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A11100988630

/NBS monograph
QC100 .U556 V25-13;1976 C.1 NBS-PUB-C 19



NBS MONOGRAPH 25 – SECTION 13

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

Standard X-ray Diffraction Powder Patterns

QC
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U556
No.25-13
1976
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Standard X-ray Diffraction Powder Patterns

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Section 13—Data for 58 Substances

+ Monograph no. 25-13

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Issued June 1976

Library of Congress Catalog Card Number: 53-61386

National Bureau of Standards Monograph 25

Section 13—Data for 58 Substances

Nat. Bur. Stand. (U.S.), Monogr. 25—Sec. 13, 114 pages (June 1976)

CODEN: NBSMA6

**U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON: 1976**

**For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402
(Order by SD Catalog No. C13.44:25/Sec. 13). Price \$1.80 (Add 25 percent additional for other than U.S. mailing).**

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 13. --- Data for 58 Substances

by

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Standard x-ray diffraction patterns are presented for 58 substances. Thirty-one of these patterns represent experimental data and 27 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 58 compounds (31 experimental and 27 calculated patterns), and is the twenty-third of the series of "Standard X-ray Diffraction Powder Patterns."²

EXPERIMENTAL POWDER PATTERNS

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

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

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

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard (approximately 5 wt. percent tungsten powder). If tungsten lines were found to interfere with sample lines, silver or silicon was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid errors associated with aberrations at the very top of peaks, the readings of 20 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 20. 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.

¹Joint 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.

²See previous page for other published volumes.

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

| Calculated 2θ Angles, CuK α_1 $\lambda = 1.540598\text{\AA}$ | | | |
|---|---|--|--|
| hkl | W a=3.16524 \AA $\pm .00004$ | Ag a=4.08651 \AA $\pm .00002$ | Si a=5.43088 \AA $\pm .00004$ |
| 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: $\lambda(\text{CuK}\alpha_1, \text{peak}) = 1.540598\text{\AA}$ [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].

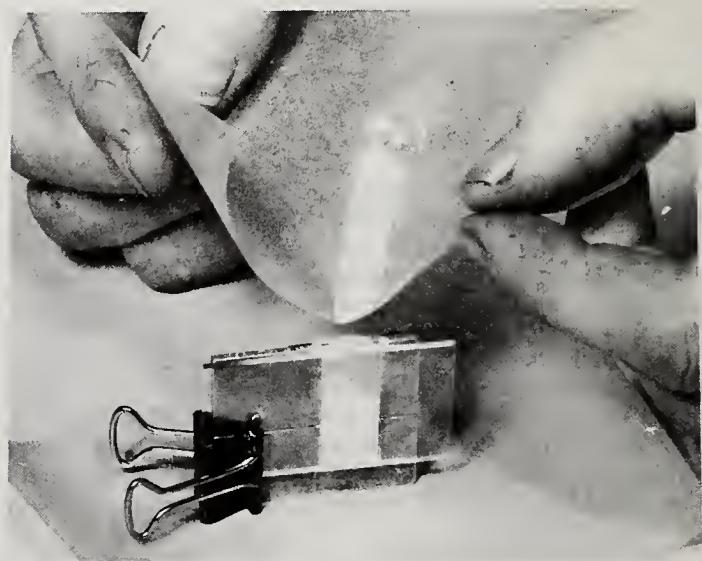
Orthorhombic cell dimensions were arranged according to the Dana convention $b > a > c$ [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of Crystal Data [1973]. For primitive cells, the transformed cell axes are an alternate labelling of the reduced cell

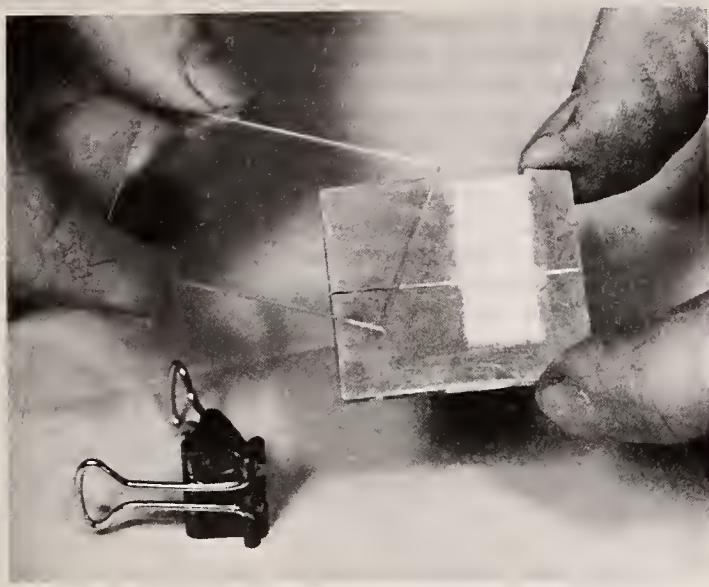
axes. For centered monoclinic cells, the transformed cell is the centered cell with the three shortest non-coplanar vectors.

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

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

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





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

Reference Intensity Ratio, I/I_{corundum} . For reference intensity measurements, $\alpha\text{-Al}_2\text{O}_3$ (corundum) was chosen as an internal standard to be mixed 1:1 by weight with the sample. This mixture of two components was mounted in our regular intensity sample holder (see Figures 1 & 2), and the pattern was taken. The reference intensity was then calculated as the direct ratio of the strongest line of the sample to the strongest line of corundum (hexagonal reflection (113)). In a few instances, the strongest line of one of the components coincided with a line of the other. In that case, the second strongest line was measured, and the value for the strongest line was then calculated.

CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by 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 $\lambda(\text{CuK}\alpha_1) = 1.540598\text{\AA}$ [Deslattes and Henins, 1973]. Both the altered and the original published values are given. Monoclinic and triclinic lattice constants

were transformed if necessary, to follow the convention of *Crystal Data* [1973]. For primitive cells, the transformed cell axes are an alternate labelling of the reduced cell axes. For centered monoclinic cells, the transformed cell is the centered cell with the three shortest non-coplanar vectors.

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

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

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

or

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

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

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

Structural information. The atom positions used in these calculated patterns varied somewhat in the degree of reliability. 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. When only the space group and structure type were given, 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:

$$\frac{I_i^{\text{abs}}}{K} = \frac{M_i L p_i |F_{i,T}|^2}{2\mu V^2}$$

where:

F is the structure factor

T is the thermal correction

$L_p = \frac{1+\cos^2\theta}{\sin^2\theta\cos\theta}$ 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]. That is:

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

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 -Al₂O₃).

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 CuK α_1 | FWHM | 2θ CuK α_1 | 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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Standard Reference Material 640, Silicon Powder, X-ray Diffraction Standard, obtainable from the Office of Standard Reference Materials, Room B311, Chemistry Building, National Bureau of Standards, Washington, D.C. 20234. \$52.00 per 10 gram unit.
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Arsenic iodide, AsI₃

Sample

The sample was obtained from the City Chemical Company of New York.

Major impurities

0.001 to 0.01% each Bi, Sb
0.0001 to 0.001% each Fe, Si

Color

Bright orange

Structure

Hexagonal, R̄3(148), Z = 6 [Braekken, 1930].

NBS lattice constants of this sample:

$$a = 7.2093(8) \text{ \AA}$$

$$c = 21.449(3)$$

Density

(calculated) 4.702 g/cm³

Reference intensity

I/I_{corundum} = 1.3

Additional patterns

1. PDF card 7-272 [Swanson et al., 1956].
2. Hanawalt et al. [1938].
3. Heyworth [1931].

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| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$ $\text{Internal standard W, } a = 3.16524 \text{ \AA}$ | | | |
|--|-----|---------------|---------------------------|
| $d(\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 7.14 | 4 | 003 | 12.39 |
| 5.39 | 9 | 012 | 16.43 |
| 3.573 | 50 | 006 | 24.90 |
| 3.218 | 100 | 113 | 27.70 |
| 2.752 | 2 | 107 | 32.51 |
| 2.539 | 20 | 116 | 35.32 |
| 2.464 | 2 | 018 | 36.43 |
| 2.384 | 1 | 009 | 37.71 |
| 2.081 | 25 | 300 | 43.46 |
| 2.028 | 3 | 1·0·10 | 44.65 |
| 1.9882 | 20 | 119 | 45.59 |
| 1.8611 | 2 | 0·1·11 | 48.90 |
| 1.7982 | 16 | 306 | 50.73 |
| 1.7873 | 8 | 0·0·12 | 51.06 |
| 1.7680 | 2 | 0·2·10 | 51.66 |
| 1.7472 | 10 | 223 | 52.32 |
| 1.6097 | 5 | 226 | 57.18 |
| 1.6012 | 6 | 1·1·12 | 57.51 |
| 1.4378 | 4 | 229 | 64.79 |
| 1.4295 | 3 | 0·0·15,321 | 65.21 |
| 1.3560 | 4 | 3·0·12 | 69.23 |
| 1.3388 | 6 | 413 | 70.25 |
| 1.3291 | 5 | 1·1·15 | 70.84 |
| 1.2730 | 3 | 416 | 74.47 |
| 1.2693 | 3 | 2·2·12 | 74.73 |
| 1.1914 | 3 | 0·0·18,3·2·10 | 80.56 |
| 1.1825 | 4 | 419 | 81.30 |
| 1.0337 | 1 | 2·4·10 | 96.35 |

Barium silicate, β -BaSiO₃

Sample

The sample was prepared by repeated grindings and heatings at about 1100 °C of a 1:1 molar mixture of Ba(OH)₂ and silica gel.

Color

Colorless

Structure

Orthorhombic, Pmmm(47), Z=4, isostructural with BaGeO₃ and NH₄BeF₃ [Liebau, 1957; Toropov and Grebenshchikov, 1956].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 5.6182(5) \text{ Å} \\ b &= 12.445(1) \\ c &= 4.5816(5) \end{aligned}$$

Density

(calculated) 4.421 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 2.6$$

Polymorphism

Funk [1958] reports a second form below about 990°. Grebenshchikov et al. [1967] confirm this and report that the transformation is irreversible. They also suggest a third form (β').

Additional patterns

1. PDF card 6-247 [Levin and Ugrinic, 1953].
2. PDF card 12-651 [Funk, 1958].
3. PDF card 21-83 [Grebenshchikov et al., 1967].
4. Austin [1947].
5. Toropov and Grebenshchikov [1956].

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| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ Å}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|---|-----|---------|----------------------|
| $\text{Internal standard Si, } a = 5.43088 \text{ Å}$ | | | |
| $d (\text{\AA})$ | I | hkl | $2\theta ({}^\circ)$ |
| 6.23 | 2 | 020 | 14.20 |
| 5.12 | 14 | 110 | 17.30 |
| 4.174 | 11 | 120 | 21.27 |
| 3.693 | 35 | 021 | 24.08 |
| 3.552 | 15 | 101 | 25.05 |
| | | | |
| 3.418 | 100 | 111 | 26.05 |
| 3.339 | 65 | 130 | 26.68 |
| 3.112 | 55 | 040 | 28.66 |
| 2.808 | 25 | 200 | 31.84 |
| 2.740 | 10 | 210 | 32.65 |
| | | | |
| 2.723 | 10 | 140 | 32.86 |
| 2.699 | 14 | 131 | 33.17 |
| 2.574 | 8 | 041 | 34.82 |
| 2.353 | 17 | 211 | 38.22 |
| 2.342 | 11 | 141 | 38.41 |
| | | | |
| 2.325 | 4 | 230 | 38.69 |
| 2.293 | 17 | 002 | 39.26 |
| 2.235 | 25 | 221 | 40.32 |
| 2.186 | 2 | 051 | 41.26 |
| 2.123 | <1 | 102 | 42.55 |
| | | | |
| 2.085 | 12 | 240 | 43.37 |
| 2.075 | 20 | 231,060 | 43.59 |
| 2.039 | 30 | 151 | 44.39 |
| 2.007 | 5 | 032 | 45.13 |
| 1.946 | 2 | 160 | 46.63 |
| | | | |
| 1.897 | 8 | 241 | 47.91 |
| 1.889 | 20 | 132,061 | 48.12 |
| 1.8629 | 4 | 250 | 48.85 |
| 1.8459 | 10 | 042 | 49.33 |
| 1.7932 | 6 | 320 | 50.88 |
| | | | |
| 1.7766 | 6 | 070,202 | 51.39 |
| 1.7588 | 5 | 212 | 51.95 |
| 1.7541 | 4 | 142 | 52.10 |
| 1.7337 | 7 | 301 | 52.76 |
| 1.7174 | 4 | 311 | 53.30 |
| | | | |
| 1.7067 | 5 | 330 | 53.66 |
| 1.6950 | 15 | 170 | 54.06 |
| 1.6685 | 2 | 260 | 54.99 |
| 1.6328 | 2 | 232 | 56.30 |
| 1.6151 | 1 | 152 | 56.97 |
| | | | |
| 1.6046 | 4 | 340 | 57.38 |
| 1.6002 | 4 | 331 | 57.55 |
| 1.5682 | 4 | 261 | 58.84 |
| 1.5554 | 1 | 080 | 59.37 |
| 1.5427 | 4 | 242 | 59.91 |
| | | | |
| 1.5387 | 4 | 062 | 60.08 |
| 1.5144 | 7 | 341 | 61.15 |
| 1.4989 | 2 | 180 | 61.85 |
| 1.4836 | 4 | 162 | 62.56 |
| 1.4734 | 6 | 081 | 63.04 |

Barium silicate, β -BaSiO₃ - continued

| d (Å) | I | hkl | 2θ (°) |
|--------|----|-----------|--------|
| 1.4649 | 4 | 113 | 63.45 |
| 1.4458 | 3 | 252 | 64.39 |
| 1.4350 | 3 | 123,033 | 64.93 |
| 1.4280 | 6 | 271 | 65.29 |
| 1.4247 | 3 | 181 | 65.46 |
| | | | |
| 1.4126 | 4 | 322 | 66.09 |
| 1.3958 | 4 | 410 | 66.99 |
| 1.3901 | 5 | 360,133 | 67.30 |
| 1.3690 | 3 | 332 | 68.48 |
| 1.3629 | 6 | 172 | 68.83 |
| | | | |
| 1.3490 | 1 | 262 | 69.64 |
| 1.3433 | <1 | 401,203 + | 69.98 |
| 1.3347 | 4 | 411,213 | 70.50 |
| 1.3304 | 5 | 430,361 | 70.76 |
| 1.3145 | 4 | 342 | 71.75 |
| | | | |
| 1.3126 | 4 | 421,223 | 71.87 |
| 1.3046 | 4 | 281 | 72.38 |
| 1.2886 | 4 | 191 | 73.42 |
| 1.2775 | 5 | 431,233 | 74.17 |
| 1.2688 | 3 | 153 | 74.76 |
| | | | |
| 1.2548 | 2 | 182 | 75.74 |
| 1.2444 | 2 | 0·10·0 | 76.49 |
| 1.2409 | 2 | 371,290 | 76.74 |
| 1.2304 | 2 | 063 | 77.52 |
| 1.2231 | 2 | 450 | 78.07 |
| 1.2009 | 1 | 0·10·1 | 79.80 |

Barium silicate (sanbornite), $\beta\text{-BaSi}_2\text{O}_5$

Sample

The sample was prepared by melting a 1:2 molar mixture of BaCO_3 and silica gel (at about 1430 °C) and annealing for 15 hours at 1325 °C. Because of the presence of a small amount of the high (α) form, the intensities are subject to a slight uncertainty.

Color

Colorless

Structure

Orthorhombic, $\text{Pmnb}(62)$, $Z=4$. The structure has been determined by Douglass [1958].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 7.6922(8)\text{\AA} \\ b &= 13.525(1) \\ c &= 4.6336(5) \end{aligned}$$

Density

(calculated) 3.769 g/cm³

Polymorphism

There is a high (α) form stable above 1350 °C [Roth and Levin, 1959]. This is given on PDF card 10-45 [Klasens et al., 1957].

Additional patterns

1. PDF card 10-46 [Klasens et al., 1957].
2. PDF card 11-170 (natural mineral) [Douglass, 1958].
3. Levin and Ugrinic [1953].
4. Oehlschlegel [1971].
5. Roth and Levin [1959].

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 Oehlschlegel, G. (1971). Glästechm. Ber. 44, 194.
 Roth, R.S. and Levin, E.M. (1959). J. Res. Nat. Bur. Stand. 62, 193.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{\AA}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|--|-----|---------|--------------------|
| $\text{Internal standard Si, } a = 5.43088 \text{\AA}$ | | | |
| $d(\text{\AA})$ | I | hkl | $2\theta (^\circ)$ |
| 6.77 | 40 | 020 | 13.06 |
| 5.08 | 25 | 120 | 17.43 |
| 3.973 | 85 | 101 | 22.36 |
| 3.844 | 6 | 200 | 23.12 |
| 3.808 | 9 | 111 | 23.34 |
| 3.424 | 50 | 121 | 26.00 |
| 3.382 | 16 | 040 | 26.33 |
| 3.343 | 70 | 220 | 26.64 |
| 3.234 | 30 | 031 | 27.56 |
| 3.097 | 100 | 140 | 28.80 |
| 2.981 | 4 | 131 | 29.95 |
| 2.892 | 5 | 211 | 30.90 |
| 2.732 | 35 | 041 | 32.75 |
| 2.712 | 40 | 221 | 33.00 |
| 2.575 | 18 | 141 | 34.81 |
| 2.539 | 6 | 240 | 35.32 |
| 2.399 | 4 | 320 | 37.46 |
| 2.337 | 8 | 051 | 38.49 |
| 2.317 | 13 | 002 | 38.83 |
| 2.285 | 3 | 012 | 39.40 |
| 2.244 | 11 | 301 | 40.16 |
| 2.236 | 13 | 151 | 40.30 |
| 2.227 | 35 | 241 | 40.47 |
| 2.192 | 14 | 022 | 41.15 |
| 2.164 | 25 | 160 | 41.70 |
| 2.130 | 35 | 321 | 42.41 |
| 2.108 | 10 | 122 | 42.86 |
| 2.059 | 4 | 032 | 43.93 |
| 2.043 | 9 | 340 | 44.31 |
| 2.027 | 20 | 061 | 44.66 |
| 1.996 | 5 | 251 | 45.40 |
| 1.9907 | 8 | 132 | 45.53 |
| 1.9845 | 6 | 202 | 45.68 |
| 1.9233 | 9 | 400 | 47.22 |
| 1.9047 | 11 | 222 | 47.71 |
| 1.8693 | 3 | 341 | 48.67 |
| 1.8547 | 12 | 142 | 49.08 |
| 1.8501 | 10 | 420 | 49.21 |
| 1.8166 | 3 | 232 | 50.18 |
| 1.7732 | 19 | 261 | 50.88 |
| 1.7367 | 3 | 171 | 52.66 |
| 1.7114 | 5 | 242 | 53.50 |
| 1.7049 | 5 | 312 | 53.72 |
| 1.6918 | 16 | 080 | 54.17 |
| 1.6716 | 3 | 440 | 54.88 |
| 1.6663 | 3 | 322 | 55.07 |
| 1.6516 | 5 | 431,180 | 55.60 |
| 1.6175 | 3 | 271 | 56.88 |
| 1.6000 | 5 | 252 | 57.56 |
| 1.5881 | 6 | 081 | 58.03 |

Barium silicate (sanbornite), $\beta\text{-BaSi}_2\text{O}_5$ - continued

| d (\AA) | I | hkl | 2θ ($^\circ$) |
|----------------------|----|------------|------------------------|
| 1.5812 | 10 | 162 | 58.31 |
| 1.5723 | 8 | 441 | 58.67 |
| 1.5552 | 6 | 181 | 59.38 |
| 1.5327 | 4 | 342 | 60.34 |
| 1.5144 | 2 | 103 | 61.15 |
| 1.5057 | 2 | 023,113 | 61.54 |
| 1.4840 | 5 | 451,072 | 62.54 |
| 1.4797 | 7 | 402 | 62.74 |
| 1.4676 | 8 | 281 | 63.32 |
| 1.4597 | 7 | 501 | 63.70 |
| 1.4508 | 4 | 511,352 | 64.14 |
| 1.4452 | 4 | 422 | 64.42 |
| 1.4352 | 2 | 133 | 64.92 |
| 1.4255 | 3 | 213 | 65.42 |
| 1.4115 | 4 | 380 | 66.15 |
| 1.4004 | 7 | 540 | 66.74 |
| 1.3953 | 8 | 461 | 67.02 |
| 1.3666 | 5 | 362,233 | 68.62 |
| 1.3555 | 3 | 442 | 69.26 |
| 1.3506 | 3 | 381 | 69.55 |
| 1.3443 | 4 | 182 | 69.92 |
| 1.3410 | 5 | 053,541 | 70.12 |
| 1.3319 | 2 | 1·10·0 | 70.67 |
| 1.3228 | 6 | 303 | 71.23 |
| 1.3196 | 5 | 243 | 71.43 |
| 1.2982 | 5 | 0·10·1,452 | 72.79 |
| 1.2801 | 8 | 1·10·1 | 73.99 |
| 1.2758 | 9 | 2·10·0,512 | 74.28 |
| 1.2696 | 5 | 480,333 | 74.71 |
| 1.2594 | 3 | 620,522 | 75.42 |
| 1.2328 | 3 | 532 | 77.34 |
| 1.2321 | 2 | 343 | 77.39 |
| 1.2244 | 3 | 481 | 77.97 |
| 1.2054 | 4 | 382 | 79.44 |

Barium silicate, Ba₂SiO₄

Sample

The sample was prepared by heating a 2:1 molar mixture of BaCO₃ and silicic acid at 1000 °C overnight, grinding and reheating at 1400 °C for 2 hours.

Color

Colorless

Structure

Orthorhombic, Pnam(62), Z=4, isostructural with α-K₂SO₄ [O'Daniel and Tscheischwili, 1942].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 7.508(1) \text{ Å} \\ b &= 10.214(1) \\ c &= 5.8091(8) \end{aligned}$$

Density

(calculated) 5.468 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 1.8$$

Additional patterns

1. PDF card 6-366 [Levin and Ugrinic, 1953].
2. Austin [1947].
3. Budnikov and Kulikova [1966].
4. Glushkova and Keler [1957].
5. Grebenschchikov et al. [1956].
6. O'Daniel and Tscheischwili [1942].
7. Shitova and Grebenschchikov [1972].
8. Toropov and Grebenschchikov [1956].

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 Toropov, N. A. and Grebenschchikov, R. G. (1956). J. Inorg. Chem. (USSR) 1 [12], 41.

| d (Å) | ° | I | hkl | 2θ (°) |
|--------|---|-----|-----|--------|
| 3.153 | | 25 | 201 | 28.28 |
| 3.098 | | 20 | 130 | 28.79 |
| 3.022 | | 70 | 220 | 29.53 |
| 3.017 | | 100 | 211 | 29.59 |
| 2.938 | | 95 | 031 | 30.40 |
| 2.905 | | 70 | 002 | 30.75 |
| 2.683 | | 13 | 221 | 33.37 |
| 2.554 | | 9 | 040 | 35.11 |
| 2.525 | | 20 | 022 | 35.53 |
| 2.431 | | 40 | 310 | 36.95 |
| 2.393 | | 20 | 122 | 37.55 |
| 2.297 | | 5 | 202 | 39.18 |
| 2.242 | | 20 | 212 | 40.19 |
| 2.233 | | 19 | 141 | 40.35 |
| 2.120 | | 20 | 132 | 42.62 |
| 2.095 | | 30 | 222 | 43.14 |
| 2.017 | | 12 | 330 | 44.91 |
| 1.984 | | 6 | 241 | 45.69 |
| 1.971 | | 16 | 150 | 46.00 |
| 1.928 | | 4 | 051 | 47.11 |
| 1.918 | | 2 | 042 | 47.37 |
| 1.904 | | 17 | 232 | 47.72 |
| 1.877 | | 3 | 400 | 48.47 |
| 1.864 | | 25 | 312 | 48.82 |
| 1.844 | | 4 | 113 | 49.38 |
| 1.795 | | 3 | 250 | 50.84 |
| 1.788 | | 6 | 340 | 51.04 |
| 1.786 | | 5 | 401 | 51.11 |
| 1.7594 | | 25 | 411 | 51.93 |
| 1.7203 | | 5 | 203 | 53.20 |
| 1.7084 | | 35 | 341 | 53.60 |
| 1.6970 | | 14 | 213 | 53.99 |
| 1.6832 | | 14 | 033 | 54.47 |
| 1.6566 | | 6 | 332 | 55.42 |
| 1.6438 | | 6 | 430 | 55.89 |
| 1.6309 | | 16 | 223 | 56.37 |
| 1.5967 | | 5 | 161 | 57.69 |
| 1.5767 | | 2 | 402 | 58.49 |
| 1.5507 | | 4 | 260 | 59.57 |
| 1.5115 | | 6 | 143 | 61.28 |
| 1.5066 | | 6 | 422 | 61.50 |
| 1.4976 | | 6 | 261 | 61.91 |
| 1.4684 | | 4 | 062 | 63.28 |
| 1.4639 | | 2 | 441 | 63.50 |
| 1.4524 | | 9 | 004 | 64.06 |
| 1.4396 | | 8 | 511 | 64.70 |
| 1.4301 | | 7 | 432 | 65.18 |
| 1.4151 | | 6 | 071 | 65.96 |
| 1.3822 | | 2 | 450 | 67.74 |
| 1.3680 | | 11 | 361 | 68.54 |
| 1.3479 | | 3 | 403 | 69.71 |
| 1.3367 | | 5 | 531 | 70.38 |

CuKα₁ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d (Å) | ° | I | hkl | 2θ (°) |
|-------|---|----|-----|--------|
| 5.11 | | 10 | 020 | 17.34 |
| 4.22 | | 16 | 120 | 21.02 |
| 4.20 | | 25 | 111 | 21.16 |
| 3.524 | | 14 | 210 | 25.25 |
| 3.415 | | 80 | 121 | 26.07 |

Barium silicate, $\text{Ba}_2\text{Si}_3\text{O}_8$

Sample

The sample was prepared by repeated grinding and heating at about 1400 °C of a 2:3 molar mixture of BaCO_3 and silica gel.

