O_4$	10	12
Beryllium cobalt, BeCo	5m	62
Beryllium germanium oxide, Be_2GeO_4	10	13
Beryllium lanthanum oxide, $Be_2La_2O_5$	9m	65
Beryllium niobium, Be_2Nb	7m	92
Beryllium oxide (bromellite), BeO	1	36
Beryllium palladium, BePd	5m	62
Beryllium silicate, phenacite, Be_2SiO_4	8	11
Bismuth, Bi	3	20
Bismuth cerium, BiCe	4m	46
Bismuth dysprosium, BiDy	4m	47
Bismuth erbium, BiEr	4m	47
Bismuth fluoride, BiF_3	1m	7
Bismuth holmium, BiHo	4m	48
Bismuth(III) iodide, BiI_3	6	20
Bismuth lanthanum, BiLa	4m	48
Bismuth neodymium, BiNd	4m	49
Bismuth oxide (bismite), α-Bi_2O_3	3m	16
Bismuth oxide bromide, BiOBr	8	14
Bismuth oxide chloride (bismoclite), BiOCl	4	54
Bismuth oxide iodide, BiOI	9	16
Bismuth phosphate, $BiPO_4$ (monoclinic)	3m	11
Bismuth phosphate, $BiPO_4$ (trigonal)	3m	13
Bismuth praseodymium, BiPr	4m	49
Bismuth sulfide (bismuthinite), Bi_2S_3	5m	13
Bismuth telluride, BiTe	4m	50
Bismuth telluride (tellurobismuthite), Bi_2Te_3	3m	16
Bismuth vanadium oxide, low form, $BiVO_4$(tetragonal)	3m	14
Bismuth vanadium oxide, high form, $BiVO_4$ (monoclinic)	3m	14
Boron oxide, B_2O_3, phase 1	10m	70
Cadmium, Cd	3	10
Cadmium ammine chloride, $Cd(NH_3)_2Cl_2$	10m	14
Cadmium bromide, $CdBr_2$	9	17
Cadmium bromide chloride, CdBrCl	11m	15
Cadmium carbonate (otavite), $CdCO_3$	7	11
Cadmium cerium, CdCe	5m	63
Cadmium chlorate hydrate, $Cd(ClO_4)_2 \cdot 6H_2O$	3m	19
Cadmium chloride, $CdCl_2$	9	18
Cadmium chromium oxide, $CdCr_2O_4$	5m	16
Cadmium copper, Cd_8Cu_5	11m	81
Cadmium cyanide, $Cd(CN)_2$	2m	8
Cadmium fluoride, CdF_2	10m	15
Cadmium iron oxide, $CdFe_2O_4$	9m	16
Cadmium lanthanum, CdLa	5m	63
Cadmium manganese oxide, $CdMn_2O_4$	10m	16
Cadmium molybdenum oxide, $CdMoO_4$	6	21
Cadmium nitrate hydrate, $Cd(NO_3)_2 \cdot 4H_2O$	7m	93
Cadmium oxide, CdO	2	27
Cadmium oxide, CdO (ref. standard)	8m	2
Cadmium praseodymium, CdPr	5m	64
Cadmium selenide (cadmoselite), CdSe (hexagonal)	7	12
Cadmium silicate, Cd_2SiO_4	13m	19
Cadmium silicate, Cd_3SiO_5	13m	20
Cadmium sulfate, $CdSO_4$	3m	20
Cadmium sulfate hydrate, $3CdSO_4 \cdot 8H_2O$	6m	8
Cadmium sulfate hydrate, $CdSO_4 \cdot H_2O$	6m	10
Cadmium sulfide (greenockite), CdS	4	15
Cadmium telluride, CdTe	3m	21
Cadmium tungsten oxide, $CdWO_4$	2m	8
Calcium, Ca	9m	68
Calcium aluminum germanium oxide, $Ca_3Al_2(GeO_4)_3$	10	15
Calcium aluminum hydroxide, $Ca_3Al_2(OH)_{12}$	11m	16
Calcium aluminum oxide, $Ca_3Al_2O_6$	5	10
Calcium aluminum oxide (mayenite), $Ca_{12}Al_{14}O_{33}$	9	20
Calcium aluminum sulfate hydrate (ettringite), $Ca_6Al_2S_3O_{18} \cdot 31H_2O$	8	3
Calcium bromide, $CaBr_2$	11m	70
Calcium bromide hydrate, $CaBr_2 \cdot 6H_2O$	8	15
Calcium carbonate (aragonite), $CaCO_3$ (orthorhombic)	3	53
Calcium carbonate (aragonite), $CaCO_3$ (orthorhombic, calculated pattern)	14m	44
Calcium carbonate (calcite), $CaCO_3$ (hexagonal)	2	51
Calcium chloride (hydrophilite), $CaCl_2$	11m	18
Calcium chloride fluoride, CaClF	10m	17
Calcium chloride hydrate, $CaCl_2 \cdot 4H_2O$	11m	73
Calcium chloride hydrate (antarcticite), $CaCl_2 \cdot 6H_2O$	12m	16
Calcium chromium germanium oxide, $Ca_3Cr_2(GeO_4)_3$	10	16
Calcium chromium oxide (chromatite), $CaCrO_4$	7	13
Calcium chromium silicate (uvarovite), $Ca_3Cr_2(SiO_4)_3$	10	17
Calcium fluoride (fluorite), CaF_2	1	69
Calcium fluoride phosphate (fluorapatite), $Ca_5F(PO_4)_3$	3m	22
Calcium gallium germanium oxide, $Ca_3Ga_2(GeO_4)_3$	10	18
Calcium hydrogen phosphate hydrate, $Ca_8H_2(PO_4)_6 \cdot 5H_2O$	13m	21
Calcium hydroxide (portlandite), $Ca(OH)_2$	1	58
Calcium iodate (lautarite), $Ca(IO_3)_2$	14m	12
Calcium iodate hydrate, $Ca(IO_3)_2 \cdot 6H_2O$	14m	13
Calcium iron germanium oxide, $Ca_3Fe_2(GeO_4)_3$	10	19
Calcium iron silicate (andradite), $Ca_3Fe_2Si_3O_{12}$	9	22
Calcium iron silicate hydroxide, julgoldite, $Ca_2Fe_3Si_3O_{10}(OH,O)_2(OH)_2$	10m	72
Calcium lead nitrate, $Ca_{.33}Pb_{.67}(NO_3)_2$	12m	44
Calcium lead nitrate, $Ca_{.67}Pb_{.33}(NO_3)_2$	12m	44

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Calcium magnesium silicate (diopside), $CaMg(SiO_3)_2$	5m	17
Calcium molybdenum oxide (powellite), $CaMoO_4$	6	22
Calcium nitrate, $Ca(NO_3)_2$	7	14
Calcium oxide, (lime), CaO	1	43
Calcium oxide, (lime), CaO (calculated pattern)	14m	49
Calcium oxide phosphate, $Ca_4O(PO_4)_2$	12m	17
Calcium phosphate, β-$Ca_2P_2O_7$	7m	95
Calcium platinum oxide, Ca_4PtO_6	10m	18
Calcium selenide, CaSe	5m	64
Calcium strontium nitrate, $Ca_{.33}Sr_{.67}(NO_3)_2$	12m	46
Calcium strontium nitrate, $Ca_{.67}Sr_{.33}(NO_3)_2$	12m	46
Calcium sulfate (anhydrite), $CaSO_4$	4	65
Calcium sulfide (oldhamite), CaS	7	15
Calcium telluride, CaTe	4m	50
Calcium titanium oxide (perovskite), $CaTiO_3$	9m	17
Calcium tungsten oxide, Ca_3WO_6	9m	19
Calcium tungsten oxide, scheelite, $CaWO_4$	6	23
Carbon, diamond, C	2	5
Cerium arsenate, $CeAsO_4$	4m	8
Cerium(III) chloride, $CeCl_3$	1m	8
Cerium cobalt, $CeCo_2$	13m	50
Cerium cobalt, $Ce_{24}Co_{11}$	13m	51
Cerium copper, $CeCu_6$	7m	99
Cerium(III) fluoride, CeF_3	8	17
Cerium gallium, $CeGa_2$	13m	54
Cerium magnesium, CeMg	5m	65
Cerium magnesium, $CeMg_3$	13m	56
Cerium nickel, $CeNi_2$	13m	58
Cerium niobium titanium oxide (aeschynite), $CeNbTiO_6$	3m	24
Cerium nitride, CeN	4m	51
Cerium(IV) oxide (cerianite), CeO_2	1	56
Cerium phosphide, CeP	4m	52
Cerium thallium, CeTl	13m	59
Cerium thallium, $CeTl_3$	13m	60
Cerium thallium, Ce_3Tl	13m	61
Cerium(III) vanadium oxide, $CeVO_4$	1m	9
Cerium zinc, CeZn	5m	65
Cerium zinc, $CeZn_3$	14m	50
Cerium zinc, $CeZn_5$	14m	53
Cerium zinc, Ce_2Zn_{17}	14m	55
Cesium aluminum sulfate hydrate, $CsAl(SO_4)_2 \cdot 12H_2O$	6	25
Cesium antimony fluoride, $CsSbF_6$	4m	9
Cesium beryllium fluoride, $CsBeF_3$	9m	69
Cesium boron fluoride, $CsBF_4$	8	22
Cesium bromate, $CsBrO_3$	8	18
Cesium bromide, CsBr	3	49
Cesium cadmium bromide, $CsCdBr_3$ (hexagonal)	10m	20
Cesium cadmium chloride, $CsCdCl_3$ (hexagonal)	5m	19
Cesium calcium chloride, $CsCaCl_3$	5m	21
Cesium calcium fluoride, $CsCaF_3$	8m	25
Cesium calcium sulfate, $Cs_2Ca_2(SO_4)_3$	7m	12
Cesium cerium chloride, Cs_2CeCl_6	14m	58
Cesium chlorate, $CsClO_3$	8	20
Cesium chlorate, $CsClO_4$, (orthorhombic)	1m	10
Cesium chloride, CsCl	2	44
Cesium chromium oxide, Cs_2CrO_4	3m	25
Cesium chromium sulfate hydrate, $CsCr(SO_4)_2 \cdot 12H_2O$	8	21
Cesium cobalt(II) chloride, $CsCoCl_3$	6m	11
Cesium cobalt chloride, Cs_2CoCl_4	11m	19
Cesium copper(II) chloride, $CsCuCl_3$	5m	22
Cesium copper chloride, Cs_2CuCl_4	11m	20
Cesium copper sulfate hydrate, $Cs_2Cu(SO_4)_2 \cdot 6H_2O$	7m	14
Cesium fluoride, CsF	3m	26
Cesium gallium sulfate hydrate, $CsGa(SO_4)_2 \cdot 12H_2O$	8	23
Cesium germanium fluoride, Cs_2GeF_6	5	17
Cesium iodide, CsI	4	47
Cesium iodine bromide, CsI_2Br	7m	103
Cesium iodine chloride, $CsICl_2$	3	50
Cesium iron chloride hydrate, $Cs_2FeCl_5 \cdot H_2O$	14m	14
Cesium iron sulfate hydrate, $Cs_2Fe(SO_4)_2 \cdot 6H_2O$	7m	16
Cesium iron sulfate hydrate, $CsFe(SO_4)_2 \cdot 12H_2O$	6	28
Cesium lead(II) chloride, $CsPbCl_3$ (tetragonal)	5m	24
Cesium lead fluoride, $CsPbF_3$	8m	26
Cesium lithium cobalt cyanide, $CsLiCo(CN)_6$	10m	79
Cesium lithium fluoride, $CsLiF_2$	7m	105
Cesium magnesium chromium oxide, $Cs_2Mg_2(CrO_4)_3$	8m	27
Cesium magnesium chromium oxide hydrate, $Cs_2Mg(CrO_4)_2 \cdot 6H_2O$	8m	29
Cesium magnesium sulfate hydrate, $Cs_2Mg(SO_4)_2 \cdot 6H_2O$	7m	18
Cesium manganese fluoride, $CsMnF_3$	10m	21
Cesium manganese sulfate hydrate, $Cs_2Mn(SO_4)_2 \cdot 6H_2O$	7m	20
Cesium mercury chloride, $CsHgCl_3$	7m	22
Cesium nickel(II) chloride, $CsNiCl_3$	6m	12
Cesium nickel sulfate hydrate, $Cs_2Ni(SO_4)_2 \cdot 6H_2O$	7m	23
Cesium nitrate, $CsNO_3$	9	25
Cesium osmium(IV) bromide, Cs_2OsBr_6	2m	10
Cesium osmium chloride, Cs_2OsCl_6	2m	11
Cesium platinum bromide, Cs_2PtBr_6	8	19
Cesium platinum chloride, Cs_2PtCl_6	5	14
Cesium platinum fluoride, Cs_2PtF_6	6	27
Cesium selenium bromide, Cs_2SeBr_6	8	20
Cesium silicon fluoride, Cs_2SiF_6	5	19
Cesium strontium chloride, $CsSrCl_3$	6m	13
Cesium sulfate, Cs_2SO_4	7	17
Cesium tellurium bromide, Cs_2TeBr_6	9	24
Cesium tin chloride, Cs_2SnCl_6	5	16
Cesium vanadium sulfate hydrate, $CsV(SO_4)_2 \cdot 12H_2O$	1m	11
Cesium zinc sulfate hydrate, $Cs_2Zn(SO_4)_2 \cdot 6H_2O$	7m	25
Chromium, Cr	5	20
Chromium chloride, $CrCl_2$	11m	77
Chromium cobalt silicide, $Co_9Cr_{15}Si_6$	14m	62
Chromium fluoride, CrF_2	10m	81