Color

Colorless

Structure

Monoclinic, $P2_1/a$ (14), $Z = 4$ [Kalscher and Liebau, 1965; Oehlschlegel, 1971]. $\text{Ba}_2\text{Si}_3\text{O}_8$ had earlier been reported with a similar cell with $a/2$ [Roth and Levin, 1959].

NBS lattice constants of this sample:

$$a = 13.960(3)\text{\AA}$$

$$b = 4.6895(9)$$

$$c = 12.486(2)$$

$$\beta = 93.54(1)^\circ$$

Density

(calculated) 3.964 g/cm³

Reference intensity

$I/I_{\text{corundum}} = 1.8$

Polymorphism

Oehlschlegel [1971] reports a reversible transformation of $\text{Ba}_2\text{Si}_3\text{O}_8$ at 1009 °C.

Additional patterns

1. PDF card 12-694 [Roth and Levin, 1959].
2. Austin [1947].

References

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 Kalscher, H. and Liebau, F. (1965). Naturwiss. 52, 512.
 Oehlschlegel, G. (1971). Glastech. Ber. 44, 194.
 Roth, R.S. and Levin, E.M. (1959). J. Res. Nat. Bur. Stand. 62, 193.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{\AA}; \text{temp. } 25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|---|-----|-----------|---------------------------|
| Internal standard Ag, $a = 4.08651 \text{\AA}$ | | | |
| $d(\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 12.51 | 10 | 001 | 7.06 |
| 6.965 | 20 | 200 | 12.70 |
| 6.245 | 5 | 201 | 14.17 |
| 5.929 | 16 | 201 | 14.93 |
| 4.512 | 2 | 202 | 19.66 |
| 4.390 | 2 | 011 | 20.21 |
| 4.162 | 2 | 111,003 | 21.33 |
| 3.890 | 4 | 210 | 22.84 |
| 3.746 | 55 | 211,012 | 23.73 |
| 3.669 | 100 | 203 | 24.24 |
| 3.478 | 5 | 400,203 | 25.59 |
| 3.415 | 5 | 401 | 26.07 |
| 3.301 | 70 | 401,310 | 26.99 |
| 3.250 | 30 | 212 | 27.42 |
| 3.121 | 40 | 402 | 28.58 |
| 3.114 | 40 | 004 | 28.64 |
| 2.864 | 1 | 312 | 31.21 |
| 2.792 | 13 | 213 | 32.03 |
| 2.782 | 60 | 204 | 32.15 |
| 2.756 | 30 | 411,403 | 32.46 |
| 2.701 | 2 | 411 | 33.14 |
| 2.598 | 3 | 412 | 34.49 |
| 2.493 | 4 | 005 | 36.00 |
| 2.475 | 1 | 214 | 36.26 |
| 2.398 | 5 | 404,510 | 37.48 |
| 2.393 | 5 | 205,214 | 37.55 |
| 2.376 | 2 | 511,413 | 37.84 |
| 2.346 | 10 | 020 | 38.34 |
| 2.310 | 3 | 601 | 38.96 |
| 2.301 | 3 | 205 | 39.11 |
| 2.268 | 19 | 121,413 | 39.71 |
| 2.221 | 13 | 220,602 | 40.58 |
| 2.201 | 9 | 015 | 40.98 |
| 2.180 | 2 | 221 | 41.38 |
| 2.133 | 30 | 602,215 + | 42.34 |
| 2.080 | 8 | 610,222 | 43.48 |
| 2.074 | 6 | 321 | 43.60 |
| 2.042 | 2 | 023 | 44.33 |
| 2.032 | 5 | 315,414 | 44.55 |
| 1.975 | 9 | 223,603 | 45.90 |
| 1.971 | 11 | 405 | 46.02 |
| 1.911 | 6 | 421 | 47.53 |
| 1.908 | 4 | 415 | 47.62 |
| 1.900 | 2 | 016 | 47.83 |
| 1.875 | 4 | 422,024 | 48.52 |
| 1.834 | 4 | 406 | 49.66 |
| 1.820 | 9 | 613 | 50.07 |
| 1.807 | 10 | 216 | 50.46 |
| 1.793 | 6 | 316,224 | 50.90 |
| 1.785 | 7 | 712,423 | 51.12 |

Barium silicate, $\text{Ba}_2\text{Si}_3\text{O}_8$ - continued

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ |
|-----------------|----|------------------------|---------------------------|
| 1.780 | 19 | 007 | 51.28 |
| 1.776 | 13 | $\bar{6}14, \bar{5}15$ | 51.42 |
| 1.753 | 6 | $\bar{6}05$ | 52.12 |
| 1.751 | 6 | $\bar{2}07$ | 52.20 |
| 1.738 | 5 | 423, 406 | 52.63 |
| 1.705 | 2 | $\bar{8}02, \bar{1}25$ | 53.73 |
| 1.649 | 8 | 620, 605 | 55.69 |
| 1.645 | 5 | $\bar{6}21$ | 55.85 |
| 1.631 | 4 | $\bar{8}11$ | 56.36 |
| 1.628 | 6 | 416 | 56.46 |
| 1.612 | 3 | $\bar{6}22, \bar{5}16$ | 57.09 |
| 1.608 | 3 | $\bar{8}11$ | 57.26 |
| 1.598 | 3 | 217, $\bar{6}06$ | 57.65 |
| 1.578 | 1 | 622 | 58.45 |
| 1.556 | 2 | $\bar{6}23, 615$ | 59.34 |
| 1.550 | 4 | 031, $\bar{8}13$ | 59.59 |
| 1.515 | 2 | 032, $\bar{7}21$ | 61.10 |
| 1.508 | 2 | 425 | 61.42 |
| 1.500 | 5 | 208 | 61.79 |
| 1.476 | 2 | 232, $\bar{3}31$ | 62.93 |
| 1.4697 | 3 | 910, $\bar{9}11 +$ | 63.22 |
| 1.4636 | 1 | 218, 033 | 63.51 |
| 1.4448 | 1 | 426 | 64.44 |
| 1.4208 | 3 | $\bar{4}31$ | 65.66 |
| 1.4180 | 3 | 027, $\bar{1}27$ | 65.81 |
| 1.4038 | 2 | 127 | 66.56 |
| 1.3914 | 10 | $\bar{6}17$ | 67.23 |
| 1.3485 | 3 | 625, $\bar{3}34$ | 69.67 |

Barium silicate, Ba_3SiO_5

Sample

The sample was prepared by repeated grindings and heatings at about 1400 °C of a 3:1 molar mixture of BaCO_3 and silica gel.

Color

Colorless

Structure

Tetragonal, I4/mcm (140), Z = 4, isostructural with Cs_3CoCl_5 and other similar compounds [Mansmann, 1965].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 7.3068(2)\text{\AA} \\ c &= 11.2275(6) \end{aligned}$$

Density

(calculated) 5.763 g/cm³

Reference Intensity

$$\frac{I}{I_{\text{corundum}}} = 2.4$$

Polymorphism

Since Glushkova and Keler [1957] and Budnikov and Kulikova [1966] report patterns which differ considerably from the present study, the possibility of polymorphism cannot be ruled out.

Additional patterns

1. PDF card 19-175 [Budnikov and Kulikova, 1966].
2. PDF card 23-1027 [Brisi and Appendino, 1966].
3. Glushkova and Keler [1957].
4. Eysel [1970].

References

- Brisi, C. and Appendino, P. (1966). Ric. Sci. 36, 369.
 Budnikov, P.P. and Kulikova, N.V. (1966). Inorg. Mater. (USSR), 2, 1717.
 Eysel, W. (1970). Neues Jahrb. Mineral. Monatsh. 1970, 534.
 Glushkova, V.B. and Keler, E.K. (1957). J. Inorg. Chem. (USSR) 2 [6], 63.
 Mansmann, M. (1965). Z. Anorg. Allg. Chem. 339, 52.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{\AA}$; temp. $25 \pm 1 \text{ }^{\circ}\text{C}$ Internal standard W, $a = 3.16524 \text{\AA}$ | | | |
|---|-----|-------|------------------------|
| $d(\text{\AA})$ | I | hkl | $2\theta ({}^{\circ})$ |
| 5.619 | 7 | 002 | 15.76 |
| 5.169 | 4 | 110 | 17.14 |
| 3.802 | 20 | 112 | 23.38 |
| 3.138 | 55 | 211 | 28.42 |
| 3.062 | 100 | 202 | 29.14 |
| 2.808 | 25 | 004 | 31.84 |
| 2.584 | 30 | 220 | 34.69 |
| 2.462 | 60 | 213 | 36.47 |
| 2.311 | 30 | 310 | 38.94 |
| 1.994 | 4 | 321 | 45.44 |
| 1.901 | 20 | 224 | 47.82 |
| 1.872 | 2 | 006 | 48.60 |
| 1.851 | 12 | 215 | 49.19 |
| 1.827 | 1 | 400 | 49.87 |
| 1.784 | 16 | 314 | 51.17 |
| 1.760 | 7 | 116 | 51.92 |
| 1.751 | 20 | 411 | 52.20 |
| 1.738 | 5 | 402 | 52.61 |
| 1.7224 | 2 | 330 | 53.13 |
| 1.6657 | 14 | 206 | 55.09 |
| 1.6465 | 16 | 332 | 55.79 |
| 1.6338 | 6 | 420 | 56.26 |
| 1.6018 | 16 | 413 | 57.49 |
| 1.5687 | 4 | 422 | 58.82 |
| 1.5311 | 3 | 404 | 60.41 |
| 1.5041 | 1 | 325 | 61.61 |
| 1.4676 | 1 | 334 | 63.32 |
| 1.4492 | 1 | 431 | 64.22 |
| 1.4402 | 4 | 217 | 64.67 |
| 1.4120 | 6 | 424 | 66.12 |
| 1.4034 | 3 | 008 | 66.58 |
| 1.3912 | 11 | 415 | 67.24 |
| 1.3881 | 10 | 512 | 67.41 |
| 1.3614 | 1 | 433 | 68.92 |
| 1.3473 | 1 | 521 | 69.74 |
| 1.3074 | 3 | 406 | 72.20 |
| 1.2917 | 2 | 440 | 73.22 |
| 1.2757 | 2 | 523 | 74.29 |
| 1.2677 | 6 | 336 | 74.84 |
| 1.2584 | 2 | 442 | 75.49 |
| 1.2534 | 5 | 530 | 75.84 |
| 1.2335 | 4 | 228 | 77.29 |
| 1.2307 | 3 | 426 | 77.50 |
| 1.2231 | 3 | 532 | 78.07 |
| 1.2179 | 4 | 600 | 78.47 |
| 1.1994 | 3 | 318 | 79.92 |
| 1.1944 | 3 | 611 | 80.32 |
| 1.1892 | 5 | 417 | 80.74 |
| 1.1737 | 1 | 444 | 82.04 |
| 1.1655 | 3 | 219 | 82.74 |

Barium silicate, Ba_3SiO_5 - continued

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ |
|-----------------|----|-----------|---------------------------|
| 1.1615 | 2 | 525 | 83.09 |
| 1.1442 | 8 | 534 | 84.63 |
| 1.1376 | 2 | 516 | 85.24 |
| 1.1350 | 2 | 541 | 85.48 |
| 1.1317 | 6 | 622 | 85.79 |
| 1.1172 | 5 | 604 | 87.18 |
| 1.1129 | 2 | 408 | 87.60 |
| 1.0916 | 1 | 543 | 89.77 |
| 1.0802 | 1 | 437 | 90.97 |
| 1.0732 | 3 | 20·10 | 91.74 |
| 1.0646 | 3 | 428 | 92.70 |
| 1.0591 | 2 | 615 | 93.32 |
| 1.0412 | 2 | 536 | 95.43 |
| 1.0335 | 1 | 710 | 96.38 |
| 1.0201 | 4 | 419 | 98.07 |
| 1.0174 | 3 | 545 | 98.42 |
| 1.0163 | 5 | 712 | 98.57 |
| 0.9997 | 2 | 721 | 100.80 |
| .9972 | 4 | 642 | 101.15 |
| .9830 | 5 | 626 | 103.19 |
| .9742 | 1 | 21·11 | 104.51 |
| .9695 | 3 | 554, 723. | 105.22 |
| .9615 | 2 | 617 | 106.48 |
| .9565 | 1 | 40·10 | 107.28 |
| .9530 | 2 | 644 | 107.85 |
| .9504 | 1 | 448 | 108.29 |
| .9457 | 2 | 732 | 109.09 |
| .9405 | 2 | 33·10 | 109.97 |
| .9347 | 6 | 538 | 111.00 |
| .9298 | 1 | 547 | 111.88 |
| .9252 | <1 | 42·10 | 112.73 |
| .9198 | 3 | 608 | 113.75 |
| .9162 | 3 | 725 | 114.43 |
| .9044 | 4 | 716 | 116.79 |
| .9033 | 5 | 741 | 117.02 |
| .9013 | 5 | 802, 637 | 117.45 |
| .8909 | 2 | 646 | 119.67 |
| .8860 | 3 | 820 | 120.78 |
| .8838 | 4 | 51·10 | 121.29 |
| .8808 | 4 | 743 | 121.99 |

Barium silicate, $\text{Ba}_3\text{Si}_5\text{O}_{13}$

Sample

The sample was prepared by heating a 3:5 molar mixture of BaCO_3 and silica gel at about 1400°C with repeated grindings and reheatings. Because of problems related to orientation, the intensities are subject to some uncertainty.

Color

Colorless

Optical data

Biaxial(+), $N_\alpha = 1.612$, $N_\beta = 1.616$, $N_\gamma = 1.636$.
 $2V$ is about 35° [Oehlschlegel, 1971].

Structure

Monoclinic, $P2_1/c$ (14), $Z = 4$ [Roth, 1966; Oehlschlegel, 1971].

NBS lattice constants of this sample:

$$a = 20.208(3) \text{ \AA}$$

$$b = 4.7106(5)$$

$$c = 13.854(2)$$

$$\beta = 98.62(1)^\circ$$

Density

(calculated) 3.874 g/cm³

Additional patterns

1. PDF card 12-547 [Roth and Levin, 1959].
2. Oehlschlegel [1971].

References

- Oehlschlegel, G. (1971). *Glastechn. Ber.* **44**, 194.
 Roth, R. (1966). *Private comm. to Crystal Data* (3rd Ed., published jointly by the U.S. Dept. of Commerce, National Bureau of Standards, Washington, D.C. 20234, and the Joint Committee on Powder Diffraction Standards, Swarthmore, Pa., 19081).
 Roth, R. and Levin, E. M. (1959). *J. Res. Nat. Bur. Stand.* **62**, 193.

| d (Å) | I | hkl | θ (°) |
|-------|-----|---------------|-------|
| 4.996 | 2 | 400 | 17.74 |
| 4.263 | 5 | 210 | 20.82 |
| 3.998 | 3 | 211, 500 | 22.22 |
| 3.870 | 11 | 112 | 22.96 |
| 3.844 | 55 | 310 | 23.12 |
| 3.773 | 100 | 402 | 23.56 |
| 3.729 | 10 | 212 | 23.84 |
| 3.622 | 2 | 311 | 24.56 |
| 3.484 | 3 | 312 | 25.55 |
| 3.424 | 7 | 410, 004 | 26.00 |
| 3.328 | 20 | 600 | 26.77 |
| 3.249 | 85 | 304, 411 + | 27.43 |
| 3.199 | 40 | 412 | 27.87 |
| 3.100 | 20 | 204 | 28.78 |
| 3.045 | 2 | 510, 404 | 29.31 |
| 2.909 | 6 | 512 | 30.71 |
| 2.875 | 13 | 304 | 31.08 |
| 2.855 | 5 | 700 | 31.31 |
| 2.788 | 75 | 114, 702 | 32.08 |
| 2.769 | 25 | 014 | 32.30 |
| 2.718 | 2 | 610 | 32.93 |
| 2.698 | 3 | 114 | 33.18 |
| 2.644 | 3 | 404 | 33.87 |
| 2.607 | 2 | 611 | 34.37 |
| 2.589 | 2 | 214, 604 | 34.62 |
| 2.558 | 1 | 414 | 35.05 |
| 2.497 | 1 | 800 | 35.93 |
| 2.469 | 3 | 802 | 36.36 |
| 2.443 | 2 | 710 | 36.76 |
| 2.429 | 4 | 612, 504 | 36.98 |
| 2.356 | 14 | 020 | 38.17 |
| 2.283 | 6 | 006 | 39.44 |
| 2.273 | 25 | 221 | 39.61 |
| 2.269 | 13 | 614 | 39.69 |
| 2.241 | 5 | 802, 215 | 40.21 |
| 2.230 | 18 | 106 | 40.41 |
| 2.224 | 15 | 122, 811 | 40.53 |
| 2.211 | 35 | 712, 902 | 40.77 |
| 2.206 | 30 | 810, 406 | 40.87 |
| 2.175 | 4 | 321 | 41.49 |
| 2.158 | 9 | 514, 206 | 41.82 |
| 2.124 | 5 | 421, 506 | 42.53 |
| 2.068 | 11 | 216, 123 + | 43.73 |
| 2.043 | 3 | 316 | 44.31 |
| 2.025 | 7 | 902, 812 | 44.72 |
| 2.008 | 8 | 910 | 45.11 |
| 2.004 | 16 | 904 | 45.20 |
| 1.999 | 15 | 422, 10·0·0 + | 45.33 |
| 1.980 | 2 | 423 | 45.79 |
| 1.923 | 2 | 620 | 47.22 |

CuK α_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

| d (Å) | I | hkl | θ (°) |
|-------|----|-----|-------|
| 9.96 | 4 | 200 | 8.87 |
| 6.80 | 16 | 102 | 13.00 |
| 6.202 | 6 | 102 | 14.27 |
| 6.091 | 15 | 202 | 14.53 |
| 5.181 | 3 | 302 | 17.10 |

Barium silicate, $\text{Ba}_3\text{Si}_5\text{O}_{13}$ - continued

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ |
|-----------------|----|------------------|---------------------------|
| 1.908 | 8 | 523, 324 | 47.61 |
| 1.888 | 5 | 804 | 48.15 |
| 1.8755 | 4 | 224 | 48.50 |
| 1.8504 | 4 | 10·0·4 | 49.20 |
| 1.8445 | 12 | 10·0·2, 914 | 49.37 |
| 1.8410 | 15 | 10·1·2, 10·1·0 | 49.47 |
| 1.8223 | 8 | 117, 324 + | 50.01 |
| 1.8162 | 35 | 11·0·0, 416 + | 50.19 |
| 1.7988 | 8 | 722 | 50.71 |
| 1.7854 | 11 | 025, 716 | 51.12 |
| 1.7635 | 4 | 125, 606 | 51.80 |
| 1.7276 | 6 | 108, 906 | 52.96 |
| 1.7040 | 2 | 822, 816 | 53.75 |
| 1.6657 | 2 | 706, 12·0·0 + | 55.09 |
| 1.6386 | 3 | 026, 914 | 56.08 |
| 1.6296 | 12 | 10·1·3, 10·0·6 | 56.42 |
| 1.6253 | 8 | 921, 218 + | 56.58 |
| 1.6209 | 8 | 916 | 56.75 |
| 1.6167 | 8 | 318, 815 + | 56.91 |
| 1.6118 | 7 | 922, 11·1·4 | 57.10 |
| 1.5984 | 3 | 418 | 57.62 |
| 1.5782 | 2 | 923, 526 | 58.43 |
| 1.5547 | 6 | 218 | 59.40 |
| 1.5509 | 9 | 230, 13·0·2 | 59.56 |
| 1.5360 | 2 | 618, 922 | 60.20 |
| 1.5284 | 4 | 330 | 60.53 |
| 1.5141 | 2 | 227, 127 + | 61.16 |
| 1.5103 | 1 | 12·1·4, 426 | 61.33 |
| 1.4948 | 2 | 508, 718 + | 62.04 |
| 1.4859 | 4 | 133, 12·1·2 | 62.45 |
| 1.4770 | 2 | 432 | 62.87 |
| 1.4732 | 2 | 923, 824 + | 63.05 |
| 1.4616 | 3 | 531, 530 + | 63.61 |
| 1.4526 | 2 | 12·0·6, 10·2·2 + | 64.05 |
| 1.4498 | 2 | 432 | 64.19 |
| 1.4418 | 7 | 11·2·2, 14·0·2 | 64.59 |
| 1.4386 | 7 | 11·2·0, 10·1·5 | 64.75 |
| 1.4272 | 2 | 034, 14·0·0 | 65.33 |
| 1.4155 | 4 | 12·0·4, 916 + | 65.94 |
| 1.4117 | 4 | 626 | 66.14 |
| 1.4003 | 3 | 918, 727 | 66.75 |
| 1.3936 | 8 | 14·0·4, 128 | 67.11 |
| 1.3852 | 2 | 2·0·10, 028 | 67.57 |
| 1.3782 | 2 | 428, 334 | 67.96 |
| 1.3662 | 4 | 135, 12·2·2 + | 68.64 |
| 1.3583 | 1 | 11·1·5, 527 | 69.10 |

Cadmium silicate, Cd_2SiO_4

Sample

The sample was prepared by heating at 1200 °C, for several hours, a 2:1 molar mixture of CdO and silica gel. The sample was ground and reheated several times at 1000 °C for one hour each time. A small amount of Cd_3SiO_5 was present and this may slightly distort the intensity measurements.

Color

Colorless

Structure

Orthorhombic, Fddd(70), Z=8. Isostructural with Na_2SO_4 (V). The structure was studied by Glasser and Glasser [1964].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 9.805(1)\text{\AA} \\ b &= 11.807(2) \\ c &= 6.013(1) \end{aligned}$$

Density

(calculated) 6.047 g/cm³

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 2.1$$

Additional pattern

1. PDF card 17-258 [Glasser and Glasser, 1964].

References

Glasser, L.S.D. and Glasser, F.P. (1964). Inorg. Chem. 3, 1228.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|---|-----|----------|--------|
| Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
| d(A) | I | hkl | 2θ (°) |
| 4.704 | 15 | 111 | 18.85 |
| 3.770 | 45 | 220 | 23.58 |
| 2.951 | 65 | 040 | 30.26 |
| 2.790 | 100 | 311 | 32.06 |
| 2.678 | 90 | 022 | 33.43 |
| 2.563 | 25 | 202 | 34.98 |
| 2.449 | 3 | 400 | 36.66 |
| 2.352 | 6 | 222 | 38.24 |
| 2.320 | 35 | 331 | 38.78 |
| 2.145 | 8 | 151 | 42.10 |
| 1.936 | 20 | 113, 242 | 46.90 |
| 1.841 | 20 | 511 | 49.48 |
| 1.824 | 35 | 260, 351 | 49.97 |
| 1.758 | 3 | 133 | 51.99 |
| 1.691 | 20 | 313 | 54.19 |
| 1.685 | 13 | 531 | 54.39 |
| 1.647 | 20 | 062 | 55.78 |
| 1.603 | 2 | 171 | 57.45 |
| 1.575 | 7 | 620 | 58.55 |
| 1.567 | 14 | 333 | 58.88 |
| 1.504 | 5 | 004 | 61.63 |
| 1.476 | 4 | 080 | 62.91 |
| 1.454 | 10 | 371 | 63.96 |
| 1.436 | 6 | 602 | 64.90 |
| 1.396 | 5 | 224 | 66.97 |
| 1.393 | 5 | 513 | 67.17 |
| 1.3843 | 6 | 353 | 67.62 |
| 1.3396 | 8 | 044 | 70.20 |
| 1.3199 | 2 | 533 | 71.41 |
| 1.2909 | 5 | 642 | 73.27 |
| 1.2789 | 3 | 282 | 74.07 |
| 1.2571 | 3 | 660 | 75.58 |
| 1.2259 | 1 | 800 | 77.86 |
| 1.2052 | 3 | 553 | 79.46 |
| 1.2003 | 4 | 373 | 79.85 |
| 1.1932 | 3 | 391 | 80.42 |

Cadmium silicate, Cd_3SiO_5

Sample

The sample was made by heating a 3:1 molar mixture of CdO and silica gel at 1100 °C for 2 hours. The product was then ground and reheated at 700 °C for 20 hours. The sample showed some hydration products after standing in air and also contained a very slight percentage of Cd_2SiO_4 ; therefore, the intensities may be slightly in error.

Color

Greenish yellow.

Structure

Tetragonal, P4/nmm (129), $Z = 2$ [Eysel, 1970]. Eysel (1970) suggested also a possible monoclinic cell. The broadening of some lines in patterns from this sample indicates that it probably is of lower symmetry.

NBS lattice constants of this sample:

$$\begin{aligned} a &= 6.842(2)\text{\AA} \\ c &= 4.952(2) \end{aligned}$$

Density

(calculated) 6.379 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 5.4$$

Additional patterns

1. PDF card 17-257 [Dent Glasser and Glasser, 1964].
2. Eysel [1970].

References

- Dent Glasser, L. S. and Glasser, F. P. (1964). Inorg. Chem. 3, 1228.
 Eysel, W. (1970). Neues Jahrb. Mineral. Monatsh. 1970, 534.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{\AA}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$ $\text{Internal standard W, } a = 3.16524 \text{\AA}$ | | | |
|---|-----|-----|--------|
| d (Å) | I | hkl | 2θ (°) |
| 4.96 | 5 | 001 | 17.88 |
| 4.85 | 8 | 110 | 18.29 |
| 4.015 | 3 | 101 | 22.12 |
| 3.462 | 5 | 111 | 25.71 |
| 3.420 | 2 | 200 | 26.03 |
| 2.814 | 100 | 201 | 31.77 |
| 2.604 | <1 | 211 | 34.41 |
| 2.476 | 11 | 002 | 36.25 |
| 2.419 | 20 | 220 | 37.14 |
| 2.327 | 4 | 102 | 38.66 |
| 2.206 | 3 | 112 | 40.88 |
| 2.173 | 5 | 221 | 41.53 |
| 2.165 | 5 | 310 | 41.68 |
| 2.071 | 2 | 301 | 43.68 |
| 2.006 | 3 | 202 | 45.16 |
| 1.982 | 3 | 311 | 45.70 |
| 1.924 | 1 | 212 | 47.20 |
| 1.730 | 20 | 222 | 52.87 |
| 1.710 | 10 | 400 | 53.55 |
| 1.677 | 1 | 302 | 54.68 |
| 1.629 | 1 | 312 | 56.44 |
| 1.616 | 1 | 401 | 56.94 |
| 1.613 | 2 | 330 | 57.04 |
| 1.562 | 1 | 113 | 59.08 |
| 1.530 | 1 | 420 | 60.44 |
| 1.5066 | 1 | 322 | 61.50 |
| 1.4861 | 7 | 203 | 62.44 |
| 1.4616 | 14 | 421 | 63.61 |
| 1.4072 | 6 | 402 | 66.38 |
| 1.3782 | 1 | 412 | 67.96 |

Calcium hydrogen phosphate hydrate, $\text{Ca}_8\text{H}_2(\text{PO}_4)_6 \cdot 5\text{H}_2\text{O}$

Sample

The sample was obtained from B. Dickens at NBS. Brown et al. [1962] prepared the sample. The intensity of the strongest line was very high compared to the other reflections. Therefore, the intensity of the second strongest line ($d=2.833$) was assigned the value of 100 and all other reflections were scaled to it. On that scale the strongest line at $d=18.67$ has $I \approx 300$.

Color

Colorless

Optical data

Biaxial(-), $N_{\alpha} = 1.576$, $N_{\beta} = 1.583$, $N_{\gamma} = 1.585$. $2V$ is $\approx 50^\circ$ [Brown et al, 1962].

Structure

Triclinic, $Z = 2$. The structure was determined by Brown et al.[1962] and refined by Dickens et al. [1973].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 9.529(3)\text{\AA} \\ b &= 18.994(4) \\ c &= 6.855(3) \\ \alpha &= 92.33(3)^\circ \\ \beta &= 90.13(3) \\ \gamma &= 79.93(2) \end{aligned}$$

Density

(calculated) 2.673 g/cm^3 .

Reference intensity

$I/I_{\text{corundum}} = 0.5$. This measurement is based on the line at 2.833\AA (designated as 100).

Additional patterns

1. PDF card 11-184 [Bjerrum, 1958].
2. PDF card 13-391 [Hayek et al, 1960].
3. Lehr et al. [1967].

References

- Bjerrum, N. (1958). Kgl. Dan. Vidensk. Selsk. Mat. Fys. Medd. 31, Nr. 7, 22.
 Brown, W.E., Smith, J.P., Lehr, J.R., and Frazier, A. W. (1962). Nature (London) 196, 1050.
 Dickens, B., Schroeder, L. W., and Brown, W. E. (1973). Am. Crys. Assoc. (Abs.-Winter Meeting) B2, 26.
 Hayek, E., Newesely, H., Hassenteufel, W., and Krismer, B. (1960). Monatsh. Chem. 91, 249.
 Lehr, J. R., Brown, E. H., Frazier, A. W., Smith, J.P., and Thrasher, R.D.(1967).Tenn. Val. Auth. (Chem. Eng. Bull.) No. 6.

| $\text{CuK}\alpha_1, \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ \text{C}$ | | | |
|--|-----|------------|-------------------|
| $\text{Internal standard W, } a = 3.16524 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I | hkl | $2\theta (\circ)$ |
| 18.67 | 300 | 010 | 4.73 |
| 9.36 | 45 | 100, 020 | 9.44 |
| 9.05 | 40 | 110 | 9.77 |
| 6.10 | 6 | 120 | 14.51 |
| 5.52 | 25 | 101 | 16.04 |
| 5.417 | 7 | 111, 021 | 16.35 |
| 5.211 | 4 | 111 | 17.00 |
| 5.101 | 12 | 111 | 17.37 |
| 4.815 | 6 | 130 | 18.41 |
| 4.706 | 5 | 031 | 18.84 |
| 4.670 | 4 | 040 | 18.99 |
| 4.514 | 10 | 031, 140 + | 19.65 |
| 4.492 | 10 | 121 | 19.75 |
| 4.294 | 7 | 131 | 20.67 |
| 4.111 | 5 | 230 | 21.60 |
| 3.919 | 16 | 220, 140 + | 22.67 |
| 3.879 | 12 | 201, 131 | 22.91 |
| 3.862 | 10 | 201 | 23.01 |
| 3.786 | 10 | 041 | 23.48 |
| 3.745 | 14 | 221 | 23.74 |
| 3.660 | 30 | 211 | 24.30 |
| 3.492 | 25 | 231 | 25.49 |
| 3.441 | 50 | 221 | 25.87 |
| 3.424 | 60 | 002 | 26.00 |
| 3.378 | 18 | 221 | 26.36 |
| 3.311 | 20 | 151 | 26.91 |
| 3.278 | 18 | 150 | 27.18 |
| 3.209 | 25 | 102, 250 + | 27.78 |
| 3.180 | 25 | 241, 310 | 28.04 |
| 3.132 | 10 | 122, 300 + | 28.48 |
| 3.117 | 7 | 112, 060 | 28.62 |
| 3.055 | 14 | 032, 240 | 29.21 |
| 3.015 | 8 | 330 | 29.61 |
| 2.946 | 14 | 122, 251 | 30.31 |
| 2.914 | 12 | 151 | 30.66 |
| 2.873 | 30 | 251 | 31.10 |
| 2.833 | 100 | 260 | 31.55 |
| 2.820 | 95 | 320, 241 | 31.70 |
| 2.779 | 45 | 142, 331 | 32.18 |
| 2.745 | 35 | 132, 331 | 32.59 |
| 2.707 | 25 | 222, 042 | 33.06 |
| 2.671 | 50 | 070 | 33.53 |
| 2.637 | 35 | 161, 350 | 33.97 |
| 2.617 | 20 | 330 | 34.23 |
| 2.606 | 20 | 222, 341 | 34.38 |
| 2.567 | 16 | 161, 152 | 34.93 |
| 2.544 | 12 | 171, 251 | 35.25 |
| 2.486 | 5 | 251 | 36.10 |
| 2.475 | 8 | 052, 171 | 36.27 |
| 2.458 | 5 | 170 | 36.52 |

Calcium hydrogen phosphate hydrate, $\text{Ca}_8\text{H}_2(\text{PO}_4)_6 \cdot 5\text{H}_2\text{O}$ - continued

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ |
|-----------------|----|---------------|---------------------------|
| 2.365 | 7 | 180 | 38.01 |
| 2.335 | 8 | 080, 271 + | 38.52 |
| 2.304 | 7 | 252, 302 + | 39.06 |
| 2.271 | 5 | 361, 312 | 39.66 |
| 2.265 | 6 | 181, 162 | 39.77 |
| 2.258 | 7 | 062, 341 | 39.89 |
| 2.215 | 16 | 162, 350 | 40.71 |
| 2.158 | 5 | 322, 441 | 41.83 |
| 2.136 | 7 | 441 | 42.27 |
| 2.106 | 9 | 190 | 42.90 |
| 2.088 | 7 | 252 | 43.29 |
| 2.063 | 6 | 272, 213 + | 43.85 |
| 2.036 | 5 | 133, 360 + | 44.46 |
| 2.002 | 8 | 262 | 45.25 |
| 1.998 | 9 | 431 | 45.35 |
| 1.990 | 10 | 191 | 45.55 |
| 1.957 | 7 | 422, 190 | 46.36 |
| 1.948 | 17 | 342, 381 + | 46.58 |
| 1.936 | 18 | 361 | 46.88 |
| 1.929 | 11 | 291, 233 | 47.06 |
| 1.914 | 11 | 053 | 47.46 |
| 1.897 | 10 | 1•10•0, 372 + | 47.92 |
| 1.891 | 10 | 530 | 48.07 |
| 1.848 | 20 | 303, 1•10•1 | 49.27 |
| 1.837 | 20 | 352, 391 + | 49.59 |
| 1.832 | 18 | 253, 511 + | 49.72 |
| 1.804 | 15 | 391, 2•10•1 | 50.54 |
| 1.745 | 8 | 291, 462 | 52.39 |
| 1.743 | 8 | 551 | 52.47 |
| 1.725 | 10 | 1•11•0 | 53.05 |
| 1.710 | 25 | 490 | 53.55 |

Cobalt phosphate, $\text{Co}(\text{PO}_3)_2$

Sample

The sample was prepared by heating a 1:2 molar mixture of CoCO_3 and H_3PO_4 to about 640 °C for 15 hours.

Color

Deep purplish red.

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:

$$\begin{aligned} a &= 11.189(3) \text{ Å} \\ b &= 8.287(2) \\ c &= 9.926(4) \\ \beta &= 112.42(3)^\circ \end{aligned}$$

Density

(calculated) 3.386 g/cm³

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 1.4$$

Additional pattern

1. PDF card 19-351 (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.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. 25 ± 1 °C Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
|---|-----|----------|----------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
| 6.45 | 6 | 110 | 13.71 |
| 6.146 | 40 | 011 | 14.40 |
| 4.576 | 20 | 211 | 19.38 |
| 4.251 | 35 | 112 | 20.88 |
| 3.742 | 6 | 121 | 23.76 |
| 3.538 | 20 | 211 | 25.15 |
| 3.378 | 30 | 112, 121 | 26.36 |
| 3.232 | 12 | 220 | 27.58 |
| 3.184 | 30 | 310 | 28.00 |
| 3.001 | 100 | 222 | 29.75 |
| 2.868 | 20 | 013 | 31.16 |
| 2.670 | 3 | 130 | 33.54 |
| 2.635 | 4 | 411 | 34.00 |
| 2.586 | 20 | 400 | 34.66 |
| 2.466 | 4 | 231 | 36.40 |
| 2.389 | 20 | 222 | 37.62 |
| 2.378 | 9 | 323 | 37.80 |
| 2.279 | 6 | 314 | 39.51 |
| 2.193 | 7 | 420, 411 | 41.13 |
| 2.177 | 7 | 404 | 41.45 |
| 2.156 | 3 | 330, 512 | 41.86 |
| 2.099 | 20 | 233 | 43.07 |
| 2.071 | 4 | 040 | 43.68 |
| 2.016 | 8 | 114, 141 | 44.93 |
| 1.956 | 6 | 402 | 46.38 |
| 1.928 | 4 | 424 | 47.10 |
| 1.895 | 2 | 523 | 47.96 |
| 1.872 | 3 | 242 | 48.61 |
| 1.854 | 3 | 433 | 49.10 |
| 1.824 | 2 | 415 | 49.97 |
| 1.799 | 5 | 334 | 50.71 |
| 1.757 | 8 | 233 | 52.00 |
| 1.754 | 6 | 431, 143 | 52.09 |
| 1.735 | 6 | 532 | 52.70 |
| 1.701 | 7 | 622 | 53.85 |
| 1.6314 | 10 | 051, 512 | 56.35 |
| 1.6167 | 7 | 440 | 56.91 |
| 1.6115 | 7 | 235, 314 | 57.11 |
| 1.5376 | 6 | 044 | 60.13 |
| 1.5295 | 6 | 006 | 60.48 |
| 1.5250 | 7 | 633 | 60.68 |
| 1.5009 | 4 | 444 | 61.76 |

Copper imidazole nitrate, Cu(C₃H₄N₂)₄(NO₃)₂

Sample

The sample was prepared at NBS by C. W. Reimann by evaporating an aqueous solution of Cu(NO₃)₂ and imidazole (C₃H₄N₂) at room temperature. It was difficult to obtain intensities because the sample deteriorated somewhat when exposed to x-rays.

Color

Unground: deep blue

Optical Data

Biaxial (-), N_α = 1.584, N_β = 1.610, N_γ = 1.645.
2V ≈ 40°. The sample shows pleochroism.

Structure

Orthorhombic, Pmn_b(62), Z=4, [Mighell, Santoro, and Reimann, private comm.].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 13.396(3) \text{ Å} \\ b &= 13.858(3) \\ c &= 9.825(2) \end{aligned}$$

Density

(calculated) 1.675 g/cm³

Reference intensity

I/I_{corundum} = 1.0

| CuK _α ₁ λ = 1.540598 Å; temp. 25±1 °C | | | |
|---|-----|-----|--------|
| Internal standard Ag, a = 4.08651 Å | | | |
| d(Å) | I | hkl | 2θ (°) |
| 8.01 | 8 | 011 | 11.04 |
| 6.87 | 19 | 111 | 12.87 |
| 6.697 | 6 | 200 | 13.21 |
| 6.159 | 25 | 120 | 14.37 |
| 5.142 | 25 | 211 | 17.23 |
| 4.911 | 5 | 002 | 18.05 |
| 4.629 | 3 | 012 | 19.16 |
| 4.375 | 16 | 112 | 20.28 |
| 4.182 | 4 | 031 | 21.23 |
| 4.066 | 10 | 301 | 21.84 |
| 3.962 | 100 | 202 | 22.42 |
| 3.906 | 25 | 311 | 22.75 |
| 3.839 | 18 | 122 | 23.15 |
| 3.807 | 18 | 212 | 23.35 |
| 3.756 | 40 | 320 | 23.67 |

| d(Å) | I | hkl | 2θ (°) |
|-------|----|------------|--------|
| 3.548 | 8 | 231 | 25.08 |
| 3.464 | 85 | 040 | 25.70 |
| 3.352 | 8 | 140, 400 | 26.57 |
| 3.264 | 9 | 041, 132 | 27.30 |
| 3.179 | 7 | 103, 141 | 28.05 |
| 3.092 | 25 | 411 | 28.85 |
| 3.051 | 7 | 331 | 29.25 |
| 3.009 | 10 | 232 | 29.67 |
| 2.984 | 10 | 322 | 29.92 |
| 2.938 | 3 | 241 | 30.40 |
| 2.883 | 8 | 421 | 30.99 |
| 2.832 | 1 | 042 | 31.57 |
| 2.768 | 16 | 142, 402 | 32.32 |
| 2.736 | 6 | 340 | 32.70 |
| 2.707 | 8 | 223 | 33.06 |
| 2.666 | 5 | 051 | 33.59 |
| 2.638 | 14 | 341 | 33.96 |
| 2.615 | 25 | 151, 431 | 34.26 |
| 2.608 | 16 | 242 | 34.36 |
| 2.541 | 2 | 511 | 35.30 |
| 2.498 | 4 | 520 | 35.92 |
| 2.477 | 4 | 251 | 36.23 |
| 2.456 | 5 | 004 | 36.56 |
| 2.379 | 4 | 114, 043 + | 37.79 |
| 2.338 | 4 | 441 | 38.47 |
| 2.306 | 13 | 204 | 39.03 |
| 2.277 | 20 | 160, 214 | 39.55 |
| 2.243 | 6 | 243 | 40.18 |
| 2.228 | 11 | 522 | 40.46 |
| 2.183 | 2 | 260 | 41.32 |
| 2.161 | 6 | 442 | 41.76 |
| 2.119 | 2 | 540 | 42.63 |
| 2.087 | 5 | 433, 451 | 43.31 |
| 2.065 | 6 | 162 | 43.80 |
| 2.050 | 10 | 360, 513 | 44.14 |
| 2.033 | 5 | 602 | 44.53 |
| 2.004 | 2 | 044 | 45.20 |
| 1.980 | 4 | 144, 404 | 45.79 |
| 1.958 | 1 | 452 | 46.33 |
| 1.941 | 3 | 071, 443 | 46.77 |
| 1.921 | 6 | 171, 244 | 47.29 |
| 1.891 | 8 | 025, 551 + | 48.08 |
| 1.866 | 4 | 461 | 48.75 |
| 1.861 | 5 | 711, 632 | 48.89 |
| 1.845 | 2 | 720, 641 | 49.36 |
| 1.828 | 4 | 613, 344 | 49.85 |
| 1.780 | 7 | 371, 543 | 51.28 |
| 1.752 | 3 | 642, 524 | 52.16 |
| 1.749 | 2 | 560 | 52.26 |
| 1.733 | 3 | 080 | 52.78 |
| 1.727 | 3 | 722 | 52.99 |
| 1.710 | 2 | 045 | 53.56 |

Lead chloride fluoride (matlockite), PbClF

Sample

The sample was prepared by melting a 1:1 molar mixture of PbCl₂ and PbF₂ at about 600 °C.

Color

Yellowish gray

Structure

Tetragonal, P4/nmm (129), Z = 2, isostructural with BaClF and other similar double halides. The structure of PbClF was determined by Bannister [1934].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 4.1104(2) \text{ Å} \\ c &= 7.2325(5) \end{aligned}$$

Density

(calculated) 7.111 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 6.2$$

Additional patterns

1. PDF card 4-460 [Swanson et al., 1953].
2. Nieuwenkamp and Bijvoet [1932].

References

- Bahnister, F.A. (1934). Mineral. Mag. 23, 587.
 Nieuwenkamp, W. and Bijvoet, J. M. (1932). Z. Krist. 81, 469.
 Swanson, H. E. and Tatge, E. (1953). Nat. Bur. Stand. (U.S.) Circ. 539, 1, 76.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ Å}$; temp. 25 ± 1 °C Internal standard W, $a = 3.16524 \text{ Å}$ | | | |
|---|-----|-------|----------------------|
| $d(\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
| 7.22 | 13 | 001 | 12.25 |
| 3.617 | 40 | 002 | 24.59 |
| 3.574 | 100 | 101 | 24.89 |
| 2.906 | 45 | 110 | 30.74 |
| 2.715 | 35 | 102 | 32.96 |
| 2.412 | 4 | 003 | 37.25 |
| 2.265 | 40 | 112 | 39.76 |
| 2.079 | 16 | 103 | 43.49 |
| 2.055 | 20 | 200 | 44.04 |
| 1.976 | 2 | 201 | 45.88 |
| 1.855 | 9 | 113 | 49.06 |
| 1.808 | 1 | 004 | 50.43 |
| 1.786 | 17 | 202 | 51.10 |
| 1.781 | 25 | 211 | 51.26 |
| 1.6552 | 11 | 104 | 55.47 |
| 1.6386 | 9 | 212 | 56.08 |
| 1.5636 | 2 | 203 | 59.03 |
| 1.5350 | 1 | 114 | 60.24 |
| 1.4618 | 7 | 213 | 63.60 |
| 1.4528 | 5 | 220 | 64.04 |
| 1.4466 | 3 | 005 | 64.35 |
| 1.4249 | 1 | 221 | 65.45 |
| 1.3645 | 1 | 105 | 68.74 |
| 1.3478 | 5 | 222 | 69.71 |
| 1.3458 | 4 | 301 | 69.83 |
| 1.3001 | 5 | 310 | 72.67 |
| 1.2952 | 6 | 115 | 72.99 |
| 1.2891 | 8 | 214 | 73.39 |
| 1.2814 | 2 | 302 | 73.90 |
| 1.2232 | 5 | 312 | 78.06 |
| 1.1910 | 1 | 303 | 80.60 |
| 1.1831 | 3 | 205 | 81.25 |
| 1.1567 | 2 | 106 | 83.51 |
| 1.1440 | 2 | 313 | 84.65 |
| 1.1368 | 1 | 215 | 85.31 |
| 1.1259 | 2 | 321 | 86.34 |
| 1.0920 | 2 | 304 | 89.72 |
| 1.0873 | 2 | 322 | 90.22 |
| 1.0331 | 1 | 007 | 96.43 |
| 1.0252 | 2 | 225 | 97.42 |
| 1.0079 | 1 | 216 | 99.68 |
| 0.9878 | 2 | 411 | 102.49 |
| 0.9736 | 1 | 117 | 104.59 |
| 0.9669 | 2 | 315 | 105.63 |
| 0.9645 | 3 | 324 | 106.01 |

Magnesium phosphate, $\text{Mg}(\text{PO}_3)_2$

Sample

The sample was prepared by heating a 1:2 molar mixture of MgCO_3 and H_3PO_4 to 710 °C. It was then reground and reheated at 710 °C several times.

Color

Colorless

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:

$$\begin{aligned} a &= 11.119(3)\text{\AA} \\ b &= 8.268(2) \\ c &= 9.920(3) \\ \beta &= 112.44(3)^\circ \end{aligned}$$

Density

(calculated) 2.872 g/cm³

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 1.4$$

Additional pattern

1. PDF card 11-41 [Sarver and Hummel, 1959].

References

- Beucher, M. and Grenier, J.-C. (1968). Mater. Res. Bull. 3, 643.
 Sarver, J. F. and Hummel, F. A. (1959). J. Electrochem. Soc. 106, 500.

| CuK α_1 $\lambda = 1.540598 \text{\AA}$; temp. 25±1 °C | | | |
|--|-----|----------|-------|
| Internal standard W, $a = 3.16524 \text{\AA}$ | | | |
| d(Å) | I | hkl | 2θ(°) |
| 6.44 | 2 | 110 | 13.75 |
| 6.14 | 16 | 011 | 14.42 |
| 5.13 | 4 | 200 | 17.26 |
| 4.59 | 60 | 002 | 19.34 |
| 4.34 | 4 | 202 | 20.47 |
| 4.243 | 35 | 112 | 20.92 |
| 3.731 | 1 | 121 | 23.83 |
| 3.519 | 20 | 211 | 25.29 |
| 3.371 | 25 | 112, 121 | 26.42 |
| 3.219 | 50 | 220 | 27.69 |
| 3.181 | 30 | 312 | 28.03 |
| 3.164 | 30 | 310 | 28.18 |
| 3.070 | 2 | 022 | 29.06 |
| 2.993 | 100 | 222 | 29.83 |
| 2.865 | 16 | 013 | 31.19 |
| 2.728 | 6 | 402 | 32.80 |
| 2.662 | 1 | 130 | 33.64 |
| 2.576 | 20 | 123 | 34.80 |
| 2.380 | 16 | 222 | 37.77 |
| 2.373 | 12 | 323 | 37.89 |
| 2.358 | 6 | 321 | 38.14 |
| 2.277 | 6 | 422, 314 | 39.55 |
| 2.248 | 4 | 231 | 40.07 |
| 2.242 | 3 | 123 | 40.19 |
| 2.181 | 8 | 420, 411 | 41.37 |
| 2.147 | 2 | 330 | 42.05 |
| 2.094 | 17 | 233 | 43.16 |
| 2.068 | 2 | 040 | 43.74 |
| 1.946 | 3 | 141, 402 | 46.63 |
| 1.938 | 3 | 521 | 46.85 |
| 1.929 | 4 | 215 | 47.07 |
| 1.885 | 3 | 042 | 48.23 |
| 1.865 | 2 | 242 | 48.78 |
| 1.848 | 2 | 433, 204 | 49.27 |
| 1.828 | 2 | 134 | 49.83 |
| 1.805 | 4 | 341 | 50.53 |
| 1.796 | 6 | 334 | 50.81 |
| 1.755 | 6 | 125 | 52.06 |
| 1.754 | 6 | 233 | 52.10 |
| 1.751 | 4 | 143 | 52.19 |
| 1.728 | 6 | 532 | 52.96 |
| 1.692 | 7 | 622 | 54.18 |
| 1.648 | 4 | 442, 530 | 55.74 |
| 1.627 | 7 | 051 | 56.51 |
| 1.623 | 8 | 512 | 56.67 |
| 1.6102 | 10 | 440 | 57.16 |
| 1.5353 | 8 | 044 | 60.23 |
| 1.5184 | 6 | 633 | 60.97 |
| 1.5148 | 6 | 631 | 61.13 |
| 1.4974 | 4 | 444 | 61.92 |

Magnesium tungsten oxide, $MgWO_4$

Sample

The sample was prepared by treating an aqueous solution of Na_2WO_4 with concentrated $MgCl_2$ at 80°C. The precipitate was filtered, washed with alcohol and heated at 850°C for 30 minutes.

Color

Colorless

Structure

Monoclinic, $P2/a$ (13), $Z=2$, isostructural with wolframite, $(Fe,Mn)WO_4$ [Broch, 1929].