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Chromium fluoride, Cr_2F_5	7m	108
Chromium(III) fluoride hydrate, $CrF_3 \cdot 3H_2O$	5m	25
Chromium iridium 3:1, Cr_3Ir	6m	14
Chromium(III) oxide, Cr_2O_3	5	22
Chromium phosphate, α-$CrPO_4$	2m	12
Chromium phosphate, β-$CrPO_4$	9	26
Chromium rhodium 3:1, Cr_3Rh	6m	15
Chromium silicide, Cr_3Si	6	29
Cobalt, Co (cubic)	4m	10
Cobalt aluminum oxide, $CoAl_2O_4$	9	27
Cobalt ammine iodide, $Co(NH_3)_6I_3$	10m	83
Cobalt antimony oxide, $CoSb_2O_6$	5m	26
Cobalt arsenide, $CoAs_2$	4m	10
Cobalt arsenide (skutterudite), $CoAs_3$	10	21
Cobalt borate, $Co_3(BO_3)_2$	12m	20
Cobalt bromide hydrate, $CoBr_2 \cdot 6H_2O$	12m	21
Cobalt(II) carbonate (spherocobaltite), $CoCO_3$	10	24
Cobalt chlorate hydrate, $Co(ClO_4)_2 \cdot 6H_2O$	3m	28
Cobalt chloride hydrate, $CoCl_2 \cdot 2H_2O$	11m	22
Cobalt chloride hydrate, $CoCl_2 \cdot 6H_2O$	11m	23
Cobalt chromium oxide, $CoCr_2O_4$	9m	21
Cobalt copper tin, $CoCu_2Sn$	14m	64
Cobalt dysprosium, Co_2Dy	13m	63
Cobalt erbium, Co_2Er	13m	64
Cobalt erbium, Co_7Er_2	13m	65
Cobalt fluoride, CoF_2	10m	85
Cobalt fluoride hydrate, $CoF_2 \cdot 4H_2O$	11m	24
Cobalt gadolinium, $CoGd_3$	13m	68
Cobalt gadolinium, Co_2Gd	13m	71
Cobalt gadolinium, Co_7Gd_2	13m	72
Cobalt gallium hafnium, Co_2GaHf	14m	65
Cobalt gallium manganese, Co_2GaMn	13m	75
Cobalt gallium niobium, Co_2GaNb	14m	66
Cobalt gallium oxide, $CoGa_2O_4$	10	27
Cobalt gallium tantalum, Co_2GaTa	13m	76
Cobalt gallium titanium, Co_2GaTi	13m	77
Cobalt gallium vanadium, Co_2GaV	13m	78
Cobalt germanium, Co_3Ge_2	14m	67
Cobalt germanium hafnium, $Co_{16}Ge_7Hf_6$	14m	69
Cobalt germanium manganese, Co_2GeMn	13m	79
Cobalt germanium niobium, $Co_{16}Ge_7Nb_6$	14m	71
Cobalt germanium oxide, Co_2GeO_4	10	27
Cobalt germanium tantalum, $Co_{16}Ge_7Ta_6$	14m	73
Cobalt germanium titanium, Co_2GeTi	13m	80
Cobalt hafnium tin, Co_2HfSn	14m	75
Cobalt holmium, Co_2Ho	14m	76
Cobalt indium, $CoIn_3$	13m	81
Cobalt iodide, CoI_2	4m	52
Cobalt iron arsenide (safflorite), $CoFeAs_4$	10	28
Cobalt iron oxide, $CoFe_2O_4$	9m	22
Cobalt iron sulfide, Co_8FeS_8	14m	77
Cobalt iron vanadium, $Co_{4.35}Fe_{13.47}V_{12.18}$	14m	79
Cobalt lanthanum, $CoLa_3$	13m	83
Cobalt lutetium, Co_2Lu	13m	86
Cobalt manganese silicide, Co_2MnSi	14m	81
Cobalt mercury thiocyanate, $Co[Hg(CNS)_4]$	2m	13
Cobalt molybdenum, Co_2Mo	14m	82
Cobalt neodymium, Co_2Nd	13m	87
Cobalt nickel tin, $Co_{.75}Ni_{.75}Sn_{.75}$	13m	88
Cobalt nitrate hydrate, α-$Co(NO_3)_2 \cdot 6H_2O$	12m	22
Cobalt(II) oxide, CoO	9	28
Cobalt(II,III) oxide, Co_3O_4	9	29
Cobalt phosphate, $Co(PO_3)_2$	13m	23
Cobalt phosphide, CoP	14m	83
Cobalt phosphide, CoP_3	14m	85
Cobalt plutonium, $CoPu_2$	14m	87
Cobalt plutonium, $CoPu_6$	14m	89
Cobalt plutonium, Co_2Pu	14m	91
Cobalt plutonium, Co_3Pu	14m	92
Cobalt plutonium, $Co_{17}Pu_2$	14m	94
Cobalt praseodymium, Co_2Pr	14m	97
Cobalt rhodium sulfide, Co_8RhS_8	14m	98
Cobalt ruthenium sulfide, Co_8RuS_8	14m	100
Cobalt samarium, Co_5Sm	13m	90
Cobalt silicate, Co_2SiO_4 (orthorhombic)	4m	11
Cobalt silicon fluoride hydrate, $CoSiF_6 \cdot 6H_2O$	3m	27
Cobalt sulfate, β-$CoSO_4$	2m	14
Cobalt tantalum silicide, $Co_{16}Ta_6Si_7$	14m	102
Cobalt thorium, $Co_{17}Th_2$	12m	64
Cobalt tin, Co_3Sn_2	13m	92
Cobalt titanium oxide, $CoTiO_3$	4m	13
Cobalt titanium silicide, $Co_{16}Ti_6Si_7$	14m	104
Cobalt tungsten oxide, $CoWO_4$	4m	13
Copper, Cu	1	15
Copper ammine selenate, $Cu(NH_3)_4SeO_4$	10m	87
Copper ammine sulfate hydrate, $Cu(NH_3)_4SO_4 \cdot H_2O$	10m	90
Copper antimony oxide, $CuSb_2O_6$	5m	27
Copper(I) bromide, CuBr	4	36
Copper(I) chloride (nantokite), CuCl	4	35
Copper fluoride hydrate, $CuF_2 \cdot 2H_2O$	11m	25
Copper hydrogen phosphite hydrate, $CuHPO_3 \cdot 2H_2O$	11m	83
Copper hydroxide carbonate, azurite, $Cu_3(OH)_2(CO_3)_2$	10	30
Copper hydroxide carbonate (malachite), $Cu_2(OH)_2CO_3$	10	31
Copper(I) iodide (marchite), CuI	4	38
Copper(I) oxide (cuprite), Cu_2O	2	23
Copper(II) oxide (tenorite), CuO	1	49
Copper phosphate, $Cu(PO_3)_2$	14m	15
Copper phosphate, α-$Cu_2P_2O_7$	7m	113
Copper sulfate (chalcocyanite), $CuSO_4$	3m	29
Copper(II) sulfide (covellite), CuS	4	13
Copper uranium oxide, $CuUO_4$	10m	93
Dysprosium arsenate, $DyAsO_4$	3m	30
Dysprosium arsenide, DyAs	4m	53
Dysprosium gallium oxide, $Dy_3Ga_5O_{12}$	2m	15
Dysprosium gold, DyAu	5m	66
Dysprosium nitride, DyN	4m	53
Dysprosium oxide, Dy_2O_3	9	30
Dysprosium silver, DyAg	5m	66
Dysprosium telluride, DyTe	4m	54
Dysprosium vanadium oxide, $DyVO_4$	4m	15
Erbium arsenate, $ErAsO_4$	3m	31
Erbium arsenide, ErAs	4m	54