NBS lattice constants of this sample:

$$a = 4.9288(6)\text{\AA}$$

$$b = 5.6751(8)$$

$$c = 4.6879(5)$$

$$\beta = 90.70(1)^\circ$$

Density

(calculated) 6.893 g/cm^3

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 3.0$$

Polymorphism

The monoclinic, wolframite type reported here is stable below 1165°C. Chang et al. [1966] reported a high temperature modification stable above 1165°C. Their data are given on PDF card 19-776. Dunning et al., [1947] reported the existence of a cubic modification, formed between 90° and 300°C.

Additional patterns

1. PDF card 7-190 [Swanson et al. 1953].
2. Broch [1929].
3. Dunning and Megaw [1946].
4. Fonda [1944].

References

- Broch, E. (1929). Skrifter Norske Videns. - Akad., Oslo I. Mat. Nat. Klasse 1929, No. 8.
 Chang, L. L. Y., Scroger, M. G., and Phillips, B. (1966). J. Amer. Ceram. Soc. 49, 385.
 Dunning, N. J. and Megaw, H. D., (1946). Trans. Faraday Soc. 42, 705.
 Fonda, G. R. (1944). J. Phys. Chem. 48, 303.
 Swanson, H. E. and Tatge, E. (1953). Nat. Bur. Stand., U.S. Circ. 539, Vol. I, 84.

| $CuK\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|--|-----|----------|--------------------|
| $\text{Internal standard W, } a = 3.16524 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I | hkl | $2\theta (^\circ)$ |
| 5.67 | 20 | 010 | 15.63 |
| 4.68 | 95 | 001 | 18.94 |
| 3.719 | 100 | 110 | 23.91 |
| 3.610 | 45 | 011 | 24.64 |
| 2.929 | 100 | 111 | 30.50 |
| 2.901 | 95 | 111 | 30.80 |
| 2.836 | 25 | 020 | 31.52 |
| 2.463 | 40 | 200 | 36.45 |
| 2.459 | 40 | 120 | 36.51 |
| 2.427 | 18 | 021 | 37.01 |
| 2.343 | 20 | 002 | 38.39 |
| 2.261 | 3 | 210 | 39.84 |
| 2.191 | 25 | 201 | 41.16 |
| 2.185 | 14 | 121 | 41.28 |
| 2.172 | 40 | 121, 201 | 41.55 |
| 2.044 | 6 | 211 | 44.28 |
| 2.027 | 11 | 211 | 44.68 |
| 1.9919 | 13 | 112 | 45.50 |
| 1.9751 | 18 | 112 | 45.91 |
| 1.8913 | 8 | 030 | 48.07 |
| 1.8600 | 13 | 220 | 48.93 |
| 1.8068 | 12 | 022 | 50.47 |
| 1.7660 | 3 | 130 | 51.72 |
| 1.7540 | 25 | 031 | 52.10 |
| 1.7346 | 6 | 221 | 52.73 |
| 1.7243 | 7 | 221 | 53.07 |
| 1.7087 | 15 | 202 | 53.59 |
| 1.7020 | 17 | 122 | 53.82 |
| 1.6909 | 20 | 122 | 54.20 |
| 1.6881 | 25 | 202 | 54.30 |
| 1.6552 | 2 | 131 | 55.47 |
| 1.6508 | 2 | 131 | 55.63 |
| 1.6360 | 2 | 212 | 56.18 |
| 1.6180 | 2 | 212 | 56.86 |
| 1.5782 | 7 | 310 | 58.43 |
| 1.5626 | 4 | 003 | 59.07 |
| 1.5061 | 3 | 013 | 61.52 |
| 1.5011 | 18 | 311, 230 | 61.75 |
| 1.4904 | 10 | 311 | 62.24 |
| 1.4720 | 7 | 032 | 63.11 |
| 1.4643 | 6 | 222 | 63.48 |
| 1.4508 | 6 | 222 | 64.14 |
| 1.4458 | 11 | 113 | 64.39 |
| 1.4360 | 14 | 113 | 64.88 |
| 1.4327 | 17 | 231 | 65.05 |
| 1.4264 | 12 | 231 | 65.37 |
| 1.4222 | 15 | 320 | 65.59 |
| 1.3690 | 3 | 023 | 68.48 |
| 1.3641 | 13 | 321, 140 | 68.76 |
| 1.3565 | 4 | 321 | 69.20 |

Magnesium tungsten oxide, MgWO_4

| d (Å) | I | hkl | 2θ (°) |
|--------|---|-------------|--------|
| 1.3271 | 2 | $\bar{2}03$ | 70.96 |
| 1.3224 | 6 | $\bar{1}23$ | 71.25 |
| 1.3160 | 4 | $\bar{3}12$ | 71.65 |
| 1.3121 | 7 | $\bar{2}03$ | 71.90 |
| 1.3102 | 8 | $\bar{1}41$ | 72.02 |
| 1.3019 | 4 | 312 | 72.55 |
| 1.2923 | 2 | $\bar{2}13$ | 73.17 |
| 1.2786 | 2 | 213 | 74.09 |
| 1.2681 | 4 | $\bar{2}32$ | 74.81 |

Mercury chloride, HgCl_2

Sample

The sample was commercially prepared mercuric chloride.

Color

Colorless

Optical data

Biaxial(-), $N_\alpha = 1.725$, $N_\beta = 1.859$, $N_\gamma = 1.965$, $2V = 85^\circ$ [Merwin, 1920].

Structure

Orthorhombic, $Pmn\bar{b}$ (62), $Z = 4$. The structure was determined by Braekken and Scholten [1934].

NBS lattice constants of this sample:

$$a = 5.9756(8)\text{\AA}$$

$$b = 12.768(2)$$

$$c = 4.3347(6)$$

Density

(calculated) 5.453 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 3.2$

Additional pattern

1. PDF card 4-331 [Swanson and Tatge, 1953].

References

Braekken, H. and Scholten, W. (1934). *Z. Krist.* 89, 448.

Merwin, H.E. (1920). *J. Am. Chem. Soc.* 42, 2432.

Swanson, H. E. and Tatge, E. (1953). *Nat. Bur. Stand. (U.S.) Circ.* 539, 1, 73.

| $d(\text{\AA})$ | $\overset{\circ}{\theta}$ | I | hkl | $2\theta (\text{)}^\circ$ |
|-----------------|---------------------------|---|---------|---------------------------|
| 2.418 | 20 | | 211 | 37.16 |
| 2.361 | 4 | | 141 | 38.08 |
| 2.295 | 3 | | 221 | 39.22 |
| 2.199 | 8 | | 051 | 41.01 |
| 2.181 | 6 | | 240 | 41.36 |
| 2.130 | 14 | | 231,060 | 42.41 |
| 2.065 | 16 | | 151 | 43.81 |
| 2.012 | 10 | | 112 | 45.01 |
| 2.006 | 16 | | 160 | 45.16 |
| 1.941 | 13 | | 122 | 46.76 |
| 1.902 | 7 | | 320 | 47.78 |
| 1.838 | 2 | | 132 | 49.55 |
| 1.820 | 1 | | 161 | 50.09 |
| 1.810 | 1 | | 301 | 50.38 |
| 1.793 | 10 | | 042,311 | 50.90 |
| 1.771 | 4 | | 251 | 51.56 |
| 1.754 | 3 | | 202 | 52.09 |
| 1.740 | 2 | | 321 | 52.54 |
| 1.738 | 2 | | 212 | 52.61 |
| 1.681 | 3 | | 071 | 54.55 |
| 1.666 | 5 | | 331 | 55.09 |
| 1.653 | 2 | | 052 | 55.55 |
| 1.621 | 4 | | 232 | 56.73 |
| 1.618 | 3 | | 171 | 56.85 |
| 1.595 | 4 | | 080 | 57.74 |
| 1.574 | 1 | | 341 | 58.61 |
| 1.537 | 5 | | 242 | 60.15 |
| 1.493 | 3 | | 400 | 62.10 |
| 1.477 | 3 | | 351 | 62.87 |
| 1.472 | 4 | | 162 | 63.09 |
| 1.454 | 4 | | 420,360 | 63.98 |
| 1.436 | 1 | | 013 | 64.89 |
| 1.429 | 4 | | 322 | 65.22 |
| 1.408 | 3 | | 280 | 66.32 |
| 1.4043 | 5 | | 103,411 | 66.53 |
| 1.3958 | 2 | | 113,072 | 66.99 |
| 1.3788 | <1 | | 421,361 | 67.93 |
| 1.3538 | 1 | | 262 | 69.36 |
| 1.3406 | 2 | | 431 | 70.14 |
| 1.3151 | 1 | | 191 | 71.71 |
| 1.2939 | 1 | | 213 | 73.07 |
| 1.2850 | 2 | | 082,371 | 73.66 |
| 1.2745 | 1 | | 223 | 74.37 |
| 1.2360 | 1 | | 451 | 77.10 |
| 1.2304 | 2 | | 153,402 | 77.52 |
| 1.1805 | 1 | | 282 | 81.46 |
| 1.1748 | 1 | | 520 | 81.94 |
| 1.1694 | 1 | | 303 | 82.40 |
| 1.1648 | 1 | | 313 | 82.80 |
| 1.1478 | 2 | | 442,511 | 84.31 |

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ \text{C}$

Internal standard W, $a = 3.16524 \text{ \AA}$

| $d(\text{\AA})$ | $\overset{\circ}{\theta}$ | I | hkl | $2\theta (\text{)}^\circ$ |
|-----------------|---------------------------|---------|-------|---------------------------|
| 4.365 | 100 | 120 | | 20.33 |
| 4.107 | 40 | 011 | | 21.62 |
| 3.587 | 7 | 021 | | 24.80 |
| 3.511 | 5 | 101 | | 25.35 |
| 3.386 | 10 | 111 | | 26.30 |
| 3.192 | 12 | 040 | | 27.93 |
| 3.075 | 12 | 121 | | 29.01 |
| 3.038 | 30 | 031 | | 29.38 |
| 2.989 | 50 | 200 | | 29.87 |
| 2.708 | 40 | 131,220 | | 33.05 |

Mercury chloride (calomel), Hg_2Cl_2

Sample

The sample was obtained from British Drug House, Ltd.

Optical data

Uniaxial(+), $N_o = 2.6559$, $N_e = 1.97325$ [Groth, 1904].

Structure

Tetragonal, I4/mmm (139), $Z = 2$, isostructural with Hg_2Br_2 , Hg_2F_2 , and Hg_2I_2 [Havighurst, 1925 and Mark and Steinback, 1926].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 4.4801(2)\text{\AA} \\ c &= 10.9060(6) \end{aligned}$$

Density

(calculated) 7.162 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 5.0$$

Additional patterns

1. PDF card 4-581 [Swanson and Tatge, 1953].
2. Havighurst [1925].
3. Hylleraas [1926].
4. Ruff et al. [1928].
5. Hanawalt et al. [1938].

References

- Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 Havighurst, R.J. (1925). Amer. J. Sci. 10, 15.
 Hylleraas, E. (1926). Z. Phys. 36, 859.
 Groth, H. (1904). Chemische Krystallographie, Vol. 1, 124, Engelmann, Leipzig.
 Mark, H. and Steinbach, J. (1926). Z. Krist. 64, 79.
 Ruff, O., Ebert, F., and Luft, F. (1928). Z. Anorg. Allg. Chem. 170, 49.
 Swanson, H.E. and Tatge, E. (1953). NBS Circular 539, 1, 72.

| $d(\text{\AA})$ | CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ | | |
|-----------------|---|----------|--------------------|
| | I | hkl | $2\theta (^\circ)$ |
| 4.147 | 75 | 101 | 21.41 |
| 3.170 | 100 | 110 | 28.13 |
| 2.824 | 12 | 103 | 31.66 |
| 2.727 | 30 | 004 | 32.81 |
| 2.240 | 15 | 200 | 40.22 |
| 2.067 | 40 | 114 | 43.76 |
| 1.970 | 17 | 211 | 46.03 |
| 1.962 | 30 | 105 | 46.24 |
| 1.818 | <1 | 006 | 50.14 |
| 1.756 | 4 | 213 | 52.05 |
| 1.732 | 12 | 204 | 52.83 |
| 1.5841 | 6 | 220 | 58.19 |
| 1.4755 | 11 | 215 | 62.94 |
| 1.4164 | 3 | 310 | 65.89 |
| 1.3815 | 1 | 303 | 67.78 |
| 1.3696 | 6 | 224 | 68.45 |
| 1.3633 | 3 | 008 | 68.81 |
| 1.2569 | 4 | 314 | 75.59 |
| 1.2522 | 5 | 118 | 75.93 |
| 1.2343 | 2 | 321 | 77.23 |
| 1.2319 | 2 | 305 | 77.41 |
| 1.1756 | 1 | 323 | 81.88 |
| 1.1697 | 5 | 109 | 82.38 |
| 1.1648 | 3 | 208 | 82.80 |
| 1.1202 | <1 | 400 | 86.89 |
| 1.0908 | <1 | 00010 | 89.85 |
| 1.0800 | 2 | 325 | 91.00 |
| 1.0563 | 1 | 330 | 93.65 |
| 1.0410 | 1 | 413 | 95.46 |
| 1.0370 | 3 | 219, 332 | 95.95 |
| 1.0312 | 2 | 1110 | 96.66 |
| 1.0018 | 1 | 420 | 100.52 |
| 0.9846 | 2 | 334 | 102.95 |
| 0.9823 | 2 | 318 | 103.29 |
| 0.9728 | 2 | 415 | 104.72 |
| 0.9405 | 1 | 424 | 109.97 |
| 0.9089 | 1 | 00012 | 115.89 |
| 0.8930 | <1 | 431 | 119.22 |
| 0.8736 | 1 | 1112 | 123.72 |
| 0.8675 | 2 | 329 | 125.23 |
| 0.8287 | 1 | 435 | 136.71 |
| 0.8246 | 2 | 10013 | 138.20 |

Nickel acetate hydrate, $\text{Ni}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution of $\text{Ni}(\text{C}_2\text{H}_3\text{O}_2)_2$.

Color

Brilliant bluish green.

Optical data

Biaxial (-). $N_\alpha = 1.441$, $N_\gamma = 1.560$. $2V$ is very small.

Structure

Monoclinic $P2_1/c(14)$, $Z = 2$, isostructural with $\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O}$. The structure was determined by van Niekerk and Schoening [1953] and refined by Downie et al. [1971].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 4.7749(9)\text{\AA} \\ b &= 11.772(2) \\ c &= 8.435(1) \\ \beta &= 93.86(1)^\circ \end{aligned}$$

Density

(calculated) 1.747 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 4.6$$

Additional patterns

1. PDF card 14-721 [Hanawalt et al., 1938].
2. PDF card 24-1360. This is data from card 14-721 indexed by University College, Cardiff, Wales.

References

- Downie, T. C., Harrison, W., Rafer, E. S., and Hepworth, M. A. (1971). Acta Crystallogr. B27, 706.
 Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 van Niekerk, J. N. and Schoening, F. R. (1953). Acta Crystallogr. 6, 609.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
|---|-----|-----------------------|-------------------|
| d (Å) | I | hkl | $2\theta (\circ)$ |
| 6.84 | 100 | 011 | 12.94 |
| 5.886 | 4 | 020 | 15.04 |
| 4.828 | 6 | 021 | 18.36 |
| 4.762 | 30 | 100 | 18.62 |
| 4.416 | 2 | 110 | 20.09 |
| 4.209 | 13 | 002 | 21.09 |
| 4.014 | 19 | $\bar{1}11$ | 22.13 |
| 3.962 | 5 | 012 | 22.42 |
| 3.811 | 7 | 111 | 23.32 |
| 3.702 | <1 | 120 | 24.02 |
| 3.555 | 11 | 031 | 25.03 |
| 3.454 | <1 | $\bar{1}21$ | 25.77 |
| 3.326 | 2 | $\bar{1}21$ | 26.78 |
| 3.265 | 2 | $\bar{1}02$ | 27.29 |
| 3.147 | 20 | $\bar{1}12$ | 28.34 |
| 3.053 | 3 | 102 | 29.23 |
| 3.029 | 2 | 130 | 29.47 |
| 2.956 | 4 | 112 | 30.21 |
| 2.946 | 2 | 040 | 30.32 |
| 2.890 | 8 | 131 | 30.92 |
| 2.869 | 7 | 032 | 31.15 |
| 2.813 | 1 | 131 | 31.79 |
| 2.711 | 5 | 122 | 33.02 |
| 2.531 | 1 | 023 | 35.44 |
| 2.504 | 8 | 140 | 35.83 |
| 2.438 | 2 | $\bar{1}13$ | 36.83 |
| 2.410 | 3 | 042, 132 | 37.28 |
| 2.383 | 2 | 200 | 37.72 |
| 2.378 | 4 | 141 | 37.80 |
| 2.304 | 7 | 113 | 39.07 |
| 2.294 | 7 | $\bar{1}23$ | 39.24 |
| 2.281 | 2 | 033 | 39.47 |
| 2.267 | 1 | 051 | 39.70 |
| 2.186 | 5 | 142, 123 | 41.27 |
| 2.136 | 1 | 202 | 42.27 |
| 2.111 | 5 | 150 | 42.81 |
| 2.104 | 4 | 004, 221, $\bar{1}33$ | 42.95 |
| 2.063 | 3 | 151 | 43.85 |
| 2.055 | 2 | 052 | 44.04 |
| 2.032 | 1 | 151, 043 | 44.56 |
| 2.016 | 3 | 202, 133 | 44.92 |
| 2.007 | 4 | $\bar{2}22$ | 45.13 |
| 1.982 | 1 | 024 | 45.75 |
| 1.953 | 1 | 231 | 46.46 |
| 1.948 | 2 | $\bar{1}14$ | 46.59 |
| 1.907 | 3 | 222 | 47.64 |
| 1.879 | 2 | 104 | 48.41 |
| 1.875 | 2 | $\bar{2}32$ | 48.51 |
| 1.872 | 2 | $\bar{1}24$ | 48.61 |
| 1.855 | 6 | 213, 114, 034 | 49.06 |

Nickel acetate hydrate, $\text{Ni}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O}$ - continued

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ |
|-----------------|----|----------|---------------------------|
| 1.852 | 5 | 240 | 49.16 |
| 1.836 | 1 | 143 | 49.61 |
| 1.803 | 2 | 053 | 50.57 |
| 1.791 | 3 | 223 | 50.95 |
| 1.789 | 2 | 124, 241 | 51.01 |
| 1.778 | 3 | 062 | 51.36 |
| 1.7645 | <1 | 161, 134 | 51.77 |
| 1.7392 | 2 | 213 | 52.58 |
| 1.7282 | 1 | 242 | 52.94 |
| 1.7108 | <1 | 044, 153 | 53.52 |
| 1.6944 | 2 | 233, 134 | 54.08 |
| 1.6812 | <1 | 162 | 54.54 |
| 1.6660 | 2 | 015 | 55.08 |
| 1.6629 | 2 | 242, 153 | 55.19 |
| 1.6272 | 1 | 251 | 56.51 |
| 1.6074 | 2 | 063, 115 | 57.27 |
| 1.6043 | 1 | 233 | 57.39 |

Potassium lead chloride, KPb_2Cl_5

Sample

The sample was prepared by melting a 1:2 molar mixture of KCl and $PbCl_2$ at 480 °C and cooling in air.

Color

Colorless

Structure

Orthorhombic, Z=4, isostructural with $RbPb_2Cl_5$ and other similar compounds [Jansen, 1968].

NBS lattice constants of this sample:

$$a = 8.865(2) \text{ \AA}$$

$$b = 12.498(2)$$

$$c = 7.934(1)$$

Density

(calculated) 4.767 g/cm³

Additional pattern

1. PDF card 23-484 [Jansen, 1968].

Reference

Jansen, P. W. J. (1968). Rec. Trav. Chim. Pays-Bas, 87, 1021.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. 25±1 °C | | | |
|---|-----|---------|--------|
| Internal standard Ag, a = 4.08651 \AA° | | | |
| d(\AA) | I | hkl | 2θ (°) |
| 8.83 | 25 | 100 | 10.01 |
| 6.69 | 11 | 011 | 13.22 |
| 6.25 | 5 | 020 | 14.16 |
| 5.90 | 7 | 101 | 15.00 |
| 5.34 | 11 | 111 | 16.58 |
| 5.10 | 10 | 120 | 17.37 |
| 4.292 | 7 | 121 | 20.68 |
| 3.968 | 25 | 002 | 22.39 |
| 3.693 | 100 | 211,031 | 24.08 |
| 3.616 | 40 | 102,220 | 24.60 |
| 3.478 | 8 | 112 | 25.59 |
| 3.406 | 9 | 131 | 26.14 |
| 3.350 | 2 | 022 | 26.59 |
| 3.290 | 3 | 221 | 27.08 |
| 3.129 | 5 | 122 | 28.50 |
| 3.478 | 8 | 112 | 25.59 |
| 3.406 | 9 | 131 | 26.14 |
| 3.350 | 2 | 022 | 26.59 |
| 3.290 | 3 | 221 | 27.08 |
| 3.129 | 5 | 122 | 28.50 |

| d(\AA) | I | hkl | 2θ (°) |
|-------------------|----|---------|--------|
| 3.123 | 3 | 040 | 28.56 |
| 2.952 | 4 | 202,300 | 30.25 |
| 2.907 | 4 | 041 | 30.73 |
| 2.876 | 11 | 310,032 | 31.07 |
| 2.836 | 6 | 231 | 31.52 |
| 2.764 | 9 | 141 | 32.36 |
| 2.733 | 9 | 132 | 32.74 |
| 2.703 | <2 | 311 | 33.11 |
| 2.671 | 50 | 222,320 | 33.52 |
| 2.587 | 5 | 013 | 34.65 |
| 2.553 | 20 | 240 | 35.12 |
| 2.534 | 9 | 103 | 35.39 |
| 2.483 | 2 | 113 | 36.14 |
| 2.454 | 2 | 042 | 36.59 |
| 2.371 | 4 | 302 | 37.91 |
| 2.350 | 14 | 123 | 38.27 |
| 2.328 | 7 | 312 | 38.65 |
| 2.303 | 10 | 151 | 39.09 |
| 2.232 | 18 | 033 | 40.38 |
| 2.216 | 16 | 400,322 | 40.68 |
| 2.166 | 6 | 133 | 41.67 |
| 2.148 | 8 | 242,340 | 42.04 |
| 2.101 | 19 | 251 | 43.02 |
| 2.083 | 7 | 060 | 43.41 |
| 2.059 | 5 | 332 | 43.94 |
| 2.027 | 3 | 160 | 44.66 |
| 1.994 | 3 | 233 | 45.44 |
| 1.968 | 7 | 143 | 46.08 |
| 1.935 | 9 | 104,402 | 46.92 |
| 1.912 | 5 | 114,412 | 47.51 |
| 1.900 | 13 | 431 | 47.84 |
| 1.879 | 6 | 323 | 48.40 |
| 1.856 | <2 | 351 | 49.04 |
| 1.848 | 5 | 422 | 49.27 |
| 1.845 | 9 | 062 | 49.36 |
| 1.817 | <2 | 053 | 50.18 |
| 1.810 | 5 | 204 | 50.38 |
| 1.805 | 3 | 162 | 50.51 |
| 1.781 | 4 | 333 | 51.24 |
| 1.762 | <2 | 441 | 51.84 |
| 1.756 | 3 | 510,134 | 52.04 |
| 1.740 | 3 | 224 | 52.56 |
| 1.680 | 2 | 253 | 54.58 |
| 1.6679 | 3 | 521 | 55.01 |
| 1.6467 | 2 | 304 | 55.78 |
| 1.6330 | <2 | 314 | 56.29 |
| 1.6232 | 2 | 451 | 56.66 |
| 1.6190 | 2 | 502 | 56.82 |
| 1.6092 | 3 | 163 | 57.20 |
| 1.5730 | 5 | 433 | 58.64 |
| 1.5624 | 2 | 080,105 | 59.08 |
| 1.5314 | 3 | 334 | 60.40 |
| 1.5177 | 4 | 460 | 61.00 |
| 1.5155 | 5 | 125 | 61.10 |

Potassium platinum chloride, K_2PtCl_6

Sample

The sample was prepared by reaction of KCl and H_2PtCl_6 .

Major impurities

0.01 to 0.1% Na and Ba
 0.001 to 0.01% Al, Ca, Cr, and Si
 0.0001 to 0.001% Ag, Fe, Mg, and Mn

Color

Bright yellow

Optical data

Isotropic, $N = 1.823$

Structure

Cubic, $Fm\bar{3}m$ (225) $Z=4$, isostructural with other similar alkali platinum halides. The structure of K_2PtCl_6 was determined by Ewing and Pauling [1928].