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Erbium gallium oxide, $Er_3Ga_5O_{12}$	1m	12
Erbium manganese oxide, $ErMnO_3$	2m	16
Erbium nitride, ErN	4m	55
Erbium oxide, Er_2O_3	8	25
Erbium phosphate, $ErPO_4$	9	31
Erbium silver, ErAg	5m	67
Erbium telluride, ErTe	4m	55
Erbium vanadium oxide, $ErVO_4$	5m	29
Europium arsenate, $EuAsO_4$	3m	32
Europium(III) chloride, $EuCl_3$	1m	13
Europium gallium oxide, $Eu_3Ga_5O_{12}$	2m	17
Europium nitride, EuN	4m	56
Europium oxide, EuO	4m	56
Europium oxychloride, EuOCl	1m	13
Europium phosphate, $EuPO_4$	11m	26
Europium(III) vanadium oxide, $EuVO_4$	4m	16
Gadolinium arsenate, $GdAsO_4$	4m	17
Gadolinium arsenide, GdAs	4m	57
Gadolinium chloride hydrate, $GdCl_3 \cdot 6H_2O$	7m	118
Gadolinium fluoride, GdF_3	1m	14
Gadolinium gallium oxide, $Gd_3Ga_5O_{12}$	2m	18
Gadolinium indium, GdIn	5m	67
Gadolinium nitride, GdN	4m	57
Gadolinium oxide, Gd_2O_3	1m	16
Gadolinium oxychloride, GdOCl	1m	17
Gadolinium silver, GdAg	6m	87
Gadolinium titanium oxide, Gd_2TiO_5	8m	32
Gadolinium vanadium oxide, $GdVO_4$	5m	30
Gallium, Ga	2	9
Gallium arsenide, GaAs	3m	33
Gallium lutetium oxide, $Ga_5Lu_3O_{12}$	2m	22
Gallium magnesium, Ga_2Mg	12m	48
Gallium magnesium, Ga_5Mg_2	12m	51
Gallium neodymium oxide, $Ga_5Nd_3O_{12}$	1m	34
Gallium oxide, α-Ga_2O_3	4	25
Gallium phosphate (α-quartz type), $GaPO_4$	8	27
Gallium phosphate hydrate, $GaPO_4 \cdot 2H_2O$	8m	34
Gallium samarium oxide, $Ga_5Sm_3O_{12}$	1m	42
Gallium ytterbium oxide, $Ga_5Yb_3O_{12}$	1m	49
Gallium yttrium oxide, $Ga_5Y_3O_{12}$	1m	50
Germanium, Ge	1	18
Germanium iodide, GeI_2	4m	58
Germanium(IV) iodide, GeI_4	5	25
Germanium oxide, GeO_2 (hexagonal) (low form)	1	51
Germanium oxide, GeO_2 (tetragonal) (high form)	8	28
Gold, Au	1	33
Gold(I) cyanide, AuCN	10	33
Gold holmium, AuHo	5m	68
Gold magnesium, AuMg	6m	83
Gold niobium, $AuNb_3$	6m	16
Gold potassium cyanide, $AuK(CN)_2$	8m	36
Gold tin 1:1, AuSn	7	19
Gold titanium 1:3, $AuTi_3$	6m	17
Gold vanadium, AuV_3	6m	18
Hafnium, Hf	3	18
Holmium arsenate, $HoAsO_4$	3m	34
Holmium fluoride, HoF_3	10m	23
Holmium nitride, HoN	4m	58
Holmium oxide, Ho_2O_3	9	32
Holmium selenide, HoSe	4m	59
Holmium silver, HoAg	5m	68
Holmium vanadium oxide, $HoVO_4$	4m	18
Hydrogen amidosulfate, H_2NSO_3H	7	54
Hydrogen arsenate, $H_5As_3O_{10}$	7m	84
Hydrogen borate, β-HBO_2	9m	71
Hydrogen borate (metaborite), HBO_2 (cubic)	4m	27
Hydrogen iodate, HIO_3	5	28
Hydrogen iodate, HI_3O_8	8m	104
Hydrogen phosphate hydrate, $H_3PO_4 \cdot \frac{1}{2}H_2O$	12m	56
Hydrogen tellurate, H_6TeO_6	12m	34
Indium, In	3	12
Indium arsenide, InAs	3m	35
Indium oxide, In_2O_3	5	26
Indium phosphate, $InPO_4$	8	29
Indium sulfide, In_2S_3	11m	30
Iodine, I_2	3	16
Iridium, Ir	4	9
Iridium niobium, $IrNb_3$	6m	19
Iridium oxide, IrO_2	4m	19
Iridium titanium 1:3, $IrTi_3$	6m	20
Iridium vanadium, IrV_3	6m	21
Iron, α-Fe	4	3
Iron arsenide, FeAs	1m	19
Iron arsenide (loellingite), $FeAs_2$	10	34
Iron bromide, $FeBr_2$	4m	59
Iron chloride hydrate, $FeCl_2 \cdot 2H_2O$	11m	32
Iron fluoride hydrate, $FeF_2 \cdot 4H_2O$	11m	90
Iron hydroxide sulfate hydrate, butlerite, $Fe(OH)SO_4 \cdot 2H_2O$	10m	95
Iron iodide, FeI_2	4m	60
Iron(II,III) oxide (magnetite), Fe_3O_4	5m	31
Iron sulfate hydrate (melanterite), $FeSO_4 \cdot 7H_2O$	8m	38
Iron sulfide (pyrite), FeS_2	5	29
Iron thorium, $Fe_{17}Th_2$	12m	67
Lanthanum arsenate, $LaAsO_4$	3m	36
Lanthanum arsenide, LaAs	4m	60
Lanthanum borate, $LaBO_3$	1m	20
Lanthanum chloride, $LaCl_3$	1m	20
Lanthanum fluoride, LaF_3	7	21
Lanthanum magnesium, LaMg	5m	69
Lanthanum niobium titanium oxide, $LaNbTiO_6$	3m	37
Lanthanum nitrate hydrate, $La(NO_3)_3 \cdot 6H_2O$	8m	40
Lanthanum nitride, LaN	4m	61
Lanthanum oxide, La_2O_3	3	33
Lanthanum oxychloride, LaOCl	7	22
Lanthanum phosphide, LaP	5m	69
Lanthanum selenide, LaSe	4m	61
Lanthanum zinc, LaZn	5m	70
Lead, Pb	1	34
Lead borate, PbB_4O_7	4m	19
Lead bromide, $PbBr_2$	2	47
Lead bromide chloride, PbBrCl	11m	33
Lead bromide fluoride, PbBrF	10m	25
Lead chloride (cotunnite), $PbCl_2$	12m	23
Lead carbonate (cerussite), $PbCO_3$	2	56
Lead chloride fluoride (matlockite), PbClF	13m	25

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Lead chromium oxide, Pb_2CrO_5	14m	16
Lead fluoride, α-PbF_2 (orthorhombic)	5	31
Lead fluoride, β-PbF_2 (cubic)	5	33
Lead fluoride iodide, PbFI	10m	26
Lead hydrogen arsenate (schultenite), $PbHAsO_4$	14m	18
Lead hydroxide phosphate, $Pb_5(PO_4)_3OH$	8	33
Lead(II) iodide, PbI_2	5	34
Lead molybdenum oxide (wulfenite), $PbMoO_4$	7	23
Lead nitrate, $Pb(NO_3)_2$	5	36
Lead oxide (litharge), PbO (red, tetragonal)	2	30
Lead oxide (massicot), PbO (yellow, orthorhombic)	2	32
Lead(II,III) oxide (minium), Pb_3O_4	8	32
Lead oxide sulfate, $Pb_5O_5SO_4$	10m	27
Lead oxybromide, $Pb_3O_2Br_2$	5m	32
Lead selenide (clausthalite), PbSe	5	38
Lead strontium nitrate, $Pb_{.33}Sr_{.67}(NO_3)_2$	12m	53
Lead strontium nitrate, $Pb_{.67}Sr_{.33}(NO_3)_2$	12m	53
Lead sulfate (anglesite), $PbSO_4$	3	67
Lead sulfide (galena), PbS	2	18
Lead tin oxide, Pb_2SnO_4	10m	29
Lead titanium oxide (macedonite), $PbTiO_3$	5	39
Lead tungsten oxide (stolzite), $PbWO_4$ (tetragonal)	5m	34
Lead uranium oxide, Pb_3UO_6	8m	109
Lithium aluminum fluoride, α-Li_3AlF_6	8m	111
Lithium arsenate, Li_3AsO_4	2m	19
Lithium azide, LiN_3	8m	113
Lithium barium fluoride, $LiBaF_3$	5m	35
Lithium beryllium fluoride, Li_2BeF_4	7m	126
Lithium borate, $Li_2B_4O_7$	8m	114
Lithium bromide, LiBr	4	30
Lithium carbonate, Li_2CO_3	8m	42
Lithium chlorate hydrate, $LiClO_4 \cdot 3H_2O$	8	34
Lithium chloride, LiCl	1	62
Lithium fluoride, LiF	1	61
Lithium gallium oxide, $LiGaO_2$	10m	31
Lithium hydroxide hydrate, $LiOH \cdot H_2O$	11m	92
Lithium iodate, $LiIO_3$ (hexagonal)	7	26
Lithium iodate, $LiIO_3$ (tetragonal)	10m	33
Lithium molybdenum oxide, Li_2MoO_4 (trigonal)	1m	23
Lithium niobium oxide, $LiNbO_3$	6m	22
Lithium nitrate, $LiNO_3$	7	27
Lithium oxide, Li_2O	1m	25
Lithium phosphate hydrate, $Li_3P_3O_9 \cdot 3H_2O$	2m	20
Lithium phosphate, low form (lithiophosphate), Li_3PO_4	4m	21
Lithium phosphate, high form, Li_3PO_4	3m	39
Lithium potassium sulfate, $KLiSO_4$	3m	43
Lithium rubidium fluoride, $LiRbF_2$	7m	128
Lithium selenide, Li_2Se	10m	100
Lithium silicate, Li_2SiO_3	14m	19
Lithium silver bromide, $Li_{.2}Ag_{.8}Br$	12m	55
Lithium silver bromide, $Li_{.4}Ag_{.6}Br$	12m	55
Lithium silver bromide, $Li_{.6}Ag_{.4}Br$	12m	55
Lithium silver bromide, $Li_{.8}Ag_{.2}Br$	12m	55
Lithium sodium aluminum fluoride, cryolithionite, $Li_3Na_3Al_2F_{12}$	9m	23
Lithium sodium sulfate, $LiNaSO_4$	6m	24
Lithium sulfate, Li_2SO_4	6m	26
Lithium sulfate hydrate, $Li_2SO_4 \cdot H_2O$	4m	22
Lithium sulfide, Li_2S	10m	101
Lithium tantalum oxide, $LiTaO_3$	14m	20
Lithium telluride, Li_2Te	10m	102
Lithium tungsten oxide, Li_2WO_4 (trigonal)	1m	25
Lithium tungsten oxide hydrate, $Li_2WO_4 \cdot \frac{1}{2}H_2O$	2m	20
Lithium uranium fluoride, $LiUF_5$	7m	131
Lutetium arsenate, $LuAsO_4$	5m	36
Lutetium manganese oxide, $LuMnO_3$	2m	23
Lutetium nitride, LuN	4m	62
Lutetium oxide, Lu_2O_3	1m	27
Lutetium vanadium oxide, $LuVO_4$	5m	37
Magnesium, Mg	1	10
Magnesium aluminum oxide (spinel), $MgAl_2O_4$	9m	25
Magnesium aluminum silicate (low cordierite), $Mg_2Al_4Si_5O_{18}$ (orthorhombic)	1m	28
Magnesium aluminum silicate (indialite) $Mg_2Al_4Si_5O_{18}$ (hexagonal)	1m	29
Magnesium aluminum silicate (pyrope), $Mg_3Al_2(SiO_4)_2$	4m	24
Magnesium borate, $Mg_2B_2O_5$ (triclinic)	4m	25
Magnesium bromide, $MgBr_2$	4m	62
Magnesium bromide hydrate, $MgBr_2 \cdot 6H_2O$	11m	35
Magnesium carbonate (magnesite), $MgCO_3$	7	28
Magnesium cerium nitrate hydrate, $Mg_3Ce_2(NO_3)_{12} \cdot 24H_2O$	10	20
Magnesium chlorate hydrate, $Mg(ClO_4)_2 \cdot 6H_2O$	7m	30
Magnesium chloride (chloromagnesite), $MgCl_2$	11m	94
Magnesium chloride hydrate, $MgCl_2 \cdot 12H_2O$	7m	135
Magnesium chloride hydrate (bischofite), $MgCl_2 \cdot 6H_2O$	11m	37
Magnesium chromium oxide (magnesiochromite), $MgCr_2O_4$	9	34
Magnesium fluoride (sellaite), MgF_2	4	33
Magnesium fluoride silicate (humite), $Mg_7F_2Si_3O_{12}$	1m	30
Magnesium fluoride silicate (norbergite), $Mg_3F_2SiO_4$	10	39
Magnesium gallium oxide, $MgGa_2O_4$	10	36
Magnesium germanium oxide, Mg_2GeO_4 (cubic)	10	37