NBS lattice constant of this sample:

$$a = 9.7560(1)\text{\AA}$$

Density

(calculated) 3.478 g/cm^3

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 5.7$$

Additional patterns

1. PDF card 7-199 [Swanson et al., 1955].
2. Hanawalt et al. [1938].

References

- Ewing, F.J. and Pauling, L. (1928). Z. Krist. 68, 223.
 Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 Swanson, H. E., Gilfrich, N.T., and Ugrinic, G.M. (1955). Nat. Bur. Stand. (U.S.) Circ. 539, 5, 49.

| $\overset{\circ}{\text{CuK}\alpha_1} \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|--|-----|--------|----------------------------|
| $\overset{\circ}{\text{Internal standard Ag, } a = 4.08651 \text{ \AA}}$ | | | |
| $d(\text{\AA})$ | I | hkl | $2\theta (\text{ }^\circ)$ |
| 5.633 | 100 | 111 | 15.72 |
| 4.878 | 40 | 200 | 18.17 |
| 3.4491 | 45 | 220 | 25.81 |
| 2.9417 | 45 | 311 | 30.36 |
| 2.8160 | 5 | 222 | 31.75 |
| 2.4391 | 40 | 400 | 36.82 |
| 2.2383 | 13 | 331 | 40.26 |
| 2.1817 | 15 | 420 | 41.35 |
| 1.9915 | 14 | 422 | 45.51 |
| 1.8773 | 14 | 511 | 48.45 |
| 1.7246 | 18 | 440 | 53.06 |
| 1.6492 | 13 | 531 | 55.69 |
| 1.6259 | 6 | 600 | 56.56 |
| 1.5425 | 5 | 620 | 59.92 |
| 1.4878 | 4 | 533 | 62.36 |
| 1.4083 | 4 | 444 | 66.32 |
| 1.3659 | 6 | 711 | 68.66 |
| 1.3531 | 3 | 640 | 69.40 |
| 1.3035 | 4 | 642 | 72.45 |
| 1.2700 | 4 | 731 | 74.68 |
| 1.2194 | 1 | 800 | 78.35 |
| 1.1918 | 1 | 733 | 80.53 |
| 1.1829 | 2 | 820 | 81.26 |
| 1.1496 | 1 | 660 | 84.14 |
| 1.1264 | 2 | 751 | 86.29 |
| 1.0907 | 3 | 840 | 89.86 |
| 1.0708 | 2 | 911 | 92.00 |
| 1.0645 | 2 | 842 | 92.71 |
| 1.0401 | 1 | 664 | 95.57 |
| 1.0226 | 2 | 931 | 97.75 |
| 0.9957 | 2 | 844 | 101.36 |
| .9805 | 2 | 933 | 103.56 |
| .9757 | 1 | 10·0·0 | 104.28 |
| .9567 | 2 | 10·2·0 | 107.25 |
| .9431 | 2 | 951 | 109.49 |
| .9098 | 1 | 953 | 115.71 |
| .9059 | 2 | 10·4·0 | 116.50 |
| .8905 | 1 | 10·4·2 | 119.76 |
| .8796 | 1 | 11·1·1 | 122.26 |
| .8624 | 1 | 880 | 126.57 |
| .8525 | 1 | 11·3·1 | 129.28 |
| .8492 | 1 | 10·4·4 | 130.22 |
| .8366 | 1 | 10·6·0 | 134.08 |
| .8275 | 1 | 11·3·3 | 137.14 |
| .8130 | 1 | 12·0·0 | 142.69 |
| .8064 | 1 | 11·5·1 | 146.40 |
| .7912 | 1 | 12·2·2 | 153.60 |
| .7835 | <1 | 11·5·3 | 158.90 |

Silicon, Si

Sample

The sample was very pure vacuum floated, zone refined silicon. This sample is NBS Standard Reference Material # 640, Silicon Powder, X-Ray Diffraction Standard.*

Major impurities (after grinding of the sample):

0.001-0.0001% each of Ca, Cu.

Color

Gray

Structure

Cubic, Fd3m (227), Z = 8 [Debye and Scherrer, 1916].

NBS lattice constant of this sample:

$$a = 5.43088 (4) \text{ \AA}$$

Density

(calculated) 2.329 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 4.7$$

Polymorphism

Kasper and Richards [1964] reported that a second, dense form with space group Ia3(206) is formed under pressure.

Additional pattern

1. PDF card 5-565 [Swanson and Fuyat, 1953]. The Swanson and Fuyat [1953] reference lists a large number of early powder patterns.

References

- Debye, P. and Scherrer, P. (1916). Phys. Z. 17, 277.
 Kasper, J. S. and Richards, S. M. (1964). Acta Crystallogr. 17, 752.
 Swanson, H. E. and Fuyat, R. K. (1953). Nat. Bur. Stand. (U.S.) Circ. 539, 2, 6.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{ C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
|--|-----|-----|---------------------------|
| d(\AA) | I | hkl | $2\theta (\text{)}^\circ$ |
| 3.13552 | 100 | 111 | 28.443 |
| 1.92011 | 55 | 220 | 47.303 |
| 1.63747 | 30 | 311 | 56.123 |
| 1.35772 | 6 | 400 | 69.131 |
| 1.24593 | 11 | 331 | 76.377 |
| 1.10857 | 12 | 422 | 88.032 |
| 1.04517 | 6 | 511 | 94.954 |
| 0.96005 | 3 | 440 | 106.710 |
| .91799 | 7 | 531 | 114.094 |
| .85870 | 8 | 620 | 127.547 |
| .82820 | 3 | 533 | 136.897 |

* Samples may be obtained from the Office of Standard Reference Materials, Room B311, Chemistry Building, National Bureau of Standards, Washington, D. C. 20234, \$52 per 10 gram unit.

Silver carbonate, Ag_2CO_3

Sample

The sample was prepared by precipitation, adding K_2CO_3 to AgNO_3 solution.

Major impurities

0.001 to 0.01%, Al and Si
0.0001 to 0.001%, Ca, Cu, Fe, and Mg

Color

Greenish yellow

Structure

Monoclinic, $\text{P}2_1(4)$, $Z=2$ [Donahue and Helmholtz, 1944].

NBS lattice constants of this sample:

$$a = 4.8510(7) \text{\AA}$$

$$b = 9.544(2)$$

$$c = 3.2533(6)$$

$$\beta = 91.96^\circ(2)$$

Density

(calculated) 6.084 g/cm^3

Additional patterns

1. PDF card 12-766 [Swanson et al., 1962].
2. Hanawalt et al [1938].

References

- Donahue, J. and Helmholtz, L. (1944). J. Am. Chem. Soc. 66, 295.
 Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 Swanson, H. E., Morris, M.C., Stinchfield, R. P., and Evans, E.H. (1962). Nat. Bur. Stand. (U.S.) Monogr. 25, Sec. 1, 44.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ \text{C}$ $\text{Internal standard W, } a = 3.16524 \text{ \AA}$ | | | |
|---|-----|----------|-------------------|
| d (Å) | I | hkl | $2\theta (\circ)$ |
| 4.85 | 15 | 100 | 18.29 |
| 4.78 | 35 | 020 | 18.56 |
| 4.32 | 30 | 110 | 20.52 |
| 3.41 | 2 | 120 | 26.14 |
| 3.252 | 3 | 001 | 27.40 |
| 3.078 | 8 | 011 | 28.99 |
| 2.745 | 60 | 101 | 32.60 |
| 2.660 | 100 | 130, 101 | 33.66 |
| 2.561 | 6 | 111 | 35.01 |
| 2.423 | 2 | 200 | 37.07 |
| 2.385 | 11 | 040 | 37.68 |
| 2.381 | 13 | 121 | 37.76 |
| 2.351 | 8 | 210 | 38.26 |
| 2.322 | 14 | 121 | 38.75 |
| 2.275 | 35 | 031 | 39.59 |
| 2.161 | 11 | 220 | 41.76 |
| 2.041 | 10 | 131 | 44.35 |
| 1.976 | 2 | 201 | 45.89 |
| 1.935 | 6 | 211 | 46.92 |
| 1.929 | 9 | 230 | 47.08 |
| 1.912 | 4 | 201 | 47.51 |
| 1.875 | 6 | 211 | 48.52 |
| 1.801 | 3 | 141 | 50.65 |
| 1.777 | 13 | 150, 141 | 51.39 |
| 1.701 | 3 | 240 | 53.87 |
| 1.678 | 9 | 231 | 54.65 |
| 1.646 | 6 | 051 | 55.82 |
| 1.639 | 10 | 231 | 56.07 |
| 1.626 | 6 | 002 | 56.56 |
| 1.616 | 1 | 300 | 56.92 |
| 1.591 | 9 | 060 | 57.93 |
| 1.538 | 2 | 022, 112 | 60.11 |
| 1.530 | 3 | 320 | 60.44 |
| 1.526 | 3 | 102 | 60.64 |
| 1.511 | 2 | 160 | 61.29 |
| 1.507 | 3 | 112 | 61.47 |
| 1.4676 | <1 | 301 | 63.32 |
| 1.4526 | <1 | 122 | 64.05 |
| 1.4500 | 1 | 311 | 64.18 |
| 1.4412 | 2 | 330 | 64.62 |
| 1.4278 | 1 | 301 | 65.30 |
| 1.4115 | 1 | 311 | 66.15 |
| 1.3987 | 5 | 132 | 66.83 |

Silver sulfate, Ag_2SO_4

Sample

The sample was obtained from J. T. Baker Chemical Company.

Major impurities

0.001 to 0.01% each of Al, Fe, Mg, and Si.
0.0001 to 0.001% each of Ca and Pb.

Color

Colorless

Optical data

Biaxial (-), $N_{\alpha} = 1.756$, $N_{\beta} = 1.775$, and $N_{\gamma} = 1.782$.

Structure

Orthorhombic, Fddd(70), Z=8, Na_2SO_4 type structure [Herrmann and Ilge, 1931].

NBS lattice constants of this sample:

$$\begin{aligned}a &= 10.2699(5)\text{\AA} \\b &= 12.7069(7) \\c &= 5.8181(3)\end{aligned}$$

Density

(calculated) 5.455 g/cm³

Reference intensity

$I/I_{\text{corundum}} = 2.2$

Additional patterns

1. PDF card 7-203 [Swanson et al., 1957].
2. Hanawalt et al. [1938].

References

- Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem., Anal. Ed. 10, 457.
Herrmann, K. and Ilge, W. (1931). Z. Krist. 80, 402.
Swanson, H. E., Gilfrich, N. T., and Cook, M. I. (1957). Nat. Bur. Stand. (U.S.) Circ. 539, 7, 46.

| CuK α_1 $\lambda = 1.540598 \text{\AA}$; temp. $25 \pm 1^\circ \text{C}$ | | | |
|--|-----|-------------|---------------------------|
| Internal standard w, $a = 3.16524 \text{\AA}$ | | | |
| d(\AA) | I | hkl | $2\theta (\text{)}^\circ$ |
| 4.699 | 10 | 111 | 18.87 |
| 3.994 | 25 | 220 | 22.24 |
| 3.249 | 3 | 131 | 27.43 |
| 3.177 | 70 | 040 | 28.06 |
| 2.873 | 100 | 311 | 31.10 |
| 2.644 | 90 | 022 | 33.87 |
| 2.568 | 1 | 400 | 34.91 |
| 2.530 | 17 | 202 | 35.45 |
| 2.421 | 30 | 331 | 37.10 |
| 2.352 | 3 | 222 | 38.24 |
| 2.272 | 8 | 151 | 39.64 |
| 1.980 | 11 | 242 | 45.78 |
| 1.957 | 8 | 260 | 46.35 |
| 1.926 | 30 | 351 | 47.15 |
| 1.915 | 12 | 511 | 47.44 |
| 1.884 | 5 | 113 | 48.26 |
| 1.762 | 3 | 531 | 51.85 |
| 1.7376 | 3 | 133 | 52.63 |
| 1.7123 | 17 | 062 | 53.47 |
| 1.6730 | 12 | 313 | 54.83 |
| 1.6527 | 4 | 620 | 55.56 |
| 1.6243 | 1 | 262 | 56.62 |
| 1.5881 | 3 | 080 | 58.03 |
| 1.5675 | 13 | 333 | 58.87 |
| 1.5462 | 8 | 371 | 59.76 |
| 1.5404 | 6 | 551 | 60.01 |
| 1.4751 | 4 | 602 | 62.96 |
| 1.4542 | 3 | 004 | 63.97 |
| 1.4057 | 6 | 353 | 66.46 |
| 1.3668 | 3 | 224 | 68.61 |
| 1.3598 | 1 | 191 | 69.01 |
| 1.3457 | 2 | 282 | 69.84 |
| 1.3380 | 6 | 642, 533 | 70.30 |
| 1.3312 | 6 | 660 | 70.71 |
| 1.3225 | 6 | 044 | 71.25 |
| 1.2837 | 1 | 800 | 73.75 |
| 1.2736 | 3 | 391 | 74.43 |
| 1.2359 | 3 | 373 | 77.11 |
| 1.2331 | 3 | 2·10·0, 553 | 77.32 |
| 1.1905 | 1 | 840 | 80.64 |
| 1.1678 | 1 | 264 | 82.54 |
| 1.1645 | 3 | 0·10·2 | 82.83 |
| 1.1549 | 1 | 822 | 83.67 |
| 1.1408 | 1 | 591 | 84.94 |
| 1.1154 | 1 | 911, 135 | 87.36 |
| 1.1136 | 1 | 573 | 87.53 |
| 1.0975 | 2 | 315 | 89.15 |
| 1.0919 | 3 | 624 | 89.73 |
| 1.0829 | 4 | 393, 931 | 90.69 |
| 1.0809 | 3 | 682 | 90.90 |

Silver sulfate, Ag_2SO_4 - continued

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ |
|-----------------|---|----------------|---------------------------|
| 1.0758 | 3 | 3·11·1 | 91.46 |
| 1.0727 | 3 | 084 | 91.80 |
| 1.0663 | 2 | 335 | 92.51 |
| 1.0589 | 1 | 0·12·0 | 93.34 |
| 1.0272 | 1 | 862 | 97.17 |
| 1.0246 | 1 | 951 | 97.49 |
| 1.0203 | 1 | 6·10·0 | 98.05 |
| 1.0138 | 1 | 10·2·0 | 98.89 |
| 1.0109 | 1 | 355 | 99.28 |
| 0.9976 | 1 | 593 | 101.10 |
| .9920 | 1 | 5·11·1 | 101.88 |
| .9820 | 2 | 664 | 103.33 |
| .9586 | 1 | 026 | 106.95 |
| .9531 | 1 | 3·11·3, 971 | 107.84 |
| .9419 | 1 | 375 | 109.74 |
| .9407 | 1 | 2·10·4, 555 | 109.94 |
| .9279 | 1 | 3·13·1, 4·12·2 | 112.23 |
| .9210 | 1 | 844 | 113.51 |

Sodium phosphate hydrate, $\alpha\text{-Na}_4\text{P}_4\text{O}_{12}\cdot 4\text{H}_2\text{O}$

Sample

The sample was prepared by H.M. Ondik by hydrolytic cleavage of the α form of P_2O_5 below 15 °C. The material was neutralized by NaOH, then purified by salting out with NaCl, followed by repeated recrystallizations with H_2O and ethanol.

Major impurities

0.001 to 0.01% each of Ba, Ca, Si, and Sr.

Color

Colorless

Optical data

Biaxial (+), $N_\alpha = 1.440$, $N_\beta = 1.458$, $N_\gamma = 1.476$.

Structure

Monoclinic, $P2_1/a$ (14), $Z=2$. The structure of $\alpha\text{-Na}_4\text{P}_4\text{O}_{12}\cdot 4\text{H}_2\text{O}$ was determined by Ondik et al. [1961].

NBS lattice constants of this sample:

$$a = 9.691(2)\text{\AA}$$

$$b = 12.342(2)$$

$$c = 6.187(2)$$

$$\beta = 92.58(1)^\circ$$

Density

(calculated) 2.156 g/cm³

Polymorphism

Thilo and Ratz [1949] reported a β , high temperature form of $\text{Na}_4\text{P}_4\text{O}_{12}\cdot 4\text{H}_2\text{O}$.

Additional patterns

1. PDF card 11-15 [Swanson et al., 1960].
2. Bell et al. [1952].
3. Thilo and Ratz [1949].

References

- Bell, R.N., Audrieth, L.F., and Hill, O.F. (1952). Ind. Eng. Chem. 44, 568.
 Ondik, H. M., MacGillavry, C. H., and Block, S. (1961). Acta Crystallogr. 14, 555.
 Swanson, H. E., Cook, M. I., Evans, E. H., and de Groot, J.H. (1960). Nat. Bur. Stand. (U.S.) Circ. 539, 10, 52.
 Thilo, E. and Ratz, R. (1949). Z. Anorg. Allg. Chem. 260, 255.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{\AA}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|--|-----|------------|----------------------------|
| $\text{Internal standard W, } a = 3.16524 \text{\AA}$ | | | |
| $d(\text{\AA})$ | I | hkl | $2\theta (\text{ }^\circ)$ |
| 7.64 | 75 | 110 | 11.58 |
| 6.17 | 90 | 001, 020 | 14.34 |
| 5.21 | 5 | 120 | 17.00 |
| 4.844 | 65 | 200 | 18.30 |
| 4.719 | 60 | 111 | 18.79 |
| 4.510 | 3 | 210 | 19.67 |
| 4.369 | 17 | 021 | 20.31 |
| 3.933 | 20 | 121 | 22.59 |
| 3.894 | 2 | 201 | 22.82 |
| 3.805 | 95 | 220 | 23.36 |
| 3.728 | 25 | 201 | 23.85 |
| 3.572 | 8 | 211 | 24.91 |
| 3.424 | 10 | 031 | 26.00 |
| 3.295 | 100 | 221 | 27.04 |
| 3.255 | 70 | 131 | 27.38 |
| 3.194 | 20 | 221 | 27.91 |
| 3.133 | 19 | 230 | 28.47 |
| 3.122 | 19 | 310 | 28.57 |
| 3.089 | 25 | 002, 040 | 28.88 |
| 2.938 | 9 | 140 | 30.40 |
| 2.827 | 70 | 231, 112 | 31.62 |
| 2.760 | 19 | 022, 041 + | 32.41 |
| 2.739 | 20 | 311 | 32.67 |
| 2.685 | 18 | 122 | 33.34 |
| 2.669 | 7 | 141 | 33.55 |
| 2.638 | 14 | 141 | 33.95 |
| 2.633 | 15 | 321 | 34.02 |
| 2.602 | 7 | 240, 212 | 34.44 |
| 2.554 | 14 | 202 | 35.11 |
| 2.539 | 35 | 330 | 35.32 |
| 2.418 | 18 | 241, 132 | 37.16 |
| 2.392 | 8 | 150 | 37.57 |
| 2.375 | 8 | 410, 132 | 37.85 |
| 2.360 | 5 | 222 | 38.10 |
| 2.293 | 5 | 051 | 39.26 |
| 2.253 | 40 | 420 | 39.98 |
| 2.247 | 25 | 312 | 40.10 |
| 2.222 | 16 | 151 | 40.56 |
| 2.199 | 11 | 250 | 41.01 |
| 2.185 | 16 | 411, 042 | 41.29 |
| 2.170 | 5 | 232 | 41.59 |
| 2.148 | 5 | 312 | 42.02 |
| 2.146 | 3 | 421, 142 | 42.08 |
| 2.120 | 4 | 341 | 42.62 |
| 2.115 | 5 | 142 | 42.71 |
| 2.087 | 4 | 430, 251 | 43.32 |
| 2.060 | 2 | 003, 251 | 43.92 |
| 2.015 | 8 | 242 | 44.94 |
| 2.001 | 6 | 431 | 45.29 |
| 1.996 | 1 | 332 | 45.40 |

Sodium phosphate hydrate, $\alpha\text{-Na}_4\text{P}_4\text{O}_{12}\cdot4\text{H}_2\text{O}$ - continued

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ |
|-----------------|----|------------|---------------------------|
| 1.968 | 8 | 242 | 46.08 |
| 1.961 | 10 | 350 | 46.25 |
| 1.955 | 8 | 023, 431 | 46.40 |
| 1.949 | 8 | 402 | 46.56 |
| 1.928 | 10 | 332, 052 + | 47.09 |
| 1.924 | 7 | 412 | 47.19 |
| 1.913 | 6 | 510 | 47.49 |
| 1.907 | 10 | 161 | 47.65 |
| 1.903 | 14 | 213, 152 + | 47.75 |
| 1.895 | 9 | 260 | 47.97 |
| 1.854 | 18 | 351 | 49.11 |
| 1.850 | 18 | 511 | 49.20 |
| 1.842 | 9 | 033 | 49.44 |
| 1.837 | 9 | 441, 342 | 49.58 |
| 1.823 | 10 | 133 | 50.00 |
| 1.786 | 8 | 223, 422 | 51.11 |
| 1.776 | 8 | 252 | 51.42 |
| 1.7547 | 6 | 313 | 52.08 |
| 1.7500 | 5 | 521 | 52.23 |
| 1.7456 | 6 | 233 | 52.37 |
| 1.7349 | 5 | 360, 170 | 52.72 |
| 1.7123 | 3 | 043, 062 | 53.47 |
| 1.6991 | 6 | 233, 432 + | 53.92 |
| 1.6806 | 12 | 361 | 54.56 |
| 1.6761 | 16 | 143, 352 | 54.72 |

Strontium hydroxide, Sr(OH)_2

Sample

The sample was prepared by heating $\text{Sr(OH)}_2 \cdot 8\text{H}_2\text{O}$ for 24 hours at about 200 °C.

Color

Colorless

Structure

Orthorhombic, Pbnm (62), $Z=4$, [Bärnighausen and Weidlein, 1965]. The structure was determined by Grueninger and Bärnighausen [1969].

NBS lattice constants of this sample:

$$a = 6.1201(6)\text{\AA}$$

$$b = 9.892(1)$$

$$c = 3.9193(5)$$

Density

(calculated) 3.405 g/cm³

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 2.7$$

Additional patterns

1. PDF card 18-1273 [Bärnighausen and Weidlein, 1965].
2. PDF card 19-1276 [Mercer and Miller, 1966]. This pattern is labeled as anhydrous but is for $\text{Sr(OH)}_2 \cdot \text{H}_2\text{O}$.
3. Berggren and Brown [1971].

References

- Bärnighausen, H. and Weidlein, J. (1965). Acta Crystallogr. 19, 1048.
 Berggren, G. and Brown, A. (1971). Acta Chem. Scand. 25, 1377.
 Grueninger, H. W. and Bärnighausen, H (1969). Z. Anorg. Allgem. Chem. 368, 53.
 Mercer, R. A. and Miller, R.P. (1966). J. Inorg. Nucl. Chem. 28, 61.

$\text{CuK}\alpha_1$ $\lambda = 1.540598 \text{\AA}$; temp. 25±1 °C

Internal standard W, $a = 3.16524 \text{\AA}$

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
|-----------------|-----|-------|----------------------|
| 5.19 | 55 | 110 | 17.06 |
| 4.94 | 25 | 020 | 17.94 |
| 3.846 | 40 | 120 | 23.11 |
| 3.300 | 40 | 101 | 27.00 |
| 3.130 | 100 | 111 | 28.49 |

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
|-----------------|----|---------|----------------------|
| 3.068 | 25 | 021,200 | 29.08 |
| 2.922 | 25 | 210 | 30.57 |
| 2.903 | 45 | 130 | 30.78 |
| 2.745 | 5 | 121 | 32.59 |
| 2.602 | 2 | 220 | 34.44 |
| 2.473 | 25 | 040 | 36.30 |
| 2.343 | 45 | 211 | 38.38 |
| 2.293 | 10 | 140 | 39.26 |
| 2.244 | 2 | 230 | 40.16 |
| 2.168 | 10 | 221 | 41.62 |
| 2.091 | 25 | 041 | 43.23 |
| 1.998 | 3 | 310 | 45.36 |
| 1.979 | 6 | 141 | 45.81 |
| 1.959 | 20 | 002 | 46.31 |
| 1.947 | 50 | 231 | 46.62 |
| 1.886 | 17 | 320 | 48.21 |
| 1.834 | 6 | 112 | 49.68 |
| 1.822 | 3 | 022 | 50.03 |
| 1.810 | 15 | 301 | 50.38 |
| 1.780 | 1 | 311 | 51.29 |
| 1.746 | 6 | 122 | 52.35 |
| 1.735 | 1 | 330 | 52.73 |
| 1.727 | 2 | 241 | 52.97 |
| 1.6970 | 17 | 151 | 53.99 |
| 1.6615 | 6 | 250 | 55.24 |
| 1.6486 | 6 | 060 | 55.71 |
| 1.6280 | 11 | 212 | 56.48 |
| 1.6245 | 16 | 132 | 56.61 |
| 1.5735 | 5 | 340 | 58.62 |
| 1.5360 | 7 | 042 | 60.20 |
| 1.5304 | 6 | 400,251 | 60.44 |
| 1.5126 | 3 | 410 | 61.23 |
| 1.4898 | 4 | 142 | 62.27 |
| 1.4751 | 3 | 232,161 | 62.96 |
| 1.4608 | 5 | 341 | 63.65 |
| 1.4518 | 1 | 260 | 64.09 |
| 1.4109 | 1 | 411 | 66.18 |
| 1.3874 | 1 | 430 | 67.45 |
| 1.3768 | 2 | 170 | 68.04 |
| 1.3696 | 2 | 421 | 68.45 |
| 1.3589 | 8 | 322 | 69.06 |
| 1.3353 | 1 | 351 | 70.46 |
| 1.3080 | 3 | 431 | 72.16 |
| 1.3012 | 4 | 440 | 72.60 |
| 1.2992 | 4 | 171,332 | 72.73 |
| 1.2829 | 4 | 270 | 73.80 |
| 1.2672 | 8 | 252,113 | 74.87 |
| 1.2618 | 5 | 062 | 75.25 |

Strontium hydroxide hydrate $\text{Sr}(\text{OH})_2 \cdot \text{H}_2\text{O}$

Sample

The sample was prepared by heating $\text{Sr}(\text{OH})_2$ in a partly closed tube with about 1 ml H_2O at 100°C for 24 hours. The sample contained a small amount of SrCO_3 . Because of this and the tendency to lose H_2O when exposed to air, the intensities may be slightly in error.

Color

Colorless

Structure

Orthorhombic, $\text{Pb}21\text{m}$ (26), $Z = 2$. Isostructural with $\text{Eu}(\text{OH})_2 \cdot \text{H}_2\text{O}$ and $\text{Ba}(\text{OH})_2 \cdot \text{H}_2\text{O}$ [Bärnighausen, 1966]. The structure of $\text{Sr}(\text{OH})_2 \cdot \text{H}_2\text{O}$ was determined by Bärnighausen and Weidlein [1967].

NBS lattice constants of this sample:

$$a = 6.201(1) \text{\AA}$$

$$b = 6.716(1)$$

$$c = 3.6483(6)$$

Density

(calculated) 3.053 g/cm^3

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 0.8$$

Additional patterns

1. PDF card 19-1276 [Mercer and Miller, 1966]. This pattern was labeled as $\text{Sr}(\text{OH})_2$
2. Bärnighausen [1966].
3. Berggren and Brown [1971].
4. Carlson [1954].
5. Lutz [1965].

References

- Bärnighausen, H. (1966). Z. Anorg. Allgem. Chem. 342, 233.
 Bärnighausen, H., and Weidlein, J. (1967). Acta. Crystallogr. 22, 252.
 Berggren, G., and Brown, A. (1971). Acta. Chem. Scand. 25, 1377.
 Carlson, E. T. (1954). J. Res. Natl. Bur. Stand. 53, 371.
 Lutz, H. D. (1965). Z. Naturforsch. 20b, 61.
 Mercer, R. A., and Miller, R. P., (1966). J. Inorg. Nucl. Chem. 28, 61.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ\text{C}$ | | | |
|--|-----|----------|---------------------------|
| $\text{Internal standard Ag, } a = 4.08651 \text{ \AA}$ | | | |
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 6.20 | 65 | 100 | 14.28 |
| 4.556 | 80 | 110 | 19.47 |
| 3.651 | 40 | 001 | 24.36 |
| 3.360 | 55 | 020 | 26.51 |
| 3.147 | 45 | 101 | 28.34 |
| 2.954 | 15 | 120 | 30.23 |
| 2.848 | 60 | 111 | 31.39 |
| 2.814 | 100 | 210 | 31.77 |
| 2.472 | 50 | 021 | 36.31 |
| 2.363 | 10 | 201 | 38.05 |
| 2.296 | 70 | 121 | 39.21 |
| 2.230 | 85 | 211 | 40.42 |
| 2.106 | 25 | 130 | 42.91 |
| 2.067 | 10 | 300 | 43.77 |
| 1.977 | 18 | 310 | 45.87 |
| 1.825 | 35 | 002, 131 | 49.94 |
| 1.816 | 25 | 230 | 50.21 |
| 1.798 | 7 | 301 | 50.72 |
| 1.760 | 11 | 320 | 51.90 |
| 1.750 | 7 | 102 | 52.24 |
| 1.738 | 12 | 311 | 52.63 |
| 1.6938 | 11 | 112 | 54.10 |
| 1.6792 | 7 | 040 | 54.61 |
| 1.6248 | 25 | 231 | 56.60 |
| 1.6033 | 9 | 022 | 57.43 |
| 1.5854 | 8 | 321 | 58.14 |
| 1.5515 | 5 | 122 | 59.53 |
| 1.5500 | 7 | 400 | 59.60 |
| 1.5311 | 13 | 212 | 60.41 |
| 1.5186 | 6 | 330 | 60.96 |
| 1.4808 | 9 | 141 | 62.69 |
| 1.4266 | 7 | 401 | 65.36 |
| 1.4073 | 7 | 420 | 66.37 |
| 1.4024 | 8 | 331 | 66.62 |
| 1.3784 | 7 | 132 | 67.95 |
| 1.3678 | 3 | 302 | 68.55 |
| 1.3398 | 7 | 312 | 70.19 |
| 1.3124 | 11 | 150 | 71.88 |
| 1.3029 | 5 | 340 | 72.49 |
| 1.2862 | 8 | 232 | 73.58 |
| 1.2664 | 6 | 322 | 74.93 |
| 1.2396 | 4 | 500 | 76.83 |
| 1.2350 | 9 | 042, 151 | 77.18 |

Strontium hydroxide hydrate, $\text{Sr}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$

Sample

The sample was prepared by treating SrCO_3 with HCl followed by NaOH at boiling temperatures. On cooling, the first crystals formed were removed, redissolved and reprecipitated by slow evaporation at room temperature.

Color

Colorless

Optical Data

Uniaxial (-), $N_o = 1.497$, $N_e = 1.475$

Structure

Tetragonal, $P4/ncc$ (130), $Z = 4$. The structure was determined by Smith [1953].

NBS lattice constants of this sample:

$$a = 9.019(2)\text{\AA}$$

$$c = 11.614(2)$$

Density

(calculated) 1.868 g/cm^3

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 1.3$$

Additional patterns

1. PDF card 1-1263 [Hanawalt et al, 1938].
2. PDF card 2-1262 [Natta, 1928].
3. Berggren and Brown [1971].

References

- Berggren, G., and Brown, A. (1971). Acta. Chem. Scand. 25, 1377.
 Hanawalt, J.D., Rinn, R.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 Natta, G. (1928). Gazz. Chim. Ital. 58, 870.
 Smith, H. G. (1953). Acta. Crystallogr. 6, 604.

| $d(\text{\AA})$ | I | CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$ | |
|-----------------|-----|--|-------------------|
| | | Internal standard W, $a = 3.16524 \text{ \AA}$ | hkl |
| $d(\text{\AA})$ | I | hkl | $2\theta (\circ)$ |
| 6.37 | 50 | 110 | 13.89 |
| 5.81 | 45 | 002 | 15.25 |
| 4.50 | 45 | 200 | 19.70 |
| 4.292 | 100 | 112 | 20.68 |
| 3.559 | 80 | 202 | 25.00 |
| 3.190 | 19 | 220 | 27.95 |
| 2.904 | 14 | 004 | 30.76 |
| 2.795 | 45 | 222, 213 | 31.99 |
| 2.768 | 60 | 311 | 32.32 |
| 2.640 | 40 | 114 | 33.93 |
| 2.560 | 55 | 312 | 35.02 |
| 2.442 | 40 | 204 | 36.78 |
| 2.357 | 6 | 214 | 38.15 |
| 2.296 | 25 | 322, 313 | 39.21 |
| 2.253 | 20 | 400 | 39.99 |
| 2.147 | 30 | 224 | 42.06 |
| 2.102 | 18 | 402, 323 | 42.99 |
| 2.035 | 65 | 314 | 44.48 |
| 2.017 | 55 | 420 | 44.91 |
| 1.997 | 15 | 332 | 45.36 |
| 1.935 | 6 | 006 | 46.92 |
| 1.905 | 20 | 422, 413 | 47.70 |
| 1.852 | 12 | 116 | 49.15 |
| 1.801 | 11 | 315 | 50.63 |
| 1.780 | 7 | 404 | 51.28 |
| 1.779 | 15 | 206 | 51.33 |
| 1.715 | 9 | 334 | 53.37 |
| 1.692 | 15 | 512 | 54.15 |
| 1.655 | 8 | 424, 226 | 55.46 |
| 1.6020 | 13 | 316 | 57.48 |
| 1.5106 | 9 | 514 | 61.32 |
| 1.4950 | 8 | 532 | 62.03 |
| 1.4690 | 6 | 406 | 63.25 |
| 1.4518 | 10 | 008 | 64.09 |
| 1.4331 | 8 | 108 | 65.03 |
| 1.4263 | 12 | 620 | 65.37 |
| 1.4157 | 7 | 118 | 65.93 |
| 1.3964 | 10 | 426 | 66.96 |
| 1.3818 | 8 | 208 | 67.76 |
| 1.3648 | 7 | 534 | 68.72 |

Strontium silicate, Sr_3SiO_5

Sample

The sample was prepared by repeated grindings and heatings of a 3:1 molar mixture of SrCO_3 and silica gel. The temperature was about 1350 °C.

Color

Colorless

Structure

Tetragonal, P4/ncc (130), Z=4 [Mansmann, 1965]. The structure of Sr_3SiO_5 was studied by Dent Glasser and Glasser [1965].

NBS lattice constants for this sample:

$$\begin{aligned} a &= 6.9476(3)\text{\AA} \\ c &= 10.7534(6) \end{aligned}$$

Density

(calculated) 4.747 g/cm³

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 3.6$$

Additional patterns

1. PDF card 18-1282 [Dear, Bull. Mat. Eng. Exp. Sta., 1957].
2. Eysel [1970].
3. Nurse [1952].

References

- Dent Glasser, L.S. and Glasser, R.P. (1965). Acta Crystallogr. 18, 453.
 Eysel, W. (1970). Neues Jahrb. Mineral. Montash. 1970, 534.
 Mansmann, M. (1965). Z. Anorg. Allg. Chem. 339, 52.
 Nurse, R. W. (1952). J. Appl. Chem. (London) 2, 244.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{\AA}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|--|-----|---------|----------------------|
| Internal standard W, $a = 3.16524 \text{\AA}$ | | | |
| $d(\text{\AA})$ | I | hkl | $2\theta ({}^\circ)$ |
| 5.38 | 4 | 002 | 16.46 |
| 4.92 | 1 | 110 | 18.02 |
| 4.249 | 1 | 102 | 20.89 |
| 3.629 | 10 | 112 | 24.51 |
| 2.984 | 30 | 211 | 29.92 |
| 2.919 | 100 | 202 | 30.60 |
| 2.690 | 30 | 212,004 | 33.29 |
| 2.508 | 2 | 104 | 35.78 |
| 2.458 | 30 | 220 | 36.53 |
| 2.348 | 55 | 213 | 38.30 |
| 2.198 | 25 | 310 | 41.04 |
| 2.035 | 1 | 312,214 | 44.49 |
| 1.897 | 4 | 321 | 47.92 |
| 1.814 | 20 | 322,224 | 50.27 |
| 1.793 | 2 | 006 | 50.89 |
| 1.7683 | 9 | 215 | 51.65 |
| 1.7550 | 1 | 304 | 52.07 |
| 1.7370 | 1 | 400 | 52.65 |
| 1.7014 | 9 | 314 | 53.84 |
| 1.6840 | 3 | 116 | 54.44 |
| 1.6646 | 17 | 411 | 55.13 |
| 1.6530 | 3 | 402 | 55.55 |
| 1.6376 | 2 | 330 | 56.12 |
| 1.5926 | 16 | 206 | 57.85 |
| 1.5662 | 10 | 332,324 | 58.92 |
| 1.5535 | 4 | 420 | 59.45 |
| 1.5366 | 1 | 421,315 | 60.17 |
| 1.5250 | 12 | 413 | 60.68 |
| 1.4926 | 4 | 422 | 62.14 |
| 1.4589 | 4 | 404 | 63.74 |
| 1.4352 | 2 | 325 | 64.92 |
| 1.3982 | 1 | 334 | 66.86 |
| 1.3889 | 1 | 316 | 67.37 |
| 1.3772 | 4 | 217 | 68.02 |
| 1.3446 | 7 | 424,008 | 69.90 |
| 1.3262 | 7 | 415 | 71.02 |
| 1.3208 | 5 | 512 | 71.35 |
| 1.2961 | 1 | 118,433 | 72.93 |
| 1.2810 | 1 | 521 | 73.93 |
| 1.2571 | 2 | 406 | 76.29 |
| 1.2338 | 1 | 218 | 77.27 |
| 1.2279 | 1 | 440,416 | 77.71 |
| 1.2140 | 3 | 523 | 78.77 |
| 1.2090 | 3 | 336 | 79.16 |
| 1.2012 | 1 | 327 | 79.77 |
| 1.1974 | 2 | 442 | 80.08 |
| 1.1913 | 3 | 530 | 80.57 |
| 1.1790 | 4 | 228 | 81.59 |
| 1.1739 | 2 | 426 | 82.02 |
| 1.1674 | 2 | 435 | 82.58 |

Strontium silicate, Sr_3SiO_5 - continued

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ |
|-----------------|----|---------------|---------------------------|
| 1.1632 | 3 | 532, 524 + | 82.94 |
| 1.1579 | 2 | 600 | 83.40 |
| 1.1468 | 1 | 318 | 84.40 |
| 1.1352 | 6 | 417 | 85.46 |
| 1.1154 | 3 | 219 | 87.36 |
| 1.0891 | 7 | 534 | 90.03 |
| 1.0846 | 4 | 516 | 90.51 |
| 1.0761 | 4 | 622 | 91.42 |
| 1.0632 | 5 | 604, 408 | 92.85 |
| 1.0504 | <1 | 1•1•10, 623 + | 94.33 |
| 1.0388 | 1 | 338 | 95.72 |
| 1.0305 | 1 | 437 | 96.75 |
| 1.0272 | 3 | 2•0•10 | 97.16 |
| 1.0161 | 2 | 428, 2•1•10 | 98.59 |
| 1.0133 | 1 | 446 | 98.96 |
| 1.0088 | 2 | 615 | 99.56 |
| 0.9922 | 1 | 536 | 101.85 |
| .9747 | 2 | 419 | 104.43 |
| .9686 | 1 | 545 | 105.36 |
| .9662 | 2 | 438, 3•1•10 + | 105.74 |
| .9597 | <1 | 641 | 106.77 |
| .9506 | 1 | 721 | 108.26 |
| .9484 | 2 | 642 | 108.63 |
| .9364 | 2 | 626 | 110.69 |
| .9324 | 2 | 2•1•11 | 111.40 |
| .9305 | 1 | 643 | 111.75 |

Tin hydrogen phosphate, SnHPO_4

Sample

The sample was made by T. H. Jordan of the American Dental Association Health Foundation. Tin Fluoride, SnF_2 , was treated with H_3PO_4 at a pH of 2, followed by slight heating.

Color

Colorless

Structure

Monoclinic, $P2_1/a(14)$, $Z = 4$. The structure was determined by Berndt and Lamberg [1971].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 5.8307(8) \text{\AA} \\ b &= 13.617 (1) \\ c &= 4.6145(6) \\ \beta &= 98.73 (1)^\circ \end{aligned}$$

Density

(calculated) 3.937 g/cm^3

Reference Intensity

$I/I_{\text{corundum}} = 2.0$.

Reference

Berndt, A. F. and Lamberg, R. (1971). Acta Crystallogr. B27, 1092.

| d (Å) | I | CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ | |
|-------|-----|---|-------------------|
| | | hkl | $2\theta (\circ)$ |
| 6.80 | 100 | 020 | 13.01 |
| 5.311 | 2 | 110 | 16.68 |
| 4.562 | 12 | 001 | 19.44 |
| 4.401 | 11 | 120 | 20.16 |
| 4.327 | 1 | 011 | 20.51 |
| 3.792 | 12 | 021 | 23.44 |
| 3.731 | 16 | 111 | 23.83 |
| 3.566 | 6 | 130 | 24.95 |
| 3.404 | 35 | 040 | 26.16 |
| 3.367 | 4 | 121 | 26.45 |
| 3.241 | 8 | 111 | 27.50 |
| 2.997 | 30 | 121 | 29.79 |
| 2.946 | 40 | 131 | 30.31 |
| 2.882 | 1 | 200 | 31.01 |
| 2.820 | 14 | 210 | 31.71 |
| 2.729 | 4 | 041 | 32.79 |
| 2.689 | 7 | 131 | 33.29 |
| 2.654 | 1 | 220 | 33.75 |
| 2.623 | 1 | 201 | 34.16 |
| 2.574 | 4 | 211 | 34.82 |
| 2.559 | 1 | 141 | 35.04 |
| 2.448 | 1 | 221 | 36.68 |
| 2.384 | 3 | 141 | 37.71 |
| 2.338 | 1 | 051 | 38.47 |
| 2.279 | 6 | 002 | 39.51 |
| 2.269 | 11 | 231,060 | 39.69 |
| 2.251 | 10 | 211,012 | 40.02 |
| 2.228 | 3 | 151 | 40.45 |
| 2.210 | 4 | 112 | 40.79 |
| 2.163 | <1 | 022 | 41.72 |
| 2.111 | 1 | 160,151 | 42.80 |
| 2.077 | 1 | 241 | 43.53 |
| 2.032 | 10 | 061 | 44.55 |
| 2.008 | 6 | 132 | 45.11 |
| 1.979 | 9 | 250 | 45.82 |
| 1.936 | 3 | 202,122 | 46.90 |
| 1.918 | 2 | 212 | 47.36 |
| 1.894 | 6 | 042 | 47.99 |
| 1.889 | 6 | 251 | 48.12 |
| 1.878 | 2 | 161 | 48.44 |
| 1.863 | 1 | 222 | 48.84 |
| 1.848 | 3 | 320 | 49.28 |
| 1.843 | 4 | 132,170 | 49.41 |
| 1.808 | 4 | 321 | 50.43 |
| 1.789 | 1 | 071 | 51.01 |
| 1.783 | 1 | 260 | 51.19 |
| 1.769 | 2 | 330 | 51.62 |
| 1.748 | 5 | 052 | 52.28 |
| 1.737 | 6 | 171 | 52.64 |
| 1.681 | 2 | 171 | 54.53 |

Tin hydrogen phosphate, SnHPO_4 - continued

| d (Å) | I | hkl | 2θ (°) |
|---------|---|------------|---------------|
| 1.669 | 1 | 202, 311 | 54.96 |
| 1.657 | 2 | 212 | 55.42 |
| 1.643 | 3 | 341 | 55.93 |
| 1.632 | 3 | 180, 321 | 56.32 |
| 1.609 | 3 | 062 | 57.22 |
| 1.578 | 2 | 2̄52 | 58.44 |
| 1.5585 | 1 | 1̄81 | 59.24 |
| 1.5514 | 1 | 322 | 59.54 |
| 1.5166 | 4 | 181 | 61.05 |
| 1.5081 | 2 | 162, 341 | 61.43 |
| 1.4989 | 1 | 242 | 61.85 |
| 1.4802 | 1 | 072 | 62.72 |
| 1.4730 | 2 | 262 | 63.06 |
| 1.4634 | 1 | 190 | 63.52 |
| 1.4486 | 2 | 133 | 64.25 |
| 1.4432 | 1 | 342 | 64.52 |
| 1.4384 | 2 | 401, 203 | 64.76 |
| 1.4303 | 1 | 351, 411 + | 65.17 |
| 1.4231 | 2 | 252 | 65.54 |
| 1.4092 | 2 | 420, 191 | 66.27 |
| 1.3943 | 1 | 1̄43 | 67.07 |
| 1.3878 | 3 | 043, 123 | 67.43 |
| 1.3781 | 1 | 191 | 67.97 |
| 1.3738 | 1 | 430, 272 | 68.21 |
| 1.3670 | 1 | 370 | 68.59 |
| 1.3615 | 1 | 0·10·0 | 68.91 |

Zinc borate, $Zn_4B_6O_{13}$

Sample

The sample was a phosphor preparation obtained from the Radio Corporation of America [Leverenz, 1944].

Color

Colorless

Structure

Cubic, $I\bar{4}3m(217)$, $Z=2$. The structure was determined by Smith et al. [1961], who found the formula to be $Zn_4O(BO_2)_6$.

NBS lattice constant of this sample:

$$a = 7.4734(2) \text{\AA}$$

Density

(calculated) 4.252 g/cm^3

Additional pattern

1. PDF card 14-2 [Swanson and Tatge, 1953]. The formula at that time was mistakenly given as ZnB_2O_4 .

References

- Leverenz, H.W. (1944). Proc. I.R.E. 32, 256.
 Smith, P., García-Blanco, S., and Rivoir, L. (1961). An. Reál Soc. Espan. Fis. Quim. Madrid, A57, 263.
 Swanson, H. E. and Tatge, E. (1953). Nat. Bur. Stand. (U.S.) Circ. 539, 1, 83.

| $CuK\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ $\text{Internal standard W, } a = 3.16524 \text{ \AA}$ | | | |
|--|-----|-------|---------------------------|
| $d(\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 5.29 | 6 | 110 | 16.74 |
| 3.74 | 4 | 200 | 23.77 |
| 3.05 | 100 | 211 | 29.28 |
| 2.364 | 25 | 310 | 38.03 |
| 2.158 | 2 | 222 | 41.82 |
| 1.997 | 20 | 321 | 45.37 |
| 1.869 | 14 | 400 | 48.68 |
| 1.761 | 40 | 330 | 51.88 |
| 1.672 | 2 | 420 | 54.86 |
| 1.594 | 4 | 332 | 57.79 |
| 1.526 | 25 | 422 | 60.63 |
| 1.466 | 6 | 510 | 63.39 |
| 1.364 | 8 | 521 | 68.76 |
| 1.321 | 4 | 440 | 71.34 |
| 1.282 | 4 | 530 | 73.86 |
| 1.246 | 2 | 600 | 76.37 |
| 1.213 | 2 | 611 | 78.84 |
| 1.1818 | 2 | 620 | 81.36 |
| 1.1532 | 4 | 541 | 83.82 |
| 1.1026 | 2 | 631 | 88.64 |
| 1.0789 | 2 | 444 | 91.12 |
| 1.0569 | 2 | 710 | 93.58 |
| 1.0366 | 2 | 640 | 96.00 |
| 1.0170 | 4 | 721 | 98.48 |
| 0.9992 | 2 | 642 | 100.88 |
| .9813 | 2 | 730 | 103.44 |
| .9491 | 2 | 732 | 108.51 |
| .9199 | 4 | 811 | 113.74 |
| .9063 | 2 | 820 | 116.42 |
| .8933 | 2 | 653 | 119.16 |
| .8808 | 2 | 822 | 121.99 |
| .8688 | 4 | 831 | 124.92 |
| .8574 | 2 | 662 | 127.91 |
| .8463 | 2 | 752 | 131.08 |
| .8253 | 2 | 910 | 137.95 |
| .8154 | 2 | 842 | 141.73 |
| .8059 | 2 | 921 | 145.83 |
| .7967 | 2 | 664 | 150.44 |
| .7878 | 2 | 930 | 155.83 |

Zinc titanium oxide, ZnTiO_3

Sample

The sample was prepared by heating an equimolar mixture of $\text{Zn}(\text{NO}_3)_2$ and TiO_2 (anatase) for about two weeks at 900° with several remixings and regrindings. Because of the lack of thermal stability above 943° [Dulin and Rase, 1960], it was impossible to obtain complete reaction and the sample contained small amounts of rutile (TiO_2) and Zn_2TiO_4 ; therefore there may be a slight error in some intensities. Intensities calculated from the structure were in good agreement with the experimental values.

Color

Colorless

Structure

Hexagonal, $R\bar{3}$ (148), $Z=6$. ZnTiO_3 is isostructural with FeTiO_3 (ilmenite) and other similar titanates [Bartram and Slepety, 1961].

NBS lattice constants of this sample:

$$a = 5.0787(3)\text{\AA}$$

$$c = 13.927(1)$$

Density

(calculated) 5.165 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 2.5$

Additional patterns

1. Bartram and Slepety [1961].
2. Kubo and Kato [1963].

References

- Bartram, S.F. and Slepety, R.A. (1961). J. Amer. Ceram. Soc. 44, 493.
 Dulin, F.H. and Rase, D.E. (1960). J. Amer. Ceram. Soc. 43, 125.
 Kubo, T. and Kato, M. (1963). Kogyo Kagaku Zasshi 66, 404.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ \text{C}$ $\text{Internal standard Ag, a} = 4.08651 \text{ \AA}$ | | | |
|---|-----|----------|--------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (^\circ)$ |
| 4.63 | 1 | 003 | 19.14 |
| 4.191 | 3 | 101 | 21.18 |
| 3.717 | 20 | 012 | 23.92 |
| 2.729 | 100 | 104 | 32.79 |
| 2.540 | 75 | 110 | 35.31 |
| 2.355 | 1 | 015 | 38.18 |
| 2.321 | 1 | 006 | 38.76 |
| 2.228 | 20 | 113 | 40.45 |
| 2.173 | 3 | 021 | 41.52 |
| 2.097 | 1 | 202 | 43.10 |
| 1.860 | 35 | 024 | 48.94 |
| 1.813 | 1 | 107 | 50.29 |
| 1.713 | 35 | 116 | 53.43 |
| 1.651 | 1 | 211 | 55.64 |
| 1.619 | 11 | 018 | 56.83 |
| 1.500 | 25 | 214 | 61.80 |
| 1.466 | 25 | 300 | 63.41 |
| 1.428 | 1 | 125 | 65.31 |
| 1.399 | 1 | 303 | 66.84 |
| 1.3650 | 4 | 208 | 68.71 |
| 1.3276 | 8 | 1·0·10 | 70.93 |
| 1.3218 | 4 | 119 | 71.29 |
| 1.2760 | 1 | 217 | 74.27 |
| 1.2696 | 6 | 220 | 74.71 |
| 1.2396 | 2 | 306 | 76.84 |
| 1.2166 | 1 | 0·1·11 | 78.57 |
| 1.2020 | 6 | 128, 312 | 79.71 |
| 1.1766 | 3 | 0·2·10 | 81.79 |
| 1.1512 | 7 | 134 | 84.00 |
| 1.1139 | 5 | 226 | 87.50 |
| 1.0862 | 1 | 042 | 90.33 |
| 1.0674 | 5 | 2·1·10 | 92.38 |
| 1.0558 | 2 | 1·1·12 | 93.71 |
| 1.0485 | 3 | 404 | 94.56 |
| 1.0069 | <1 | 1·2·11 | 99.82 |
| 0.9990 | 3 | 318 | 100.90 |
| .9816 | <1 | 229 | 103.39 |
| .9702 | 4 | 0·1·14 | 105.12 |
| .9692 | 7 | 324 | 105.27 |
| .9599 | 5 | 410 | 106.74 |
| .9296 | 2 | 048 | 111.92 |
| .9175 | 3 | 1·3·10 | 114.19 |
| .9064 | 2 | 2·0·14 | 116.39 |
| .8868 | 5 | 416 | 120.59 |

Cerium cobalt, CeCo₂

Structure

Cubic, Fd3m(227), Z=8, C15 type, isostructural with Cu₂Mg [Fülling et al., 1942].