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Magnesium germanium oxide, Mg_2GeO_4 (orthorhombic)	10	38
Magnesium hydrogen phosphate hydrate, newberyite, $MgHPO_4 \cdot 3H_2O$	7m	139
Magnesium hydroxide (brucite), $Mg(OH)_2$	6	30
Magnesium iron hydroxide carbonate hydrate, pyroaurite, $Mg_6Fe_2(OH)_{16}CO_3 \cdot 4H_2O$, phase II	10m	104
Magnesium iron hydroxide carbonate hydrate, sjögrenite, $Mg_6Fe_2(OH)_{16}CO_3 \cdot 4H_2O$, phase I	10m	103
Magnesium lanthanum nitrate hydrate, $Mg_3La_2(NO_3)_{12} \cdot 24H_2O$	1m	22
Magnesium manganese oxide, $MgMn_2O_4$	10m	35
Magnesium mercury, MgHg	6m	84
Magnesium molybdenum oxide, $MgMoO_4$	7m	28
Magnesium nickel oxide, $MgNiO_2$	10m	36
Magnesium oxide (periclase), MgO	1	37
Magnesium phosphate, $Mg(PO_3)_2$	13m	26
Magnesium phosphate, α-$Mg_2P_2O_7$	9m	73
Magnesium selenide, MgSe	5m	70
Magnesium selenite hydrate, $MgSeO_3 \cdot 6H_2O$	8m	116
Magnesium silicate, enstatite, $MgSiO_3$	6	32
Magnesium silicate (forsterite), Mg_2SiO_4	1	83
Magnesium sulfate hydrate (epsomite), $MgSO_4 \cdot 7H_2O$	7	30
Magnesium sulfide, MgS	7	31
Magnesium sulfite hydrate, $MgSO_3 \cdot 6H_2O$	9m	26
Magnesium tin, Mg_2Sn	5	41
Magnesium tin oxide, Mg_2SnO_4	10m	37
Magnesium titanium oxide (geikielite), $MgTiO_3$	5	43
Magnesium titanium oxide, Mg_2TiO_4	12m	25
Magnesium tungsten oxide, $MgWO_4$	13m	27
Manganese, α-Mn	7m	142
Manganese aluminum oxide (galaxite), $MnAl_2O_4$	9	35
Manganese bromide, $MnBr_2$	4m	63
Manganese(II) carbonate (rhodochrosite), $MnCO_3$	7	32
Manganese chloride (scacchite), $MnCl_2$	8m	43
Manganese chloride hydrate, $MnCl_2 \cdot 2H_2O$	11m	38
Manganese chloride hydrate, $MnCl_2 \cdot 4H_2O$	9m	28
Manganese cobalt oxide, $MnCo_2O_4$	9m	30
Manganese fluoride, MnF_2	10m	105
Manganese iodide, MnI_2	4m	63
Manganese iron oxide (jacobsite), $MnFe_2O_4$	9	36
Manganese(II) oxide (manganosite), MnO	5	45
Manganese oxide (hausmannite), Mn_3O_4	10m	38
Manganese oxide (bixbyite), α-Mn_2O_3	11m	95
Manganese oxide (pyrolusite), β-MnO_2	10m	39
Manganese oxide hydroxide, groutite, α-MnOOH	11m	97
Manganese phosphate, $Mn(PO_3)_2$	14m	21
Manganese selenide, MnSe	10	41
Manganese sulfide (alabandite), α-MnS	4	11
Manganese(II) tungsten oxide (huebnerite), $MnWO_4$	2m	24
Manganese vanadium oxide, $Mn_2V_2O_7$	9m	75
Mercury amide chloride, $HgNH_2Cl$	10m	40
Mercury ammine chloride, $Hg(NH_3)_2Cl_2$	11m	39
Mercury bromate, $Hg(BrO_3)_2$	10m	107
Mercury(II) bromide, $HgBr_2$	10m	110
Mercury(I) bromide, Hg_2Br_2	7	33
Mercury(I) chloride (calomel), Hg_2Cl_2	13m	30
Mercury(II) chloride, $HgCl_2$	13m	29
Mercury chloride sulfide, α-$Hg_3Cl_2S_2$	8m	118
Mercury(II) cyanide, $Hg(CN)_2$	6	35
Mercury(II) fluoride, HgF_2	2m	25
Mercury(I) iodide, HgI	4	49
Mercury(II) iodide, HgI_2 (tetragonal)	7m	32
Mercury(II) oxide (montroydite), HgO	9	39
Mercury(II) selenide (tiemannite), HgSe	7	35
Mercury(II) sulfide (cinnabar), HgS (hexagonal)	4	17
Mercury(II) sulfide (metacinnabar), HgS (cubic)	4	21
Molybdenum, Mo	1	20
Molybdenum arsenide, Mo_2As_3	10m	115
Molybdenum osmium 3:1, Mo_3Os	6m	28
Molybdenum oxide (molybdite), MoO_3	3	30
Molybdenum sulfide (molybdenite), MoS_2	5	47
Neodymium arsenate, $NdAsO_4$	4m	28
Neodymium arsenide, NdAs	4m	64
Neodymium borate, $NdBO_3$	1m	32
Neodymium chloride, $NdCl_3$	1m	33
Neodymium fluoride, NdF_3	8	36
Neodymium oxide, Nd_2O_3	4	26
Neodymium oxychloride, NdOCl	8	37
Neodymium phosphate, $NdPO_4$	11m	40
Neodymium selenide, NdSe	5m	71
Neodymium silver, NdAg	5m	71
Neodymium vanadium oxide, $NdVO_4$	4m	30
Neptunium nitride, NpN	4m	64
Nickel, Ni	1	13
Nickel aluminum oxide, $NiAl_2O_4$	9	42
Nickel arsenide 1:2 (rammelsbergite), $NiAs_2$	10	42
Nickel arsenic sulfide (gersdorffite), NiAsS	1m	35
Nickel bromide, $NiBr_2$	10m	119
Nickel(II) carbonate, $NiCO_3$ (trigonal)	1m	36
Nickel chloride, $NiCl_2$	9m	81
Nickel chloride hydrate, $NiCl_2 \cdot 6H_2O$	11m	42
Nickel fluoride, NiF_2	10m	121
Nickel fluoride hydrate, $NiF_2 \cdot 4H_2O$	11m	43
Nickel gallium oxide, $NiGa_2O_4$	10	45
Nickel germanium oxide, Ni_2GeO_4	9	43
Nickel iron oxide (trevorite), $NiFe_2O_4$	10	44

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Nickel nitrate hydrate, $Ni(NO_3)_2 \cdot 6H_2O$	12m	26
Nickel(II) oxide (bunsenite), NiO	1	47
Nickel phosphate, $Ni(PO_3)_2$	14m	22
Nickel phosphide, $Ni_{12}P_5$	9m	83
Nickel silicon fluoride hydrate, $NiSiF_6 \cdot 6H_2O$	8	38
Nickel sulfate, $NiSO_4$	2m	26
Nickel sulfate hydrate(retgersite), $NiSO_4 \cdot 6H_2O$	7	36
Nickel sulfide, millerite, NiS	1m	37
Nickel tungsten oxide, $NiWO_4$	2m	27
Nickel yttrium, Ni_3Y	10m	123
Niobium osmium, Nb_3Os	6m	30
Niobium oxychloride, $NbOCl_3$	7m	148
Niobium platinum, Nb_3Pt	6m	31
Niobium silicide, $NbSi_2$	8	39
Osmium, Os	4	8
Osmium titanium, OsTi	6m	85
Palladium, Pd	1	21
Palladium hydride, $PdH_{0.706}$	5m	72
Palladium oxide, PdO	4	27
Palladium vanadium, PdV_3	6m	32
Phosphorus bromide, PBr_7	7m	150
Phosphorus oxide (stable form I), P_2O_5 (orthorhombic)	9m	86
Phosphorus oxide (stable form II), P_2O_5 (orthorhombic)	9m	88
Phosphorus oxide (metastable form), P_4O_{10} (rhombohedral)	9m	91
Platinum, Pt	1	31
Platinum titanium 1:3, $PtTi_3$	6m	33
Platinum vanadium, PtV_3	6m	34
Plutonium arsenide, PuAs	4m	65
Plutonium phosphide, PuP	4m	65
Plutonium telluride, PuTe	4m	66
Potassium aluminum sulfate, $KAl(SO_4)_2$	9m	31
Potassium aluminum sulfate hydrate (potash alum), $KAl(SO_4)_2 \cdot 12H_2O$	6	36
Potassium barium chromium oxide, $K_2Ba(CrO_4)_2$	14m	23
Potassium barium molybdenum oxide, $K_2Ba(MoO_4)_2$	14m	24
Potassium barium nickel nitrite, $K_2BaNi(NO_2)_6$	9m	32
Potassium borohydride, KBH_4	9	44
Potassium bromate, $KBrO_3$	7	38
Potassium bromide, KBr	1	66
Potassium bromide chloride, $KBr_{0.5}Cl_{0.5}$	8m	46
Potassium bromide iodide, $KBr_{.33}I_{.67}$	11m	44
Potassium bromide iodide, $KBr_{.67}I_{.33}$	11m	45
Potassium cadmium fluoride, $KCdF_3$	8m	47
Potassium cadmium sulfate, $K_2Cd_2(SO_4)_3$	7m	34
Potassium calcium carbonate (fairchildite), $K_2Ca(CO_3)_2$	8m	48
Potassium calcium chloride, $KCaCl_3$	7m	36
Potassium calcium fluoride, $KCaF_3$	8m	49
Potassium calcium magnesium sulfate, $K_2CaMg(SO_4)_3$	7m	37
Potassium calcium nickel nitrite, $K_2CaNi(NO_2)_6$	9m	33
Potassium calcium sulfate, $K_2Ca_2(SO_4)_3$	7m	39
Potassium calcium sulfate hydrate (syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$	14m	25
Potassium cerium fluoride, β-$KCeF_4$	12m	59
Potassium chlorate, $KClO_3$	3m	42
Potassium chlorate, $KClO_4$	6	43
Potassium chloride (sylvite), KCl	1	65
Potassium chromium oxide, K_3CrO_8	3m	44
Potassium chromium oxide sulfate, $K_2(CrO_4)_{.33}(SO_4)_{.67}$	12m	28
Potassium chromium oxide sulfate, $K_2(CrO_4)_{.67}(SO_4)_{.33}$	12m	27
Potassium chromium sulfate hydrate, $KCr(SO_4)_2 \cdot 12H_2O$	6	39
Potassium cobalt(II) fluoride, $KCoF_3$	6m	37
Potassium cobalt fluoride, K_2CoF_4	11m	46
Potassium cobalt nitrite, $K_3Co(NO_2)_6$	9	45
Potassium cobalt(II) sulfate, $K_2Co_2(SO_4)_3$	6m	35
Potassium copper chloride, $KCuCl_3$	7m	41
Potassium copper chloride hydrate (mitscherlichite), $K_2CuCl_4 \cdot 2H_2O$	9m	34
Potassium copper(II) fluoride, $KCuF_3$	6m	38
Potassium cyanate, KCNO	7	39
Potassium cyanide, KCN	1	77
Potassium fluoride, KF	1	64
Potassium germanium fluoride, K_2GeF_6	6	41
Potassium hydrogen arsenate, KH_2AsO_4	1m	38
Potassium hydrogen phosphate, KH_2PO_4	3	69
Potassium hydroxide, KOH at 300 °C	4m	66
Potassium iodate, KIO_4	7	41
Potassium iodide, KI	1	68
Potassium iron chloride hydrate (erythrosiderite), $K_2FeCl_5 \cdot H_2O$	14m	27
Potassium iron cyanide, $K_3Fe(CN)_6$	9m	35
Potassium iron(II) fluoride, $KFeF_3$	6m	39
Potassium iron fluoride, K_3FeF_6	9m	37
Potassium lead chloride, KPb_2Cl_5	13m	33
Potassium lead chromium oxide, $K_2Pb(CrO_4)_2$	14m	28
Potassium lead molybdenum oxide, $K_2Pb(MoO_4)_2$	14m	29
Potassium lead sulfate (palmierite), $K_2Pb(SO_4)_2$	14m	30
Potassium magnesium chloride hydrate (carnallite), $KMgCl_3 \cdot 6H_2O$	8m	50
Potassium magnesium chromium oxide, $K_2Mg_2(CrO_4)_3$	8m	52
Potassium magnesium fluoride, $KMgF_3$	6m	42
Potassium magnesium fluoride, K_2MgF_4	10m	42
Potassium magnesium selenate hydrate, $K_2Mg(SeO_4)_2 \cdot 6H_2O$	10m	43
Potassium magnesium sulfate (langbeinite), $K_2Mg_2(SO_4)_3$	6m	40

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Potassium magnesium sulfate hydrate (picromerite), $K_2Mg(SO_4)_2 \cdot 6H_2O$	8m	54
Potassium manganese(II) fluoride, $KMnF_3$	6m	45
Potassium manganese oxide, $KMnO_4$	7	42
Potassium manganese(II) sulfate (manganolangbeinite), $K_2Mn_2(SO_4)_3$	6m	43
Potassium molybdenum oxide phosphate hydrate, $K_2(MoO_3)_{12}PO_4 \cdot 4H_2O$	8	43
Potassium nickel fluoride, $KNiF_3$	7m	42
Potassium nickel fluoride, K_2NiF_4	10m	45
Potassium nickel(II) sulfate, $K_2Ni_2(SO_4)_3$	6m	46
Potassium niobium fluoride, K_2NbF_7	8m	120
Potassium nitrate (niter), KNO_3	3	58
Potassium nitrite, KNO_2	9m	38
Potassium nitroso ruthenium chloride, $K_2(NO)RuCl_5$	2m	29
Potassium oxide, K_2O	10m	125
Potassium platinum bromide, K_2PtBr_6	8	40
Potassium platinum chloride, K_2PtCl_6	13m	34
Potassium platinum fluoride, K_2PtF_6	6	42
Potassium rhenium chloride, K_2ReCl_6	2m	28
Potassium rhenium oxide, $KReO_4$	8	41
Potassium rubidium chloride, $K_{0.5}Rb_{0.5}Cl$	8m	76
Potassium rubidium chromium oxide, $KRbCrO_4$	12m	29
Potassium ruthenium chloride, K_2RuCl_6	10	46
Potassium ruthenium oxide chloride hydrate, $K_4Ru_2OCl_{10} \cdot H_2O$	10	47
Potassium selenate, K_2SeO_4	9m	41
Potassium selenide, K_2Se	10m	126
Potassium selenium bromide, K_2SeBr_6	8	41
Potassium silicon fluoride (hieratite), K_2SiF_6	5	50
Potassium silver cyanide, $KAg(CN)_2$	8m	78
Potassium sodium aluminum fluoride (elpasolite), K_2NaAlF_6	9m	43
Potassium sodium bromide, $K_{.2}Na_{.8}Br$	12m	62
Potassium sodium bromide, $K_{.4}Na_{.6}Br$	12m	62
Potassium sodium bromide, $K_{.6}Na_{.4}Br$	12m	62
Potassium sodium bromide, $K_{.8}Na_{.2}Br$	12m	62
Potassium sodium chloride, $K_{.2}Na_{.8}Cl$	12m	63
Potassium sodium chloride, $K_{.4}Na_{.6}Cl$	12m	63
Potassium sodium chloride, $K_{.6}Na_{.4}Cl$	12m	63
Potassium sodium chloride, $K_{.8}Na_{.2}Cl$	12m	63
Potassium sodium sulfate, $K_{.67}Na_{1.33}SO_4$	6m	48
Potassium sodium sulfate, $KNaSO_4$	6m	50
Potassium sodium sulfate (aphthitalite), $K_3Na(SO_4)_2$	6m	52
Potassium strontium sulfate (kalistrontite), $K_2Sr(SO_4)_2$	14m	31
Potassium sulfate, $K_2S_2O_7$	9m	99
Potassium sulfate (arcanite), K_2SO_4	3	62
Potassium sulfide, K_2S	10m	127
Potassium telluride, K_2Te	10m	128
Potassium thiocyanate, KCNS	8	44
Potassium tin chloride, K_2SnCl_6	6	38
Potassium titanium fluoride, K_2TiF_6	7	40
Potassium tungsten oxide, K_2WO_4	11m	47
Potassium vanadium oxide, KV_3O_8	8m	56
Potassium zinc bromide hydrate, $KZnBr_3 \cdot 2H_2O$	11m	104
Potassium zinc fluoride, $KZnF_3$	5	51
Potassium zinc fluoride, K_2ZnF_4	10m	46
Potassium zinc iodide hydrate, $KZnI_3 \cdot 2H_2O$	11m	107
Potassium zinc sulfate, $K_2Zn_2(SO_4)_3$	6m	54
Potassium zinc sulfate hydrate, $K_2Zn(SO_4)_2 \cdot 6H_2O$	7m	43
Potassium zinc vanadium oxide hydrate, $K_2Zn_2V_{10}O_{28} \cdot 16H_2O$	3m	45
Potassium zirconium fluoride, K_3ZrF_7	9	46
Praseodymium arsenate, $PrAsO_4$	4m	32
Praseodymium arsenide, PrAs	4m	67
Praseodymium chloride, $PrCl_3$	1m	39
Praseodymium fluoride, PrF_3	5	52
Praseodymium oxychloride, PrOCl	9	47
Praseodymium sulfide, PrS	4m	67
Praseodymium vanadium oxide, $PrVO_4$	5m	40
Praseodymium zinc, PrZn	5m	72
Rhenium, Re	2	13
Rhodium, Rh	3	9
Rhodium vanadium, RhV_3	6m	56
Rubidium aluminum sulfate hydrate, $RbAl(SO_4)_2 \cdot 12H_2O$	6	44
Rubidium amide, $RbNH_2$	5m	73
Rubidium barium chromium oxide, $Rb_2Ba(CrO_4)_2$	14m	32
Rubidium bromate, $RbBrO_3$	8	45
Rubidium bromide, RbBr	7	43
Rubidium cadmium chloride, high form, $RbCdCl_3$ (tetragonal)	5m	43
Rubidium cadmium chloride, low form, $RbCdCl_3$ (orthorhombic)	5m	41
Rubidium cadmium sulfate, $Rb_2Cd_2(SO_4)_3$	7m	45
Rubidium calcium chloride, $RbCaCl_3$	7m	47
Rubidium calcium fluoride, $RbCaF_3$	8m	57
Rubidium calcium sulfate, $Rb_2Ca_2(SO_4)_3$	7m	48
Rubidium chlorate, $RbClO_3$	8	47
Rubidium chlorate, $RbClO_4$	2m	30
Rubidium chloride, RbCl	4	41
Rubidium chromium oxide, Rb_2CrO_4	3m	46
Rubidium chromium sulfate hydrate, $RbCr(SO_4)_2 \cdot 12H_2O$	6	47
Rubidium cobalt(II) chloride, $RbCoCl_3$	6m	57
Rubidium cobalt fluoride, $RbCoF_3$	8m	58
Rubidium cobalt sulfate, $Rb_2Co_2(SO_4)_3$	8m	59
Rubidium copper chloride hydrate, $Rb_2CuCl_4 \cdot 2H_2O$	10m	47

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Rubidium copper sulfate hydrate, $Rb_2Cu(SO_4)_2 \cdot 6H_2O$	8m	61
Rubidium fluoride, RbF	8m	63
Rubidium iodate, $RbIO_4$	2m	31
Rubidium iodide, RbI	4	43
Rubidium iron chloride hydrate, $Rb_2FeCl_5 \cdot H_2O$	14m	33
Rubidium iron sulfate hydrate, $Rb_2Fe(SO_4)_2 \cdot 6H_2O$	8m	64
Rubidium lead chromium oxide, $Rb_2Pb(CrO_4)_2$	14m	34
Rubidium magnesium chromium oxide, $Rb_2Mg_2(CrO_4)_3$	8m	66
Rubidium magnesium chromium oxide hydrate, $Rb_2Mg(CrO_4)_2 \cdot 6H_2O$	8m	68
Rubidium magnesium sulfate, $Rb_2Mg_2(SO_4)_3$	7m	50
Rubidium magnesium sulfate hydrate, $Rb_2Mg(SO_4)_2 \cdot 6H_2O$	8m	70
Rubidium manganese(II) fluoride, $RbMnF_3$	5m	44
Rubidium manganese sulfate, $Rb_2Mn_2(SO_4)_3$	7m	52
Rubidium nickel(II) chloride, $RbNiCl_3$	6m	58
Rubidium nickel sulfate, $Rb_2Ni_2(SO_4)_3$	8m	72
Rubidium nickel sulfate hydrate, $Rb_2Ni(SO_4)_2 \cdot 6H_2O$	8m	74
Rubidium nitrate, $RbNO_3$ (trigonal)	5m	45
Rubidium platinum chloride, Rb_2PtCl_6	5	53
Rubidium platinum fluoride, Rb_2PtF_6	6	48
Rubidium selenate, Rb_2SeO_4	9m	44
Rubidium silicon fluoride, Rb_2SiF_6	6	49
Rubidium strontium chloride, $RbSrCl_3$	7m	54
Rubidium sulfate, Rb_2SO_4	8	48
Rubidium tellurium bromide, Rb_2TeBr_6	8	46
Rubidium tellurium chloride, Rb_2TeCl_6	8	48
Rubidium tin chloride, Rb_2SnCl_6	6	46
Rubidium zinc fluoride, $RbZnF_3$	7m	57
Rubidium zinc sulfate hydrate, $Rb_2Zn(SO_4)_2 \cdot 6H_2O$	7m	55
Ruthenium, Ru	4	5
Ruthenium titanium, RuTi	6m	86
Samarium arsenate, $SmAsO_4$	4m	33
Samarium arsenide, SmAs	4m	68
Samarium chloride, $SmCl_3$	1m	40
Samarium fluoride, SmF_3	1m	41
Samarium oxide, Sm_2O_3 (cubic)	4m	34
Samarium oxychloride, SmOCl	1m	43
Samarium silver, SmAg	5m	73
Samarium tin oxide, $Sm_2Sn_2O_7$	8m	77
Samarium vanadium oxide, $SmVO_4$	5m	47
Scandium arsenate, $ScAsO_4$	4m	35
Scandium arsenide, ScAs	4m	68
Scandium oxide, Sc_2O_3	3	27
Scandium phosphate, $ScPO_4$	8	50
Scandium silicate (thortveitite), $Sc_2Si_2O_7$	7m	58
Selenium, Se	5	54
Selenium oxide (selenolite), SeO_2	7m	60
Silicon, Si	13m	35
Silicon, Si (reference standard)	12m	2
Silicon nitride, β-Si_3N_4	14m	116
Silicon oxide (α or low cristobalite), SiO_2 (tetragonal)	10	48
Silicon oxide (α or low quartz), SiO_2 (hexagonal)	3	24
Silicon oxide (β or high cristobalite), SiO_2 (cubic)	1	42
Silver, Ag	1	23
Silver, Ag (reference standard)	8m	2
Silver arsenate, Ag_3AsO_4	5	56
Silver arsenic sulfide, xanthoconite, Ag_3AsS_3	8m	126
Silver bromate, $AgBrO_3$	5	57
Silver bromide (bromargyrite), AgBr	4	46
Silver carbonate, Ag_2CO_3	13m	
Silver chlorate, $AgClO_3$	7	44
Silver chloride (chlorargyrite), AgCl	4	44
Silver chromium oxide, Ag_2CrO_4	12m	30
Silver cyanide, AgCN	9m	48
Silver fluoride, Ag_2F	5m	53
Silver iodate, $AgIO_4$	9	49
Silver iodide (iodargyrite), AgI (hexagonal)	8	51
Silver iodide, γ-AgI (cubic)	9	48
Silver manganese oxide, $AgMnO_4$	7m	155
Silver molybdenum oxide, Ag_2MoO_4	7	45
Silver nitrate, $AgNO_3$	5	59
Silver nitrite, $AgNO_2$	5	60
Silver oxide, Ag_2O	1m	45
Silver(II) oxide nitrate, $Ag_7O_8NO_3$	4	61
Silver phosphate, Ag_3PO_4	5	62
Silver rhenium oxide, $AgReO_4$	8	53
Silver selenate, Ag_2SeO_4	2m	32
Silver sodium chloride, $Ag_{0.5}Na_{0.5}Cl$	8m	79
Silver sulfate, Ag_2SO_4	13m	37
Silver sulfide (acanthite), Ag_2S	10	51
Silver terbium, AgTb	5m	74
Silver thulium, AgTm	5m	74
Silver yttrium, AgY	5m	75
Sodium, Na	9m	105
Sodium aluminum chloride silicate, sodalite, $Na_8Al_6Cl_2(SiO_4)_6$	7m	158
Sodium azide, α-NaN_3, at -90 to -100 °C	8m	129
Sodium azide, β-NaN_3	8m	130
Sodium beryllium calcium aluminum fluoride oxide silicate, meliphanite, $(Na_{0.63}Ca_{1.37})Be(Al_{0.13}Si_{1.87})(F_{0.75}O_{6.25})$	8m	135
Sodium beryllium calcium fluoride silicate, leucophanite, $NaBeCaFSi_2O_6$	8m	138
Sodium borate, $Na_2B_8O_{13}$	7m	160
Sodium boron hydride, $NaBH_4$	9	51
Sodium bromate, $NaBrO_3$	5	65
Sodium bromide, NaBr	3	47
Sodium bromide chloride, $NaBr_{.33}Cl_{.67}$	11m	49
Sodium bromide chloride, $NaBr_{.67}Cl_{.33}$	11m	50