Lattice constant: [Wernick and Geller, 1960]

$$a = 7.161(5)\text{\AA}$$

Density
(calculated) 9.333 g/cm³

Thermal parameters

Overall isotropic B = 1.0

Scattering factors

Ce⁰ and Co⁰ [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)

$$\gamma = 0.501 \times 10^{-3}$$

$$I/I_C \text{ (calculated)} = 10.3$$

Additional pattern

1. Fülling, Moeller and Vogel [1942].

References

- Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
 Fülling, W., Moeller, K., and Vogel, R. (1942). Z. Metallk. 34, 253.
 Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.
 Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-------|-------|---|---------------|
| d(A) | I | hkl | 2θ(°) | | λ = 1.540598A |
| 4.13 | 12 | 1 1 1 | 1 | 1 | 21.48 |
| 2.532 | 66 | 2 2 0 | 2 | 2 | 35.43 |
| 2.159 | 100 | 3 1 1 | 3 | 1 | 41.80 |
| 2.067 | 15 | 2 2 2 | 2 | 2 | 43.76 |
| 1.643 | 3 | 3 3 1 | 3 | 1 | 55.92 |
| 1.462 | 20 | 4 2 2 | 4 | 2 | 63.60 |
| 1.378 | 19 | 5 1 1 | 5 | 1 | 67.97 |
| 1.378 | 6 | 3 3 3 | 3 | 3 | 67.97 |
| 1.266 | 18 | 4 4 0 | 4 | 0 | 74.96 |
| 1.210 | 2 | 5 3 1 | 5 | 1 | 79.05 |
| 1.132 | 8 | 6 2 0 | 6 | 2 | 85.74 |
| 1.092 | 8 | 5 3 3 | 5 | 3 | 89.72 |
| 1.080 | 4 | 6 2 2 | 6 | 2 | 91.05 |
| .957 | 10 | 6 4 2 | 6 | 2 | 107.21 |
| .932 | 12 | 7 3 1 | 7 | 1 | 111.43 |
| .932 | 6 | 5 5 3 | 5 | 3 | 111.43 |
| .895 | 4 | 8 0 0 | 8 | 0 | 118.76 |
| .844 | 3 | 6 6 0 | 6 | 0 | 131.78 |
| .844 | 6 | 8 2 2 | 8 | 2 | 131.78 |
| .827 | 14 | 7 5 1 | 7 | 1 | 137.36 |
| .827 | 2 | 5 5 5 | 5 | 5 | 137.36 |
| .821 | 3 | 6 6 2 | 6 | 2 | 139.36 |
| .786 | 3 | 7 5 3 | 7 | 3 | 157.04 |
| .786 | 1 | 9 1 1 | 9 | 1 | 157.04 |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|-------|-------|---|---------------|
| d(A) | I | hkl | 2θ(°) | | λ = 1.540598A |
| 4.13 | 16 | 1 1 1 | 1 | 1 | 21.48 |
| 2.532 | 68 | 2 2 0 | 2 | 2 | 35.42 |
| 2.159 | 100 | 3 1 1 | 3 | 1 | 41.80 |
| 2.067 | 15 | 2 2 2 | 2 | 2 | 43.76 |
| 1.643 | 3 | 3 3 1 | 3 | 1 | 55.92 |
| 1.462 | 16 | 4 2 2 | 4 | 2 | 63.60 |
| 1.378 | 20 | 5 1 1 | 5 | 1 | 67.96 |
| 1.266 | 13 | 4 4 0 | 4 | 0 | 74.96 |
| 1.211 | 1 | 5 3 1 | 5 | 1 | 79.04 |
| 1.132 | 5 | 6 2 0 | 6 | 2 | 85.74 |
| 1.092 | 5 | 5 3 3 | 5 | 3 | 89.72 |
| 1.080 | 2 | 6 2 2 | 6 | 2 | 91.04 |
| 1.003 | 1 | 7 1 1 | 7 | 1 | 100.38 |
| .957 | 6 | 6 4 2 | 6 | 2 | 107.22 |
| .932 | 9 | 7 3 1 | 7 | 1 | 111.44 |
| .895 | 2 | 8 0 0 | 8 | 0 | 118.76 |
| .844 | 4 | 8 2 2 | 8 | 2 | 131.78 |
| .827 | 6 | 7 5 1 | 7 | 1 | 137.36 |
| .821 | 1 | 6 6 2 | 6 | 2 | 139.36 |
| .786 | 1 | 7 5 3 | 7 | 3 | 157.04 |

Cerium cobalt, Ce₂₄Co₁₁

Structure

Hexagonal, P6₃mc (186), Z = 2. The structure was determined by Larson and Cromer [1962].

Lattice constants:

$$a = 9.588 \text{ \AA}$$

$$c = 21.827$$

(published values: a = 9.587, c = 21.825 \AA [ibid.]).

Density

(calculated) 7.666 g/cm³

Thermal parameters

Isotropic [Larson and Cromer, 1962].

Scattering factors

Ce⁰, Co⁰ [International Tables, 1962].

Scale factors (integrated intensities)

$$\gamma = 0.170 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 3.63$$

References

International Tables for X-ray Crystallography III (1962), 210, 211.

Larson, A. C. and Cromer, D. T. (1962). Acta Crystallogr. 15, 1224.

| d(Å) | ° | I | hkl | | | 2θ(°) | λ = 1.540598Å |
|-------|---|----|-----|---|------|-------|---------------|
| 2.280 | | 18 | 2 | 0 | 8 | 39.50 | |
| 2.253 | | 1 | 3 | 1 | 2 | 39.98 | |
| 2.212 | | 2 | 2 | 1 | 7 | 40.76 | |
| 2.203 | | 4 | 3 | 0 | 6 | 40.94 | |
| 2.196 | | 3 | 3 | 1 | 3 | 41.06 | |
| 2.122 | | 8 | 3 | 1 | 4 | 42.58 | |
| 2.111 | | 2 | 1 | 0 | 10 | 42.80 | |
| 2.094 | | 2 | 2 | 0 | 9 | 43.16 | |
| 2.066 | | 3 | 4 | 0 | 1 | 43.78 | |
| 2.059 | | 4 | 2 | 1 | 8 | 43.94 | |
| 2.039 | | 1 | 4 | 0 | 2 | 44.40 | |
| 1.996 | | 1 | 4 | 0 | 3 | 45.40 | |
| 1.946 | | 2 | 3 | 1 | 6 | 46.64 | |
| 1.940 | | 3 | 4 | 0 | 4 + | 46.78 | |
| 1.932 | | 2 | 2 | 0 | 10 + | 47.00 | |
| 1.919 | | 3 | 2 | 1 | 9 | 47.34 | |
| 1.905 | | 1 | 3 | 2 | 0 | 47.70 | |
| 1.876 | | 3 | 3 | 2 | 2 + | 48.48 | |
| 1.843 | | 1 | 3 | 2 | 3 | 49.42 | |
| 1.824 | | 2 | 3 | 0 | 9 | 49.96 | |
| 1.812 | | 1 | 4 | 1 | 0 | 50.32 | |
| 1.800 | | 5 | 2 | 2 | 8 + | 50.66 | |
| 1.798 | | 6 | 3 | 2 | 4 | 50.72 | |
| 1.791 | | 6 | 2 | 0 | 11 + | 50.96 | |
| 1.777 | | 2 | 1 | 0 | 12 | 51.38 | |
| 1.758 | | 9 | 4 | 1 | 3 + | 51.96 | |
| 1.746 | | 1 | 3 | 2 | 5 | 52.36 | |
| 1.728 | | 5 | 4 | 0 | 7 | 52.94 | |
| 1.701 | | 1 | 1 | 1 | 12 | 53.86 | |
| 1.687 | | 2 | 3 | 2 | 6 | 54.32 | |
| 1.677 | | 1 | 2 | 1 | 11 | 54.68 | |
| 1.673 | | 1 | 4 | 1 | 5 | 54.82 | |
| 1.666 | | 4 | 2 | 0 | 12 | 55.08 | |
| 1.661 | | 5 | 5 | 0 | 0 | 55.26 | |
| 1.656 | | 5 | 5 | 0 | 1 | 55.44 | |
| 1.652 | | 4 | 4 | 0 | 8 | 55.58 | |
| 1.646 | | 2 | 1 | 0 | 13 | 55.82 | |
| 1.642 | | 4 | 5 | 0 | 2 | 55.96 | |
| 1.625 | | 27 | 3 | 2 | 7 | 56.58 | |
| 1.621 | | 18 | 5 | 0 | 3 + | 56.74 | |
| 1.613 | | 25 | 3 | 0 | 11 | 57.06 | |
| 1.598 | | 17 | 3 | 3 | 0 | 57.64 | |
| 1.589 | | 17 | 5 | 0 | 4 | 58.00 | |
| 1.577 | | 1 | 4 | 0 | 9 | 58.48 | |
| 1.562 | | 3 | 3 | 2 | 8 | 59.10 | |
| 1.559 | | 5 | 0 | 0 | 14 | 59.22 | |
| 1.555 | | 4 | 2 | 0 | 13 | 59.38 | |
| 1.552 | | 5 | 5 | 0 | 5 | 59.50 | |
| 1.532 | | 1 | 1 | 0 | 14 | 60.36 | |
| 1.520 | | 1 | 3 | 0 | 12 | 60.90 | |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|---|-----|---------|-------|---------------|
| d(Å) | ° | I | hkl | 2θ(°) | λ = 1.540598Å |
| 10.91 | | 2 | 0 0 2 | 8.10 | |
| 8.29 | | 1 | 1 0 0 | 10.66 | |
| 6.60 | | 3 | 1 0 2 | 13.40 | |
| 4.79 | | 1 | 1 1 0 | 18.50 | |
| 3.88 | | 1 | 2 0 2 | 22.90 | |
| 3.60 | | 2 | 2 0 3 + | 24.70 | |
| 3.33 | | 10 | 1 0 6 | 26.74 | |
| 3.30 | | 28 | 2 0 4 | 26.96 | |
| 3.14 | | 32 | 2 1 0 | 28.42 | |
| 3.11 | | 28 | 2 1 1 | 28.72 | |
| 3.02 | | 28 | 2 1 2 | 29.60 | |
| 3.01 | | 23 | 2 0 5 | 29.66 | |
| 2.919 | | 60 | 1 0 7 | 30.60 | |
| 2.899 | | 12 | 1 1 6 | 30.82 | |
| 2.882 | | 19 | 2 1 3 | 31.00 | |
| 2.768 | | 22 | 3 0 0 | 32.32 | |
| 2.745 | | 8 | 3 0 1 | 32.60 | |
| 2.736 | | 22 | 2 0 6 | 32.70 | |
| 2.720 | | 100 | 2 1 4 + | 32.90 | |
| 2.587 | | 63 | 3 0 3 + | 34.64 | |
| 2.548 | | 22 | 2 1 5 | 35.20 | |
| 2.493 | | 56 | 2 0 7 | 36.00 | |
| 2.396 | | 56 | 2 2 0 | 37.50 | |
| 2.377 | | 5 | 2 1 6 | 37.82 | |
| 2.338 | | 4 | 3 0 5 | 38.48 | |

Cerium cobalt, Ce₂₄Co₁₁ - continued

| d(A) | I | hkl | 2θ(°) | λ = 1.540598Å |
|-------|---|----------|-------|---------------|
| 1.511 | 1 | 5 0 6 | 61.32 | |
| 1.504 | 1 | 4 0 10 | 61.60 | |
| 1.477 | 1 | 5 1 2 | 62.86 | |
| 1.463 | 1 | 3 3 6 | 63.54 | |
| 1.449 | 1 | 2 2 12 | 64.24 | |
| 1.441 | 1 | 4 2 6 | 64.64 | |
| 1.438 | 2 | 5 1 4 | 64.76 | |
| 1.435 | 3 | 3 2 10 + | 64.92 | |
| 1.427 | 1 | 3 1 12 | 65.32 | |
| 1.379 | 3 | 3 3 8 + | 67.92 | |
| 1.375 | 2 | 3 2 11 | 68.14 | |
| 1.373 | 2 | 2 0 15 | 68.24 | |
| 1.370 | 1 | 5 0 9 | 68.42 | |
| 1.365 | 1 | 4 3 0 | 68.70 | |
| 1.359 | 3 | 6 0 3 + | 69.04 | |
| 1.345 | 3 | 5 1 7 | 69.86 | |
| 1.338 | 5 | 4 1 11 | 70.30 | |
| 1.330 | 2 | 5 2 0 | 70.80 | |
| 1.324 | 4 | 4 3 4 | 71.14 | |
| 1.320 | 3 | 2 1 15 + | 71.38 | |
| 1.316 | 2 | 3 2 12 | 71.68 | |
| 1.308 | 7 | 5 2 3 + | 72.16 | |
| 1.274 | 1 | 4 2 10 | 74.40 | |
| 1.272 | 1 | 5 2 5 | 74.54 | |
| 1.260 | 2 | 3 2 13 | 75.40 | |
| 1.251 | 1 | 4 3 7 | 76.04 | |
| 1.249 | 1 | 5 2 6 | 76.18 | |
| 1.206 | 2 | 3 2 14 | 79.36 | |
| 1.192 | 1 | 5 1 11 | 80.50 | |
| 1.164 | 1 | 2 0 18 | 82.86 | |
| 1.159 | 3 | 5 3 4 | 83.30 | |
| 1.156 | 3 | 3 2 15 | 83.54 | |
| 1.153 | 2 | 5 1 12 | 83.80 | |
| 1.151 | 1 | 6 2 0 | 83.98 | |
| 1.150 | 2 | 6 2 1 | 84.12 | |
| 1.137 | 1 | 6 2 3 | 85.28 | |
| 1.135 | 3 | 6 0 11 | 85.48 | |
| 1.131 | 4 | 2 1 18 | 85.84 | |
| 1.128 | 3 | 5 3 6 | 86.16 | |
| 1.127 | 4 | 6 2 4 | 86.26 | |
| 1.116 | 2 | 3 3 14 + | 87.30 | |
| 1.113 | 2 | 6 2 5 | 87.56 | |
| 1.109 | 5 | 5 3 7 + | 88.02 | |
| 1.105 | 5 | 5 2 11 | 88.44 | |
| 1.100 | 3 | 7 1 0 | 88.92 | |
| 1.095 | 1 | 5 0 15 | 89.46 | |
| 1.088 | 2 | 5 3 8 | 90.16 | |
| 1.079 | 1 | 2 1 19 | 91.12 | |
| 1.042 | 1 | 5 3 10 | 95.32 | |

| Calculated Pattern (Integrated) | | | | |
|---------------------------------|-----|--------|-------|---------------|
| d(A) | I | hkl | 2θ(°) | λ = 1.540598Å |
| 10.91 | 1 | 0 0 2 | 8.09 | |
| 8.30 | 1 | 1 0 0 | 10.65 | |
| 6.61 | 2 | 1 0 2 | 13.39 | |
| 4.79 | 1 | 1 1 0 | 18.49 | |
| 3.88 | 1 | 2 0 2 | 22.90 | |
| 3.61 | 1 | 2 0 3 | 24.67 | |
| 3.60 | 1 | 1 1 4 | 24.70 | |
| 3.33 | 9 | 1 0 6 | 26.73 | |
| 3.30 | 28 | 2 0 4 | 26.96 | |
| 3.14 | 32 | 2 1 0 | 28.42 | |
| 3.11 | 28 | 2 1 1 | 28.71 | |
| 3.02 | 27 | 2 1 2 | 29.59 | |
| 3.01 | 7 | 2 0 5 | 29.67 | |
| 2.919 | 62 | 1 0 7 | 30.60 | |
| 2.898 | 10 | 1 1 6 | 30.83 | |
| 2.882 | 19 | 2 1 3 | 31.01 | |
| 2.768 | 23 | 3 0 0 | 32.32 | |
| 2.746 | 4 | 3 0 1 | 32.58 | |
| 2.736 | 16 | 2 0 6 | 32.70 | |
| 2.728 | 12 | 0 0 8 | 32.80 | |
| 2.721 | 100 | 2 1 4 | 32.90 | |
| 2.592 | 1 | 1 0 8 | 34.58 | |
| 2.587 | 70 | 3 0 3 | 34.65 | |
| 2.548 | 24 | 2 1 5 | 35.19 | |
| 2.493 | 63 | 2 0 7 | 35.99 | |
| 2.397 | 65 | 2 2 0 | 37.49 | |
| 2.376 | 4 | 2 1 6 | 37.83 | |
| 2.338 | 4 | 3 0 5 | 38.48 | |
| 2.280 | 21 | 2 0 8 | 39.49 | |
| 2.253 | 1 | 3 1 2 | 39.98 | |
| 2.212 | 2 | 2 1 7 | 40.76 | |
| 2.203 | 5 | 3 0 6 | 40.94 | |
| 2.196 | 2 | 3 1 3 | 41.08 | |
| 2.122 | 10 | 3 1 4 | 42.58 | |
| 2.111 | 2 | 1 0 10 | 42.80 | |
| 2.094 | 2 | 2 0 9 | 43.16 | |
| 2.067 | 3 | 4 0 1 | 43.77 | |
| 2.059 | 4 | 2 1 8 | 43.94 | |
| 2.039 | 1 | 4 0 2 | 44.39 | |
| 1.996 | 1 | 4 0 3 | 45.40 | |
| 1.946 | 2 | 3 1 6 | 46.64 | |
| 1.943 | 2 | 3 0 8 | 46.71 | |
| 1.940 | 2 | 4 0 4 | 46.78 | |
| 1.932 | 2 | 2 0 10 | 47.00 | |
| 1.930 | 1 | 1 0 11 | 47.05 | |
| 1.919 | 4 | 2 1 9 | 47.33 | |
| 1.905 | 2 | 3 2 0 | 47.70 | |
| 1.877 | 3 | 3 2 2 | 48.47 | |
| 1.875 | 1 | 4 0 5 | 48.52 | |
| 1.843 | 1 | 3 2 3 | 49.42 | |

Cerium cobalt, Ce₂₄Co₁₁ - continued

| d(Å) | I | hkl | | | 2θ(°) | λ = 1.540598Å |
|-------|----|-----|---|----|-------|---------------|
| | | h | k | l | ° | ° |
| 1.824 | 3 | 3 | 0 | 9 | 49.96 | |
| 1.812 | 1 | 4 | 1 | 0 | 50.32 | |
| 1.806 | 1 | 4 | 1 | 1 | 50.50 | |
| 1.803 | 1 | 4 | 0 | 6 | 50.58 | |
| 1.801 | 4 | 2 | 2 | 8 | 50.65 | |
| 1.799 | 5 | 3 | 2 | 4 | 50.72 | |
| 1.792 | 3 | 2 | 1 | 10 | 50.92 | |
| 1.790 | 5 | 2 | 0 | 11 | 50.97 | |
| 1.777 | 2 | 1 | 0 | 12 | 51.38 | |
| 1.760 | 3 | 3 | 1 | 8 | 51.92 | |
| 1.758 | 10 | 4 | 1 | 3 | 51.97 | |
| 1.746 | 1 | 3 | 2 | 5 | 52.36 | |
| 1.728 | 7 | 4 | 0 | 7 | 52.95 | |
| 1.701 | 1 | 1 | 1 | 12 | 53.87 | |
| 1.688 | 3 | 3 | 2 | 6 | 54.32 | |
| 1.677 | 1 | 2 | 1 | 11 | 54.68 | |
| 1.674 | 1 | 4 | 1 | 5 | 54.81 | |
| 1.666 | 5 | 2 | 0 | 12 | 55.08 | |
| 1.661 | 4 | 5 | 0 | 0 | 55.27 | |
| 1.656 | 4 | 5 | 0 | 1 | 55.44 | |
| 1.652 | 3 | 4 | 0 | 8 | 55.58 | |
| 1.646 | 2 | 1 | 0 | 13 | 55.82 | |
| 1.642 | 3 | 5 | 0 | 2 | 55.96 | |
| 1.626 | 37 | 3 | 2 | 7 | 56.57 | |
| 1.622 | 2 | 4 | 1 | 6 | 56.71 | |
| 1.619 | 3 | 5 | 0 | 3 | 56.82 | |
| 1.613 | 32 | 3 | 0 | 11 | 57.06 | |
| 1.598 | 22 | 3 | 3 | 0 | 57.64 | |
| 1.589 | 22 | 5 | 0 | 4 | 58.01 | |
| 1.577 | 1 | 4 | 0 | 9 | 58.48 | |
| 1.562 | 2 | 3 | 2 | 8 | 59.10 | |
| 1.559 | 6 | 0 | 0 | 14 | 59.22 | |
| 1.557 | 2 | 2 | 0 | 13 | 59.32 | |
| 1.552 | 5 | 5 | 0 | 5 | 59.51 | |
| 1.532 | 2 | 1 | 0 | 14 | 60.36 | |
| 1.520 | 1 | 3 | 0 | 12 | 60.90 | |
| 1.511 | 2 | 5 | 0 | 6 | 61.31 | |
| 1.504 | 1 | 4 | 0 | 10 | 61.61 | |
| 1.478 | 1 | 5 | 1 | 2 | 62.84 | |
| 1.463 | 1 | 3 | 3 | 6 | 63.54 | |
| 1.449 | 1 | 2 | 2 | 12 | 64.23 | |
| 1.441 | 1 | 4 | 2 | 6 | 64.63 | |
| 1.439 | 2 | 5 | 1 | 4 | 64.75 | |
| 1.435 | 2 | 3 | 2 | 10 | 64.92 | |
| 1.433 | 1 | 1 | 0 | 15 | 65.02 | |
| 1.427 | 1 | 3 | 1 | 12 | 65.32 | |
| 1.402 | 1 | 4 | 2 | 7 | 66.67 | |
| 1.379 | 4 | 3 | 3 | 8 | 67.92 | |
| 1.374 | 1 | 3 | 2 | 11 | 68.19 | |
| 1.373 | 1 | 2 | 0 | 15 | 68.24 | |

| d(Å) | I | hkl | | | 2θ(°) | λ = 1.540598Å |
|-------|---|-----|---|----|-------|---------------|
| | | h | k | l | ° | ° |
| 1.370 | 1 | 5 | 0 | 9 | 68.41 | |
| 1.365 | 1 | 4 | 3 | 0 | 68.71 | |
| 1.360 | 3 | 6 | 0 | 3 | 69.03 | |
| 1.358 | 2 | 3 | 0 | 14 | 69.09 | |
| 1.345 | 4 | 5 | 1 | 7 | 69.86 | |
| 1.338 | 7 | 4 | 1 | 11 | 70.30 | |
| 1.330 | 2 | 5 | 2 | 0 | 70.81 | |
| 1.324 | 5 | 4 | 3 | 4 | 71.14 | |
| 1.322 | 1 | 5 | 0 | 10 | 71.30 | |
| 1.320 | 2 | 2 | 1 | 15 | 71.39 | |
| 1.316 | 2 | 3 | 2 | 12 | 71.68 | |
| 1.309 | 3 | 5 | 1 | 8 | 72.12 | |
| 1.308 | 7 | 5 | 2 | 3 | 72.16 | |
| 1.307 | 4 | 2 | 2 | 14 | 72.23 | |
| 1.303 | 1 | 4 | 3 | 5 | 72.49 | |
| 1.296 | 1 | 2 | 0 | 16 | 72.93 | |
| 1.278 | 1 | 4 | 3 | 6 | 74.13 | |
| 1.274 | 1 | 4 | 2 | 10 | 74.40 | |
| 1.272 | 1 | 5 | 2 | 5 | 74.55 | |
| 1.260 | 3 | 3 | 2 | 13 | 75.40 | |
| 1.250 | 1 | 4 | 3 | 7 | 76.05 | |
| 1.249 | 1 | 5 | 2 | 6 | 76.17 | |
| 1.207 | 3 | 3 | 2 | 14 | 79.35 | |
| 1.192 | 1 | 5 | 1 | 11 | 80.50 | |
| 1.164 | 1 | 2 | 0 | 18 | 82.87 | |
| 1.159 | 4 | 5 | 3 | 4 | 83.30 | |
| 1.156 | 3 | 3 | 2 | 15 | 83.54 | |
| 1.153 | 2 | 5 | 1 | 12 | 83.82 | |
| 1.151 | 1 | 6 | 2 | 0 | 83.97 | |
| 1.150 | 2 | 6 | 2 | 1 | 84.12 | |
| 1.137 | 2 | 6 | 2 | 3 | 85.26 | |
| 1.135 | 4 | 6 | 0 | 11 | 85.47 | |
| 1.131 | 5 | 2 | 1 | 18 | 85.84 | |
| 1.128 | 2 | 5 | 3 | 6 | 86.16 | |
| 1.127 | 7 | 6 | 2 | 4 | 86.27 | |
| 1.116 | 4 | 3 | 3 | 14 | 87.30 | |
| 1.115 | 1 | 5 | 1 | 13 | 87.39 | |
| 1.113 | 1 | 6 | 2 | 5 | 87.55 | |
| 1.109 | 2 | 3 | 2 | 16 | 87.98 | |
| 1.109 | 2 | 7 | 0 | 7 | 88.02 | |
| 1.109 | 6 | 5 | 3 | 7 | 88.02 | |
| 1.107 | 1 | 2 | 0 | 19 | 88.17 | |
| 1.105 | 7 | 5 | 2 | 11 | 88.43 | |
| 1.100 | 6 | 7 | 1 | 0 | 88.92 | |
| 1.094 | 1 | 5 | 0 | 15 | 89.47 | |
| 1.088 | 3 | 5 | 3 | 8 | 90.16 | |
| 1.079 | 2 | 2 | 1 | 19 | 91.13 | |
| 1.042 | 1 | 5 | 3 | 10 | 95.31 | |
| 1.042 | 1 | 5 | 1 | 15 | 95.40 | |

Cerium gallium, CeGa₂

Structure

Hexagonal, P6/mmm(191), Z=1, isostructural with AlB₂ [Laves, 1943].