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Sodium calcium aluminum fluoride hydrate, thomsenolite, $NaCaAlF_6 \cdot H_2O$	8m	132
Sodium calcium carbonate hydrate, pirssonite, $Na_2Ca(CO_3)_2 \cdot 2H_2O$	9m	106
Sodium calcium silicate, Na_2CaSiO_4	10m	48
Sodium calcium sulfate (glauberite), $Na_2Ca(SO_4)_2$	6m	59
Sodium carbonate hydrate (thermonatrite), $Na_2CO_3 \cdot H_2O$	8	54
Sodium carbonate sulfate, $Na_4CO_3SO_4$	11m	51
Sodium carbonate sulfate (burkeite), $Na_6CO_3(SO_4)_2$	11m	52
Sodium carbonate sulfate, $Na_6CO_3(SO_4)_2$	11m	53
Sodium carbonate sulfate, $Na_6(CO_3)_2SO_4$	11m	54
Sodium chlorate, $NaClO_3$	3	51
Sodium chlorate, $NaClO_4$ (orthorhombic)	7	49
Sodium chloride (halite), NaCl	2	41
Sodium chromium oxide, Na_2CrO_4	9m	48
Sodium chromium oxide hydrate, $Na_2CrO_4 \cdot 4H_2O$	9m	50
Sodium chromium oxide hydrate, $Na_2Cr_2O_7 \cdot 2H_2O$	7m	62
Sodium chromium oxide sulfate, $Na_4(CrO_4)(SO_4)$	11m	55
Sodium cobalt(II) sulfate hydrate, $Na_2Co(SO_4)_2 \cdot 4H_2O$	6m	61
Sodium cyanate, NaCNO	2m	33
Sodium cyanide, NaCN (cubic)	1	78
Sodium cyanide, NaCN (orthorhombic) at 6 °C	1	79
Sodium fluoride (villiaumite), NaF	1	63
Sodium hydrogen fluoride, $NaHF_2$	5	63
Sodium hydrogen phosphate, $Na_3H(PO_3)_4$	10m	130
Sodium hydrogen silicate hydrate, $Na_2H_2SiO_4 \cdot 4H_2O$	7m	163
Sodium hydrogen sulfate hydrate, $NaHSO_4 \cdot H_2O$	9m	52
Sodium hydroxide, NaOH at 300 °C	4m	69
Sodium iodate, $NaIO_3$	7	47
Sodium iodate, $NaIO_4$	7	48
Sodium iodide, NaI	4	31
Sodium iron fluoride, Na_3FeF_6	9m	54
Sodium lanthanum fluoride silicate, $(Na_2La_8)F_2(SiO_4)_6$	7m	64
Sodium lanthanum molybdenum oxide, $NaLa(MoO_4)_2$	10m	49
Sodium magnesium aluminum boron hydroxide silicate, dravite, $NaMg_3Al_6B_3(OH)_4Si_6O_{27}$	3m	47
Sodium magnesium carbonate (eitelite), $Na_2Mg(CO_3)_2$	11m	56
Sodium magnesium sulfate hydrate, bloedite, $Na_2Mg(SO_4)_2 \cdot 4H_2O$	6m	63
Sodium magnesium sulfate hydrate (loeweite), $Na_{12}Mg_7(SO_4)_{13} \cdot 15H_2O$	14m	35
Sodium manganese(II) fluoride, $NaMnF_3$	6m	65
Sodium manganese sulfate hydrate, $Na_{12}Mn_7(SO_4)_{13} \cdot 15H_2O$	14m	37
Sodium mercury(II) chloride hydrate, $NaHgCl_3 \cdot 2H_2O$	6m	66
Sodium molybdenum oxide, Na_2MoO_4	1m	46
Sodium molybdenum oxide, $Na_2Mo_2O_7$	9m	110
Sodium neodymium fluoride silicate, $(Na_2Nd_8)F_2(SiO_4)_6$	7m	66
Sodium nickel(II) sulfate hydrate, $Na_2Ni(SO_4)_2 \cdot 4H_2O$	6m	68
Sodium nitrate (soda-niter), $NaNO_3$	6	50
Sodium nitrite, $NaNO_2$	4	62
Sodium oxide, Na_2O	10m	134
Sodium phosphate, $Na_3P_3O_9$	3m	49
Sodium phosphate hydrate, $Na_3P_3O_9 \cdot H_2O$	3m	50
Sodium phosphate hydrate, α-$Na_4P_4O_{12} \cdot 4H_2O$ (monoclinic)	13m	39
Sodium phosphate hydrate, β-$Na_4P_4O_{12} \cdot 4H_2O$ (triclinic)	2m	35
Sodium phosphate hydrate, $Na_6P_6O_{18} \cdot 6H_2O$	5m	54
Sodium praseodymium fluoride silicate, $(Na_2Pr_8)F_2(SiO_4)_6$	7m	68
Sodium selenate, Na_2SeO_4	9m	55
Sodium selenide, Na_2Se	10m	135
Sodium silicate, α(III), $Na_2Si_2O_5$	8m	141
Sodium silicate, β-$Na_2Si_2O_5$	10m	136
Sodium sulfate, Na_2SO_4	11m	57
Sodium sulfate (thenardite), Na_2SO_4	2	59
Sodium sulfide, Na_2S	10m	140
Sodium sulfite, Na_2SO_3	3	60
Sodium telluride, Na_2Te	10m	141
Sodium tin fluoride, $NaSn_2F_5$	7m	166
Sodium tungsten oxide, Na_2WO_4	1m	47
Sodium tungsten(VI) oxide hydrate, $Na_2WO_4 \cdot 2H_2O$	2m	33
Sodium zinc fluoride, $NaZnF_3$	6m	74
Sodium zinc sulfate hydrate, $Na_2Zn(SO_4)_2 \cdot 4H_2O$	6m	72
Sodium zirconium fluoride, $Na_7Zr_6F_{31}$	8m	144
Strontium aluminum hydroxide, $Sr_3Al_2(OH)_{12}$	10m	50
Strontium aluminum oxide, $Sr_3Al_2O_6$	10m	52
Strontium arsenate, $Sr_3(AsO_4)_2$	2m	36
Strontium azide, $Sr(N_3)_2$	8m	146
Strontium borate, SrB_2O_4	3m	53
Strontium borate, SrB_4O_7	4m	36
Strontium bromide fluoride, SrBrF	10m	54
Strontium bromide hydrate, $SrBr_2 \cdot 6H_2O$	4	60
Strontium carbonate (strontianite), $SrCO_3$	3	56
Strontium chloride, $SrCl_2$	4	40
Strontium chloride fluoride, SrClF	10m	55
Strontium chloride hydrate, $SrCl_2 \cdot 2H_2O$	11m	58
Strontium chloride hydrate, $SrCl_2 \cdot 6H_2O$	4	58
Strontium chloride hydroxide phosphate, $Sr_5Cl_{.65}(OH)_{.35}(PO_4)_3$	11m	60
Strontium fluoride, SrF_2	5	67
Strontium hydroxide, $Sr(OH)_2$	13m	41
Strontium hydroxide hydrate, $Sr(OH)_2 \cdot H_2O$	13m	42
Strontium hydroxide hydrate, $Sr(OH)_2 \cdot 8H_2O$	13m	43
Strontium indium hydroxide, $Sr_3In_2(OH)_{12}$	6m	76

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Strontium iodide hydrate, $SrI_2 \cdot 6H_2O$	8	58
Strontium manganese oxide, $SrMnO_3$ (cubic)	10m	56
Strontium manganese oxide, $SrMnO_3$ (hexagonal)	10m	58
Strontium molybdenum oxide, $SrMoO_4$	7	50
Strontium nitrate, $Sr(NO_3)_2$	12m	31
Strontium oxide, SrO	5	68
Strontium oxide, SrO_2	6	52
Strontium oxide hydrate, $SrO_2 \cdot 8H_2O$	11m	61
Strontium phosphate, α-$Sr_2P_2O_7$	11m	62
Strontium phosphate, α-$Sr_3(PO_4)_2$	11m	64
Strontium scandium oxide hydrate, $Sr_3Sc_2O_6 \cdot 6H_2O$	6m	78
Strontium silicate, Sr_3SiO_5	13m	44
Strontium sulfate (celestite), $SrSO_4$	2	61
Strontium sulfide, SrS	7	52
Strontium telluride, SrTe	4m	69
Strontium tin oxide, $SrSnO_3$	8m	80
Strontium titanium oxide, $SrTiO_3$	3	44
Strontium tungsten oxide, $SrWO_4$	7	53
Strontium tungsten oxide, Sr_2WO_5	12m	32
Strontium zirconium oxide, $SrZrO_3$	9	51
Sulfamic acid, H_2NSO_3H	7	54
Sulfur, S (orthorhombic)	9	54
Tantalum, Ta	1	29
Tantalum silicide, $TaSi_2$	8	59
Tellurium, Te	1	26
Tellurium(IV) oxide (paratellurite), TeO_2 (tetragonal)	7	56
Tellurium(IV) oxide, paratellurite, TeO_2 (tetragonal)	10	55
Tellurium(IV) oxide, tellurite, TeO_2 (orthorhombic)	9	57
Terbium arsenate, $TbAsO_4$	3m	54
Terbium arsenide, TbAs	5m	75
Terbium nitride, TbN	4m	70
Terbium phosphide, TbP	5m	76
Terbium selenide, TbSe	5m	76
Terbium sulfide, TbS	5m	77
Terbium telluride, TbTe	5m	77
Terbium vanadium oxide, $TbVO_4$	5m	56
Thallium aluminum sulfate hydrate, $TlAl(SO_4)_2 \cdot 12H_2O$	6	53
Thallium(I) arsenate, Tl_3AsO_4	2m	37
Thallium azide, TlN_3	8m	82
Thallium(I) bromate, $TlBrO_3$	8	60
Thallium bromide, TlBr	7	57
Thallium cadmium sulfate, $Tl_2Cd_2(SO_4)_3$	8m	83
Thallium(I) chlorate, $TlClO_4$	2m	38
Thallium(I) chlorate, $TlClO_3$	8	61
Thallium(I) chloride, TlCl	4	51
Thallium chromium oxide, Tl_2CrO_4	3m	54
Thallium chromium sulfate hydrate, $TlCr(SO_4)_2 \cdot 12H_2O$	6	55
Thallium cobalt sulfate, $Tl_2Co_2(SO_4)_3$	8m	85
Thallium cobalt sulfate hydrate, $Tl_2Co(SO_4)_2 \cdot 6H_2O$	7m	70
Thallium copper sulfate hydrate, $Tl_2Cu(SO_4)_2 \cdot 6H_2O$	7m	72
Thallium gallium sulfate hydrate, $TlGa(SO_4)_2 \cdot 12H_2O$	6	57
Thallium(I) iodate, $TlIO_3$	8	62
Thallium(I) iodide, TlI (orthorhombic)	4	53
Thallium iron sulfate hydrate, $Tl_2Fe(SO_4)_2 \cdot 6H_2O$	8m	87
Thallium magnesium chromium oxide, $Tl_2Mg_2(CrO_4)_3$	8m	89
Thallium magnesium sulfate hydrate, $Tl_2Mg(SO_4)_2 \cdot 6H_2O$	7m	74
Thallium manganese sulfate, $Tl_2Mn_2(SO_4)_3$	7m	76
Thallium nickel sulfate hydrate, $Tl_2Ni(SO_4)_2 \cdot 6H_2O$	7m	78
Thallium(I) nitrate, $TlNO_3$	6	58
Thallium(III) oxide, Tl_2O_3	2	28
Thallium(I) phosphate, Tl_3PO_4	7	58
Thallium(III) phosphate, $TlPO_4$	7	59
Thallium platinum chloride, Tl_2PtCl_6	5	70
Thallium silicon fluoride, Tl_2SiF_6	6	56
Thallium(I) sulfate, Tl_2SO_4	6	59
Thallium(I) thiocyanate, TlCNS	8	63
Thallium tin chloride, Tl_2SnCl_6	6	54
Thallium(I) tungsten oxide, Tl_2WO_4	1m	48
Thallium zinc sulfate hydrate, $Tl_2Zn(SO_4)_2 \cdot 6H_2O$	7m	80
Thorium arsenide, ThAs	4m	70
Thorium oxide (thorianite), ThO_2	1	57
Thulium arsenate, $TmAsO_4$	3m	56
Thulium arsenide, TmAs	4m	71
Thulium nitride, TmN	4m	71
Thulium oxide, Tm_2O_3	9	58
Thulium telluride, TmTe	4m	72
Thulium vanadium oxide, $TmVO_4$	5m	57
Tin, α-Sn (cubic)	2	12
Tin, β-Sn (tetragonal)	1	24
Tin arsenide, SnAs	4m	37
Tin(II) fluoride, SnF_2	3m	51
Tin hydrogen phosphate, $SnHPO_4$	13m	46
Tin(IV) iodide, SnI_4	5	71
Tin(II) oxide (romarchite), SnO	4	28
Tin(IV) oxide (cassiterite), SnO_2	1	54
Tin sulfide (berndtite), β-SnS_2	9m	57
Tin(II) telluride, SnTe	7	61
Titanium, Ti	3	1
Titanium oxide (anatase), TiO_2	7m	82
Titanium oxide, brookite, TiO_2 (orthorhombic)	3m	57
Titanium oxide (rutile), TiO_2	7m	83
Titanium(III) oxide, $TiO_{1.515}$	9	59
Titanium silicide, Ti_5Si_3	8	64
Titanium sulfide, TiS_2	4m	72
Titanium sulfide, Ti_2S	8m	149
Tungsten, W	1	28
Tungsten, W (reference standard)	8m	2
Tungsten sulfide (tungstenite), WS_2	8	65
Uranium oxide, UO	5m	78
Uranium oxide (uraninite), UO_2	2	33
Uranium selenide, USe	5m	78
Uranium telluride, UTe	4m	73
Vanadium, V	9m	58
Vanadium(V) oxide (shcherbinaite), V_2O_5	8	66
Vanadium sulfide, α-V_3S	14m	118

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Vanadium sulfide, β-V_3S	14m	120
Ytterbium arsenate, $YbAsO_4$	4m	38
Ytterbium arsenide, YbAs	4m	73
Ytterbium nitride, YbN	4m	74
Ytterbium oxide, Yb_2O_3	6m	80
Ytterbium selenide, YbSe	5m	79
Ytterbium telluride, YbTe	5m	79
Ytterbium(III) vanadium oxide, $YbVO_4$	5m	58
Yttrium arsenate, $YAsO_4$	2m	39
Yttrium arsenide, YAs	4m	74
Yttrium chloride oxide. YClO	1m	51
Yttrium oxide, Y_2O_3	3	28
Yttrium phosphate (xenotime), YPO_4	8	67
Yttrium sulfide, YS	5m	80
Yttrium telluride, YTe	4m	75
Yttrium titanium oxide, Y_2TiO_5	11m	113
Yttrium vanadium oxide, YVO_4	5m	59
Zinc, Zn	1	16
Zinc aluminum oxide (gahnite), $ZnAl_2O_4$	2	38
Zinc ammine bromide, $Zn(NH_3)_2Br_2$	11m	68
Zinc ammine chloride, $Zn(NH_3)_2Cl_2$	10m	59
Zinc antimony oxide, $ZnSb_2O_4$	4m	39
Zinc borate, ZnB_2O_4	1	83
Zinc borate, $Zn_4B_6O_{13}$	13m	48
Zinc carbonate, smithsonite, $ZnCO_3$	8	69
Zinc chromium oxide, $ZnCr_2O_4$	9m	59
Zinc cobalt oxide, $ZnCo_2O_4$	10m	60
Zinc cyanide, $Zn(CN)_2$	5	73
Zinc fluoride, ZnF_2	6	60
Zinc fluoride hydrate, $ZnF_2 \cdot 4H_2O$	11m	69
Zinc germanium oxide, Zn_2GeO_4	10	56
Zinc hydroxide silicate hydrate, hemimorphite, $Zn_4(OH)_2Si_2O_7 \cdot H_2O$	2	62
Zinc iodide, ZnI_2	9	60
Zinc iron oxide (franklinite), $ZnFe_2O_4$	9m	60
Zinc manganese oxide (hetaerolite), $ZnMn_2O_4$	10m	61
Zinc molybdenum oxide, $Zn_2Mo_3O_8$	7m	173
Zinc nitrate hydrate, α-$Zn(NO_3)_2 \cdot 6H_2O$	12m	36
Zinc oxide (zincite), ZnO	2	25
Zinc selenide, ZnSe	3	23
Zinc silicate (willemite), Zn_2SiO_4	7	62
Zinc silicon fluoride hydrate, $ZnSiF_6 \cdot 6H_2O$	8	70
Zinc sulfate (zinkosite), $ZnSO_4$	7	64
Zinc sulfate hydrate (goslarite), $ZnSO_4 \cdot 7H_2O$	8	71
Zinc sulfide (wurtzite), α-ZnS (hexagonal)	2	14
Zinc sulfide (sphaelerite), β-ZnS (cubic)	2	16
Zinc telluride, ZnTe	3m	58
Zinc tin oxide, Zn_2SnO_4	10m	62
Zinc titanium oxide, $ZnTiO_3$	13m	49
Zinc titanium oxide, Zn_2TiO_4	12m	37
Zinc tungsten oxide (sanmartinite), $ZnWO_4$	2m	40
Zirconium, α-Zr	2	11
Zirconium hydride, ZrH_2	5m	60
Zirconium iodate, $Zr(IO_3)_4$	1m	51
Zirconium nitride, ZrN	5m	80
Zirconium oxide, ZrO	5m	81
Zirconium phosphide, ZrP	4m	75
Zirconium silicate, zircon, $ZrSiO_4$	4	68
Zirconium sulfate hydrate (zircosulfate), $Zr(SO_4)_2 \cdot 4H_2O$	7	66

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Acetanilide, $C_6H_5NHCOCH_3$	14m	38
4-Acetyl-2'-fluorodiphenyl, $C_{14}H_{11}FO$	8m	91
Alanine, L-, $CH_3CHNH_2CO_2H$	8m	93
Allobarbital, $C_{10}H_{12}N_2O_3$	14m	41
Ammonium acetate, $NH_4 \cdot CH_3CO_2$	8m	95
Ammonium formate, NH_4HCO_2	11m	9
Ammonium oxalate hydrate (oxammite), $(NH_4)_2C_2O_4 \cdot H_2O$	7	5
Ammonium yttrium oxalate hydrate, $NH_4Y(C_2O_4)_2 \cdot H_2O$	8m	97
Ascorbic acid, L-, $C_6H_8O_6$	8m	99
Azobenzene, $C_6H_5NNC_6H_5$	7m	86
Cadmium hexaimidazole nitrate, $Cd(C_3H_4N_2)_6(NO_3)_2$	8m	23
Calcium formate, $Ca(HCO_2)_2$	8	16
Calcium malate hydrate, $Ca(O_2C)_2(CH_2CHOH) \cdot 2H_2O$	10m	76
Chlorpromazine, $C_{17}H_{19}ClN_2S$	14m	60
Cobalt acetate hydrate, $Co(C_2H_3O_2)_2 \cdot 4H_2O$	12m	19
Copper glutamate hydrate, $Cu(O_2C)_2(H_2NCHCH_2CH_2) \cdot 2H_2O$	7m	110
Copper tetraimidazole nitrate, $Cu(C_3H_4N_2)_4(NO_3)_2$	13m	24
Copper tetrapyrazole chloride, $Cu(C_3H_4N_2)_4Cl_2$	8m	31
Cysteine, L-, $HSCH_2 \cdot CH(NH_2) \cdot COOH$	11m	86
Diazepam, $C_{16}H_{13}ClN_2O$	14m	106
Dibenzoylmethane, $(C_6H_5CO)_2CH_2$	7m	115
(N,N)-Dimethyltryptamine, $C_{12}H_{16}N_2$	14m	109
bis-(o-Dodecacarborane), $C_4B_{20}H_{22}$	6m	7
Glucose, D-, α,(dextrose), $C_6H_{12}O_6$	11m	28
Glyoxime, $H_2C_2(NOH)_2$	8m	102
Hexamethylenediammonium adipate, $(CH_2)_4(CO_2H_3N)_2(CH_2)_6$	7m	121
Holmium ethylsulfate hydrate, $Ho[(C_2H_5)SO_4]_3 \cdot 9H_2O$	1m	18
Hydroquinone, γ-HOC_6H_4OH	8m	107
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 o-phthalate, $C_6H_4(CO_2Hg)_2$	10m	113
Methapyrilene hydrochloride, $C_{14}H_{20}ClN_3S$	14m	112
Methyl sulfonanilide, $C_6H_5NHSO_2CH_3$	9m	78
N-Methylphenazinium-7,7,8,8-tetracyanoquinodimethanide, $C_{25}H_{15}N_6$	7m	146
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
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
Palladium bis-(N-isopropyl-3-ethyl-salicylaldiminate), $Pd(C_{12}H_{16}NO)_2$	7m	144
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 oxalate hydrate, $K_2C_2O_4 \cdot H_2O$	9m	39
Potassium oxalate perhydrate, $K_2C_2O_4 \cdot H_2O_2$	9m	96
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 D-tartrate hydrate, $(CHOH\text{-}CO_2Na)_2 \cdot 2H_2O$	11m	110
Sodium oxalate, $Na_2C_2O_4$	6m	70
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
Trimethylammonium chloride, $(CH_3)_3NHCl$	9m	113
2,4,6-Trinitrophenetole, $C_2H_5OC_6H_2(NO_2)_3$	8m	152
Urea, $CO(NH_2)_2$	7	61
Uric acid, $C_5H_4N_4O_3$	8m	154
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

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Acanthite, Ag_2S (monoclinic)	10	51
Aeschynite $CeNbTiO_6$	3m	24
Alabandite, MnS	4	11
Anatase, TiO_2	7m	82
Andradite, $Ca_3Fe_2Si_3O_{12}$	9	22
Anglesite, $PbSO_4$	3	67
Anhydrite, $CaSO_4$	4	65
Antarcticite, $CaCl_2 \cdot 6H_2O$	12m	16
Antimony, Sb	3	14
Aphthitalite, $K_3Na(SO_4)_2$	6m	52
Aragonite, $CaCO_3$	3	53
Aragonite, $CaCO_3$ (orthorhombic, calculated pattern)	14m	44
Arcanite, K_2SO_4	3	62
Arsenic, As	3	6
Arsenolite, As_2O_3	1	51
Aurostibite, $AuSb_2$	7	18
*Azurite, $Cu_3(OH)_2(CO_3)_2$	10	30
Baryte, $BaSO_4$	10m	12
Berlinite, $AlPO_4$	10	3
Berndtite, SnS_2	9m	57
*Beryl, $Be_3Al_2Si_6O_{18}$	9	13
Bischofite, $MgCl_2 \cdot 6H_2O$	11m	37
Bismite, α-Bi_2O_3	3m	17
Bismoclite, BiOCl	4	54
Bismuth, Bi	3	20
Bismuthinite, Bi_2S_3	5m	13
Bixbyite, α-Mn_2O_3	11m	95
*Bloedite, $Na_2Mg(SO_4)_2 \cdot 4H_2O$	6m	63
Boehmite, $Al_2O_3 \cdot H_2O$	3	38
Bromargyrite, AgBr	4	46
Bromellite, BeO	1	36
*Brookite, TiO_2	3m	57
Brucite, $Mg(OH)_2$	6	30
Bunsenite, NiO	1	47
Burkeite, $Na_6CO_3(SO_4)_2$	11m	52
*Butlerite, $Fe(OH)SO_4 \cdot 2H_2O$	10m	95
Cadmoselite, CdSe	7	12
Calcite, $CaCO_3$	2	51
Calomel, Hg_2Cl_2	13m	30
Carnallite, $KMgCl_3 \cdot 6H_2O$	8m	50
Cassiterite, SnO_2	1	54
Celestite, $SrSO_4$	2	61
Cerianite, CeO_2	1	56
Cerussite, $PbCO_3$	2	56
Cervantite, Sb_2O_4	10	8
Chalcokyanite, $CuSO_4$	3m	29
Chloraluminite, $AlCl_3 \cdot 6H_2O$	7	3
Chlorargyrite, AgCl	4	44
Chloromagnesite, $MgCl_2$	11m	94
Chromatite, $CaCrO_4$	7	13
Chrysoberyl, $BeAl_2O_4$	9	10
Cinnabar, HgS	4	17
*Claudetite, As_2O_3	3m	9
Clausthalite, PbSe	5	38
Copper, Cu	1	15
Cordierite, $Mg_2Al_4Si_5O_{18}$ (orthorhombic)	1m	28
Corundum, Al_2O_3	9	3
Cotunnite, $PbCl_2$	12m	23
Covellite, CuS	4	13
Cristobalite (α or low) SiO_2	10	48
Cristobalite (β or high) SiO_2	1	42
*Cryolithionite, $Li_3Na_3Al_2F_{12}$	9m	23
Cryptohalite, $(NH_4)_2SiF_6$	5	5
Cuprite, Cu_2O	2	23
*Diamond, C	2	5
*Diaspore, $Al_2O_3 \cdot H_2O$	3	41
Diopside, $CaMg(SiO_3)_2$	5m	17
*Dravite, $NaMg_3Al_6B_3Si_6O_{27}(OH)_4$	3m	47
Eitelite, $Na_2Mg(CO_3)_2$	11m	56
Elpasolite, K_2NaAlF_6	9m	43
*Enstatite, $MgSiO_3$	6	32
Epsomite, $MgSO_4 \cdot 7H_2O$	7	30
Erythrosiderite, $K_2FeCl_5 \cdot H_2O$	14m	27
Eskolaite, Cr_2O_3	5	22
Ettringite, $Ca_6Al_2S_3O_{18} \cdot 31H_2O$	8	3
Fairchildite, $K_2Ca(CO_3)_2$	8m	48
Fluorapatite, $Ca_5F(PO_4)_3$	3m	22
Fluorite, CaF_2	1	69
Forsterite, Mg_2SiO_4	1	83
Franklinite, $ZnFe_2O_4$	9m	60
Fresnoite, $Ba_2TiSi_2O_8$	9m	14
Gahnite, $ZnAl_2O_4$	2	38
Galaxite, $MnAl_2O_4$	9	35
Galena, PbS	2	18
Geikielite, $MgTiO_3$	5	43
Gersdorffite, NiAsS	1m	35
Glauberite, $Na_2Ca(SO_4)_2$	6m	59
Gold, Au	1	33
Goslarite, $ZnSO_4 \cdot 7H_2O$	8	71
Greenockite, CdS	4	15
*Groutite, MnO(OH)	11m	97
Halite, NaCl	2	41
Hausmannite, Mn_3O_4	10m	38
*Hemimorphite, $Zn_4(OH)_2Si_2O_7 \cdot H_2O$	2	62
Hetaerolite, $ZnMn_2O_4$	10m	61
Hieratite, K_2SiF_6	5	50
Huebnerite, $MnWO_4$	2m	24
Humboldtine, $FeC_2O_4 \cdot 2H_2O$	10m	24
Humite, $Mg_7F_2Si_3O_{12}$	1m	30
Hydrophilite, $CaCl_2$	11m	18
Indialite, $Mg_2Al_4Si_5O_{18}$ (hexagonal)	1m	29
Iodargyrite, AgI	8	51
Iron, α-Fe	4	3
Jacobsite, $MnFe_2O_4$	9	36
*Julgoldite, $Ca_2Fe_3Si_3O_{10}(OH,O)_2(OH)_2$	10m	72
Kalistrontite, $K_2Sr(SO_4)_2$	14m	31
Kremersite, $(NH_4,K)_2FeCl_5 \cdot H_2O$	14m	8
Langbeinite, $K_2Mg_2(SO_4)_3$	6m	40
Lautarite, $Ca(IO_3)_2$	14m	12
Lead, Pb	1	34
*Leucophanite, $NaCaBeFSi_2O_6$	8m	138
Lime, CaO (see Vol. 1, p. 43)	14m	49
Litharge, PbO (red)	2	30
Lithiophosphate, Li_3Po_4	4m	21
Loellingite, $FeAs_2$	10	34
Loeweite, $Na_{12}Mg_7(SO_4)_{13} \cdot 15H_2O$	14m	35
Macedonite, $PbTiO_3$	5	39
Magnesiochromite, $MgCr_2O_4$	9	34
Magnesite, $MgCO_3$	7	28
Magnetite, Fe_3O_4	5m	31
Malachite, $Cu_2(OH)_2CO_3$	10	31
Manganolangbeinite, $K_2Mn_2(SO_4)_3$	6m	43
Manganosite, MnO	5	45
Marshite, CuI	4	38
Mascagnite, $(NH_4)_2SO_4$	9	8
Massicot, PbO (yellow)	2	32
Matlockite, PbFCl	13m	25

*Natural mineral.

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Mayenite, $Ca_{12}Al_{14}O_{33}$	9	20
Melanterite, $FeSO_4 \cdot 7H_2O$	8m	38
*Meliphanite, $Na_{.63}Ca_{1.37}BeAl_{1.13}Si_{1.87}O_{6.25}F_{.75}$	8m	135
Metaborite, HBO_2 (cubic)	4m	27
Metacinnabar, HgS	4	21
Miargyrite, $AgSbS_2$	5m	49
*Millerite, NiS	1m	37
Minium, Pb_3O_4	8	32
Mitscherlichite, $K_2CuCl_4 \cdot 2H_2O$	9m	34
Molybdenite, MoS_2	5	47
Molybdite, MoO_3	3	30
Montroydite, HgO	9	39
Mullite, $Al_6Si_2O_{13}$	3m	3
Nantokite, CuCl	4	35
*Newberyite, $MgHPO_4 \cdot 3H_2O$	7m	139
Niter, KNO_3	3	58
Nitrammite, NH_4NO_3	7	4
Nitrobarite, $Ba(NO_3)_2$	11m	14
Norbergite, $Mg_3F_2SiO_4$	10	39
Oldhamite, CaS	7	15
Otavite, $CdCO_3$	7	11
Oxammite, $(NH_4)_2C_2O_4 \cdot H_2O$	7	5
Palladium, Pd	1	21
Palmierite, $K_2Pb(SO_4)_2$	14m	30
*Paratellurite, TeO_2	10	55
Paratellurite, TeO_2	7	56
Periclase, MgO	1	37
Perovskite, $CaTiO_3$	9m	17
*Phenakite, Be_2SiO_4	8	11
Picromerite, $K_2Mg(SO_4)_2 \cdot 6H_2O$	8m	54
*Pirssonite, $Na_2Ca(CO_3)_2 \cdot 2H_2O$	9m	106
Platinum, Pt	1	31
Portlandite, $Ca(OH)_2$	1	58
Potash alum, $KAl(SO_4)_2 \cdot 12H_2O$	6	36
Powellite, $CaMoO_4$	6	22
Pyrargyrite, Ag_3SbS_3	5m	51
Pyrite, FeS_2	5	29
*Pyroaurite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$, phase II	10m	104
Pyrolusite, β-MnO_2	10m	39
Pyrope, $Mg_3Al_2(SiO_4)_3$	4m	24
*Quartz, SiO_2 (α or low)	3	24
Rammelsbergite, $NiAs_2$	10	42
Retgersite, $NiSO_4 \cdot 6H_2O$	7	36
Rhodochrosite, $MnCO_3$	7	32
Romarchite, SnO	4	28
Rutile, TiO_2	7m	83
Safflorite, $CoFeAs_4$	10	28
Sal-ammoniac, NH_4Cl	1	59
Sanbornite, β-$BaSi_2O_5$	13m	10
Sanmartinite, $ZnWO_4$	2m	40
Scacchite, $MnCl_2$	8m	43
*Scheelite, $CaWO_4$	6	23
Schultenite, $PbHAsO_4$	14m	18
Selenium, Se	5	54
Selenolite, SeO_2	7m	60
Sellaite, MgF_2	4	33
Senarmontite, Sb_2O_3	3	31
Shcherbinaite, V_2O_5	8	66
Silver, Ag	1	23
Silver, Ag (reference standard)	8m	2
*Sjögrenite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$, phase I	10m	103
Skutterudite, $CoAs_3$	10	21
*Smithsonite, $ZnCO_3$	8	69
*Sodalite, $Na_8Si_6Al_6O_{24}Cl_2$	7m	158
Soda-niter, $NaNO_3$	6	50
Sphaerocobaltite, $CoCO_3$	10	24
Sphalerite, ZnS	2	16
Spinel, $MgAl_2O_4$	9m	25
Stibnite, Sb_2S_3	5	6
Stolzite, $PbWO_4$	5m	34
Strontianite, $SrCO_3$	3	56
Struvite, $MgNH_4PO_4 \cdot 6H_2O$	3m	41
Sulfur, S (orthorhombic)	9	54
Sylvite, KCl	1	65
Syngenite, $K_2Ca(SO_4)_2 \cdot H_2O$	14m	25
*Tellurite, TeO_2	9	57
Tellurium, Te	1	26
Tellurobismuthite, Bi_2Te_3	3m	16
Tenorite, CuO	1	49
Teschemacherite, NH_4HCO_3	9	5
Thenardite, Na_2SO_4	2	59
Thermonatrite, $Na_2CO_3 \cdot H_2O$	8	54
*Thomsenolite, $NaCaAlF_6 \cdot H_2O$	8m	132
Thorianite, ThO_2	1	57
Thortveitite, $Sc_2Si_2O_7$	7m	58
Tiemannite, HgSe	7	35
Tin, α-Sn (cubic)	2	12
Tin, β-Sn (tetragonal)	1	24
*Topaz, $Al_2SiO_4(F,OH)_2$	1m	4
Trevorite, $NiFe_2O_4$	10	44
Tschermigite, $NH_4Al(SO_4)_2 \cdot 12H_2O$	6	3
Tungstenite, WS_2	8	65
Uraninite, UO_2	2	33
Uvarovite, $Ca_3Cr_2(SiO_4)_3$	10	17
*Valentinite, Sb_2O_3	10	6
Valentinite, Sb_2O_3	10	6
Villiaumite, NaF	1	63
Willemite, Zn_2SiO_4	7	62
Witherite, $BaCO_3$	2	54
Wulfenite, $PbMoO_4$	7	23
Wurtzite, ZnS	2	14
*Xanthoconite, Ag_3AsS_3	8m	126
Xenotime, YPO_4	8	67
Zinc, Zn	1	16
Zincite, ZnO	2	25
Zinkosite, $ZnSO_4$	7	64
*Zircon, $ZrSiO_4$	4	68
Zircosulfate, $Zr(SO_4)_2 \cdot 4H_2O$	7	66

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

Standard x-ray diffraction patterns are presented for 68 substances. Twenty-seven of these patterns represent experimental data and 41 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

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

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

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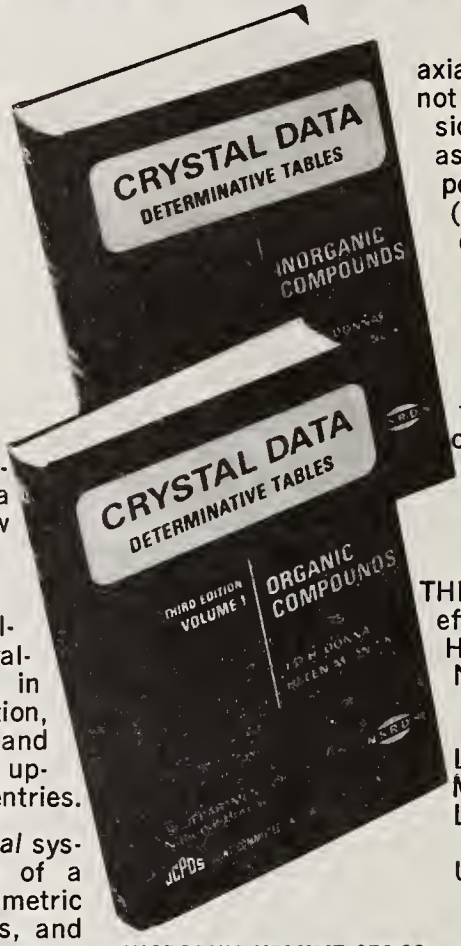

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