Lattice constants: Haszko [1961]

$$a = 4.32 \text{ \AA}$$

$$c = 4.34$$

Density

(calculated) 6.62 g/cm³

Thermal parameters

Overall isotropic B = 1.0

Scattering factors

Ce⁰ and Ga⁰ [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)

$$\gamma = 0.988 \times 10^{-3}$$

$$I/I_c \text{ (calculated) } = 12.8$$

References

- Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
 Haszko, S. E. (1961). Trans. AIME 221, 201.
 Laves, F. (1943). Naturwissenschaften 31, 145.
 Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.

| d (Å) | I | Calculated Pattern (Peak heights) | | | 2θ (°) λ = 1.540598 Å |
|-------|-----|-----------------------------------|---|---|--------------------------|
| | | h | k | l | |
| 3.74 | 13 | 1 | 0 | 0 | 23.76 |
| 2.834 | 100 | 1 | 0 | 1 | 31.54 |
| 2.170 | 14 | 0 | 0 | 2 | 41.58 |
| 2.160 | 37 | 1 | 1 | 0 | 41.78 |
| 1.877 | 3 | 1 | 0 | 2 | 48.46 |
| 1.871 | 2 | 2 | 0 | 0 | 48.62 |
| 1.718 | 17 | 2 | 0 | 1 | 53.28 |
| 1.531 | 18 | 1 | 1 | 2 | 60.42 |
| 1.417 | 1 | 2 | 0 | 2 | 65.86 |
| 1.414 | 1 | 2 | 1 | 0 | 66.02 |
| 1.349 | 6 | 1 | 0 | 3 | 69.62 |
| 1.345 | 12 | 2 | 1 | 1 | 69.90 |
| 1.247 | 3 | 3 | 0 | 0 | 76.30 |
| 1.185 | 1 | 2 | 1 | 2 | 81.12 |
| 1.144 | 3 | 2 | 0 | 3 | 84.62 |
| 1.085 | 1 | 0 | 0 | 4 | 90.46 |
| 1.081 | 4 | 3 | 0 | 2 | 90.86 |
| 1.080 | 3 | 2 | 2 | 0 | 91.00 |
| 1.011 | 3 | 2 | 1 | 3 | 99.24 |
| 1.009 | 4 | 3 | 1 | 1 | 99.52 |
| .970 | 2 | 1 | 1 | 4 | 105.22 |
| .967 | 3 | 2 | 2 | 2 | 105.62 |
| .914 | 1 | 4 | 0 | 1 | 114.80 |
| .846 | 1 | 1 | 0 | 5 | 131.30 |
| .843 | 3 | 3 | 1 | 3 | 132.00 |
| .842 | 2 | 3 | 2 | 1 | 132.38 |
| .819 | 2 | 3 | 0 | 4 | 140.46 |
| .816 | 3 | 4 | 1 | 0 | 141.30 |
| .787 | 1 | 2 | 0 | 5 | 156.10 |
| .785 | 2 | 4 | 0 | 3 | 157.46 |

Cerium gallium, CeGa₂ - continued

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-------|--------|---------------|--|
| d(A) | I | hkl | 2θ(°) | λ = 1.540598A | |
| 3.74 | 11 | 1 0 0 | 23.76 | | |
| 2.834 | 100 | 1 0 1 | 31.55 | | |
| 2.170 | 13 | 0 0 2 | 41.58 | | |
| 2.160 | 38 | 1 1 0 | 41.79 | | |
| 1.877 | 3 | 1 0 2 | 48.46 | | |
| | | | | | |
| 1.871 | 2 | 2 0 0 | 48.63 | | |
| 1.718 | 20 | 2 0 1 | 53.28 | | |
| 1.531 | 22 | 1 1 2 | 60.42 | | |
| 1.417 | 1 | 2 0 2 | 65.87 | | |
| 1.414 | 1 | 2 1 0 | 66.01 | | |
| | | | | | |
| 1.349 | 8 | 1 0 3 | 69.62 | | |
| 1.344 | 15 | 2 1 1 | 69.91 | | |
| 1.247 | 5 | 3 0 0 | 76.29 | | |
| 1.185 | 1 | 2 1 2 | 81.11 | | |
| 1.144 | 4 | 2 0 3 | 84.62 | | |
| | | | | | |
| 1.085 | 1 | 0 0 4 | 90.46 | | |
| 1.081 | 6 | 3 0 2 | 90.86 | | |
| 1.080 | 3 | 2 2 0 | 91.00 | | |
| 1.011 | 6 | 2 1 3 | 99.24 | | |
| 1.009 | 6 | 3 1 1 | 99.51 | | |
| | | | | | |
| .970 | 5 | 1 1 4 | 105.21 | | |
| .967 | 5 | 2 2 2 | 105.63 | | |
| .936 | 1 | 3 1 2 | 110.75 | | |
| .914 | 3 | 4 0 1 | 114.81 | | |
| .861 | 1 | 2 1 4 | 126.98 | | |
| | | | | | |
| .846 | 3 | 1 0 5 | 131.29 | | |
| .843 | 6 | 3 1 3 | 132.01 | | |
| .842 | 6 | 3 2 1 | 132.37 | | |
| .819 | 6 | 3 0 4 | 140.46 | | |
| .816 | 6 | 4 1 0 | 141.31 | | |
| | | | | | |
| .798 | 1 | 3 2 2 | 149.65 | | |
| .787 | 5 | 2 0 5 | 156.10 | | |
| .785 | 5 | 4 0 3 | 157.46 | | |

Cerium magnesium, CeMg₃

Structure

Cubic, face centered, Z=4. [Rossi and Iandelli, 1934]. Their atomic positions indicate Fm3m; other references include Fd3m as a possibility.

Lattice constant: [Vogel and Heumann, 1947]

$$a = 7.438 \text{ \AA}$$

Density

(calculated) 3.439 g/cm³

Thermal parameters

Overall isotropic B = 1.0

Scattering factors

Ce⁰, Mg⁰ [International Tables, 1962].

Atom positions

Rossi and Iandelli [1934].

Scale factors (integrated intensities)

$$\gamma = 0.716 \times 10^{-3}$$

I/I_c (calculated) = 10.8

References

International Tables for X-ray Crystallography III (1962), 202, 211.

Rossi, A. and Iandelli, A. (1934). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. Ser. 6, V.19, 415.

Vogel, R. and Heumann, Th. (1947). Z. Metallk. 38, 1 (1947).

| d(\text{\AA}) | I | Calculated Pattern (Peak heights) | | | | $\lambda = 1.540598\text{\AA}$ |
|---------------|-----|-----------------------------------|---|-----|---------------------------|--------------------------------|
| | | h | k | l | $2\theta (\text{\\circ})$ | |
| 4.30 | 75 | 1 | 1 | 1 | 20.66 | |
| 3.72 | 38 | 2 | 0 | 0 | 23.92 | |
| 2.63 | 100 | 2 | 2 | 0 | 34.06 | |
| 2.243 | 33 | 3 | 1 | 1 | 40.18 | |
| 2.148 | 9 | 2 | 2 | 2 | 42.04 | |
| 1.860 | 15 | 4 | 0 | 0 | 48.94 | |
| 1.706 | 11 | 3 | 3 | 1 | 53.68 | |
| 1.663 | 10 | 4 | 2 | 0 | 55.18 | |
| 1.518 | 25 | 4 | 2 | 2 | 60.98 | |
| 1.431 | 7 | 5 | 1 | 1 + | 65.12 | |
| 1.315 | 6 | 4 | 4 | 0 | 71.72 | |
| 1.257 | 6 | 5 | 3 | 1 | 75.56 | |
| 1.240 | 3 | 4 | 4 | 2 + | 76.84 | |
| 1.176 | 7 | 6 | 2 | 0 | 81.84 | |
| 1.134 | 2 | 5 | 3 | 3 | 85.54 | |
| 1.121 | 2 | 6 | 2 | 2 | 86.78 | |
| 1.074 | 2 | 4 | 4 | 4 | 91.70 | |
| 1.041 | 3 | 7 | 1 | 1 + | 95.40 | |
| 1.032 | 1 | 6 | 4 | 0 | 96.62 | |
| .994 | 7 | 6 | 4 | 2 | 101.60 | |
| .968 | 3 | 7 | 3 | 1 + | 105.40 | |
| .930 | 1 | 8 | 0 | 0 | 111.90 | |
| .909 | 1 | 7 | 3 | 3 | 115.92 | |
| .902 | 2 | 8 | 2 | 0 + | 117.30 | |
| .877 | 4 | 8 | 2 | 2 + | 122.98 | |
| .859 | 2 | 7 | 5 | 1 + | 127.50 | |
| .853 | 1 | 6 | 6 | 2 | 129.06 | |
| .832 | 3 | 8 | 4 | 0 | 135.72 | |
| .816 | 3 | 7 | 5 | 3 + | 141.30 | |
| .812 | 2 | 8 | 4 | 2 | 143.30 | |
| .793 | 3 | 6 | 6 | 4 | 152.58 | |

Cerium magnesium, CeMg₃ - continued

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-----|---|--------|---------------|
| d(Å) | I | hkl | | 2θ (°) | λ = 1.540598Å |
| 4.29 | 66 | 1 | 1 | 1 | 20.67 |
| 3.72 | 35 | 2 | 0 | 0 | 23.91 |
| 2.63 | 100 | 2 | 2 | 0 | 34.07 |
| 2.243 | 34 | 3 | 1 | 1 | 40.18 |
| 2.147 | 10 | 2 | 2 | 2 | 42.05 |
| 1.860 | 16 | 4 | 0 | 0 | 48.94 |
| 1.706 | 14 | 3 | 3 | 1 | 53.67 |
| 1.663 | 12 | 4 | 2 | 0 | 55.18 |
| 1.518 | 31 | 4 | 2 | 2 | 60.98 |
| 1.431 | 7 | 5 | 1 | 1 | 65.11 |
| 1.431 | 2 | 3 | 3 | 3 | 65.11 |
| 1.315 | 9 | 4 | 4 | 0 | 71.72 |
| 1.257 | 9 | 5 | 3 | 1 | 75.57 |
| 1.240 | 1 | 6 | 0 | 0 | 76.83 |
| 1.240 | 4 | 4 | 4 | 2 | 76.83 |
| 1.176 | 11 | 6 | 2 | 0 | 81.84 |
| 1.134 | 3 | 5 | 3 | 3 | 85.55 |
| 1.121 | 3 | 6 | 2 | 2 | 86.78 |
| 1.074 | 3 | 4 | 4 | 4 | 91.70 |
| 1.042 | 2 | 5 | 5 | 1 | 95.39 |
| 1.042 | 2 | 7 | 1 | 1 | 95.39 |
| 1.031 | 2 | 6 | 4 | 0 | 96.63 |
| .994 | 13 | 6 | 4 | 2 | 101.61 |
| .968 | 4 | 7 | 3 | 1 | 105.40 |
| .968 | 2 | 5 | 5 | 3 | 105.40 |
| .930 | 2 | 8 | 0 | 0 | 111.89 |
| .909 | 2 | 7 | 3 | 3 | 115.92 |
| .902 | 2 | 8 | 2 | 0 | 117.30 |
| .902 | 2 | 6 | 4 | 4 | 117.30 |
| .877 | 3 | 6 | 6 | 0 | 122.99 |
| .877 | 6 | 8 | 2 | 2 | 122.99 |
| .859 | 4 | 7 | 5 | 1 | 127.50 |
| .859 | 1 | 5 | 5 | 5 | 127.50 |
| .853 | 2 | 6 | 6 | 2 | 129.07 |
| .832 | 7 | 8 | 4 | 0 | 135.73 |
| .816 | 6 | 7 | 5 | 3 | 141.30 |
| .816 | 3 | 9 | 1 | 1 | 141.30 |
| .812 | 6 | 8 | 4 | 2 | 143.31 |
| .793 | 10 | 6 | 6 | 4 | 152.58 |

Cerium nickel, CeNi₂

Structure

Cubic, Fd3m(227), Z=8, C15 type, isostructural with Cu₂Mg [Fülling et al., 1942].

Lattice constant: [Wernick and Geller, 1960]

$$a = 7.202(5) \text{ \AA}$$

Density

(calculated) 9.158 g/cm³

Thermal parameters

Overall isotropic B = 1.0

Scattering factors

Ce⁰ and Ni⁰ [Thomas and Umeda, 1957], corrected for dispersion [Dabben and Templeton, 1955].

Scale factors (integrated intensities)

$$\gamma = 0.774 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 10.1$$

Additional patterns

1. Fülling, Moeller, and Vogel [1942].
2. Nowotny [1942].

References

- Dabben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
 Fülling W., Moeller, K., and Vogel, R. (1942). Z. Metallk. 34, 253.
 Nowotny, H. (1942). Z. Metallk. 34 #11, 247.
 Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.
 Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

| d (Å) | I | Calculated Pattern (Integrated) | | | | λ = 1.540598 Å |
|-------|-----|---------------------------------|---|---|--------|----------------|
| | | h | k | l | 2θ (°) | |
| 4.16 | 13 | 1 | 1 | 1 | 21.35 | |
| 2.546 | 67 | 2 | 2 | 0 | 35.22 | |
| 2.171 | 100 | 3 | 1 | 1 | 41.55 | |
| 2.079 | 15 | 2 | 2 | 2 | 43.49 | |
| 1.652 | 3 | 3 | 3 | 1 | 55.58 | |
| 1.470 | 21 | 4 | 2 | 2 | 63.20 | |
| 1.386 | 19 | 5 | 1 | 1 | 67.53 | |
| 1.386 | 6 | 3 | 3 | 3 | 67.53 | |
| 1.273 | 18 | 4 | 4 | 0 | 74.46 | |
| 1.217 | 3 | 5 | 3 | 1 | 78.51 | |
| 1.139 | 8 | 6 | 2 | 0 | 85.13 | |
| 1.098 | 8 | 5 | 3 | 3 | 89.07 | |
| 1.086 | 3 | 6 | 2 | 2 | 90.38 | |
| 1.008 | 1 | 7 | 1 | 1 | 99.60 | |
| 1.008 | 1 | 5 | 5 | 1 | 99.60 | |
| .962 | 11 | 6 | 4 | 2 | 106.33 | |
| .938 | 11 | 7 | 3 | 1 | 110.48 | |
| .938 | 6 | 5 | 5 | 3 | 110.48 | |
| .900 | 3 | 8 | 0 | 0 | 117.66 | |
| .880 | 1 | 7 | 3 | 3 | 122.20 | |
| .849 | 3 | 6 | 6 | 0 | 130.34 | |
| .849 | 6 | 8 | 2 | 2 | 130.34 | |
| .832 | 13 | 7 | 5 | 1 | 135.72 | |
| .832 | 2 | 5 | 5 | 5 | 135.72 | |
| .826 | 2 | 6 | 6 | 2 | 137.63 | |
| .805 | 1 | 8 | 4 | 0 | 146.13 | |
| .791 | 3 | 7 | 5 | 3 | 154.02 | |
| .791 | 2 | 9 | 1 | 1 | 154.02 | |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|----------------|---|-----|--------|
| d (Å) | I | h | k | l | 2θ (°) |
| | | λ = 1.540598 Å | | | |
| 4.16 | 16 | 1 | 1 | 1 | 21.36 |
| 2.546 | 72 | 2 | 2 | 0 | 35.22 |
| 2.171 | 100 | 3 | 1 | 1 | 41.56 |
| 2.079 | 14 | 2 | 2 | 2 | 43.50 |
| 1.652 | 3 | 3 | 3 | 1 | 55.58 |
| 1.470 | 17 | 4 | 2 | 2 | 63.20 |
| 1.386 | 20 | 5 | 1 | 1 + | 67.52 |
| 1.273 | 13 | 4 | 4 | 0 | 74.46 |
| 1.217 | 2 | 5 | 3 | 1 | 78.50 |
| 1.139 | 5 | 6 | 2 | 0 | 85.14 |
| 1.098 | 5 | 5 | 3 | 3 | 89.08 |
| 1.086 | 2 | 6 | 2 | 2 | 90.38 |
| 1.009 | 1 | 7 | 1 | 1 + | 99.60 |
| .962 | 6 | 6 | 4 | 2 | 106.34 |
| .938 | 8 | 7 | 3 | 1 + | 110.48 |
| .900 | 2 | 8 | 0 | 0 | 117.66 |
| .849 | 4 | 8 | 2 | 2 + | 130.34 |
| .832 | 6 | 7 | 5 | 1 + | 135.72 |
| .826 | 1 | 6 | 6 | 2 | 137.64 |
| .791 | 1 | 7 | 5 | 3 + | 154.02 |

Cerium thallium, CeTl

Structure

Cubic, Pm3m (221), Z = 1, CsCl type [Bruzzone and Ferro Ruggiero, 1962].

Lattice constant: [ibid.]

$$a = 3.893 \text{ \AA}$$

Density

(calculated) 9.695 g/cm^3

Thermal parameters

Overall isotropic B = 1.0

Scattering factors

Ce^0 , Tl^0 [International Tables, 1962].

Scale factors (integrated intensities)

$$\gamma = 1.90 \times 10^{-3}$$

I/I_c (calculated) = 32.3

| $d(\text{\AA})$ | I | Calculated Pattern (Integrated) | | | $2\theta (\text{^\circ})$ | $\lambda = 1.540598\text{\AA}$ |
|-----------------|-----|---------------------------------|---|---|---------------------------|--------------------------------|
| | | h | k | l | | |
| 3.89 | 4 | 1 | 0 | 0 | 22.82 | |
| 2.753 | 100 | 1 | 1 | 0 | 32.50 | |
| 2.248 | 1 | 1 | 1 | 1 | 40.08 | |
| 1.947 | 17 | 2 | 0 | 0 | 46.62 | |
| 1.741 | 2 | 2 | 1 | 0 | 52.52 | |
| 1.589 | 34 | 2 | 1 | 1 | 57.98 | |
| 1.376 | 10 | 2 | 2 | 0 | 68.06 | |
| 1.231 | 13 | 3 | 1 | 0 | 77.47 | |
| 1.124 | 3 | 2 | 2 | 2 | 86.54 | |
| 1.040 | 15 | 3 | 2 | 1 | 95.52 | |
| .973 | 2 | 4 | 0 | 0 | 104.65 | |
| .918 | 3 | 3 | 3 | 0 | 114.17 | |
| .918 | 6 | 4 | 1 | 1 | 114.17 | |
| .871 | 7 | 4 | 2 | 0 | 124.48 | |
| .830 | 8 | 3 | 3 | 2 | 136.28 | |
| .795 | 11 | 4 | 2 | 2 | 151.56 | |

References

International Tables for X-ray Crystallography
III (1962), 211, 212.

Bruzzone, G. and Ferro Ruggiero, A. (1962). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. 33, 465.

Calculated Pattern (Peak heights)

| $d(\text{\AA})$ | I | Calculated Pattern (Peak heights) | | | $2\theta (\text{^\circ})$ | $\lambda = 1.540598\text{\AA}$ |
|-----------------|-----|-----------------------------------|---|---|---------------------------|--------------------------------|
| | | h | k | l | | |
| 3.89 | 4 | 1 | 0 | 0 | 22.82 | |
| 2.753 | 100 | 1 | 1 | 0 | 32.50 | |
| 2.248 | 1 | 1 | 1 | 1 | 40.08 | |
| 1.947 | 15 | 2 | 0 | 0 | 46.62 | |
| 1.741 | 1 | 2 | 1 | 0 | 52.52 | |
| 1.589 | 27 | 2 | 1 | 1 | 57.98 | |
| 1.376 | 7 | 2 | 2 | 0 | 68.06 | |
| 1.231 | 8 | 3 | 1 | 0 | 77.46 | |
| 1.124 | 2 | 2 | 2 | 2 | 86.54 | |
| 1.040 | 8 | 3 | 2 | 1 | 95.52 | |
| .973 | 1 | 4 | 0 | 0 | 104.64 | |
| .918 | 4 | 4 | 1 | 1 | + 114.18 | |
| .870 | 3 | 4 | 2 | 0 | 124.48 | |
| .830 | 3 | 3 | 3 | 2 | 136.28 | |
| .795 | 3 | 4 | 2 | 2 | 151.56 | |

Cerium thallium, CeTl₃

Structure

Cubic, Pm3m (221), z = 1, AuCu₃ type [Bruzzone and Ferro Ruggiero, 1962].

Lattice constant: [ibid.]

$$a = 4.767 \text{ \AA}$$

Density
(calculated) 11.55 g/cm³

Thermal parameters

Overall isotropic B = 1.0

Scattering factors

Ce⁰, Tl⁰ [International Tables, 1962].

Scale factors (integrated intensities)

$$\gamma = 1.66 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 25.4$$

References

International Tables for X-ray Crystallography
III (1962), 211, 212.

Bruzzone, G. and Ferro Ruggiero, A. (1962). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. 33, 465.

| d(Å) | I | Calculated Pattern (Integrated) | | | | $\lambda = 1.540598\text{\AA}$ |
|-------|-----|---------------------------------|---|---|--------|--------------------------------|
| | | hkl | | | 20 (°) | |
| 4.77 | 2 | 1 | 0 | 0 | 18.60 | |
| 3.37 | 2 | 1 | 1 | 0 | 26.42 | |
| 2.752 | 100 | 1 | 1 | 1 | 32.51 | |
| 2.384 | 49 | 2 | 0 | 0 | 37.71 | |
| 2.132 | 1 | 2 | 1 | 0 | 42.36 | |
| 1.046 | 1 | 2 | 1 | 1 | 46.63 | |
| 1.685 | 32 | 2 | 2 | 0 | 54.39 | |
| 1.437 | 35 | 3 | 1 | 1 | 64.81 | |
| 1.376 | 10 | 2 | 2 | 2 | 68.08 | |
| 1.192 | 4 | 4 | 0 | 0 | 80.54 | |
| 1.094 | 13 | 3 | 3 | 1 | 89.55 | |
| 1.066 | 12 | 4 | 2 | 0 | 92.55 | |
| .973 | 10 | 4 | 2 | 2 | 104.68 | |
| .917 | 10 | 5 | 1 | 1 | 114.21 | |
| .917 | 3 | 3 | 3 | 3 | 114.21 | |
| .843 | 6 | 4 | 4 | 0 | 132.15 | |
| .806 | 29 | 5 | 3 | 1 | 145.87 | |
| .795 | 17 | 4 | 4 | 2 | 151.64 | |
| .795 | 4 | 6 | 0 | 0 | 151.64 | |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|-----|---|---|--------------------------------|
| d(Å) | I | hkl | | | 20 (°) |
| | | | | | $\lambda = 1.540598\text{\AA}$ |
| 4.77 | 2 | 1 | 0 | 0 | 18.60 |
| 3.37 | 2 | 1 | 1 | 0 | 26.42 |
| 2.753 | 100 | 1 | 1 | 1 | 32.50 |
| 2.383 | 47 | 2 | 0 | 0 | 37.72 |
| 2.132 | 1 | 2 | 1 | 0 | 42.36 |
| 1.685 | 26 | 2 | 2 | 0 | 54.40 |
| 1.437 | 27 | 3 | 1 | 1 | 64.82 |
| 1.376 | 7 | 2 | 2 | 2 | 68.08 |
| 1.192 | 3 | 4 | 0 | 0 | 80.54 |
| 1.094 | 8 | 3 | 3 | 1 | 89.56 |
| 1.066 | 7 | 4 | 2 | 0 | 92.54 |
| .973 | 5 | 4 | 2 | 2 | 104.68 |
| .917 | 6 | 5 | 1 | 1 | + 114.20 |
| .843 | 2 | 4 | 4 | 0 | 132.16 |
| .806 | 9 | 5 | 3 | 1 | 145.88 |
| .795 | 6 | 4 | 4 | 2 | + 151.64 |

Cerium thallium, Ce₃Tl

Structure

Cubic, Pm3m (221), Z = 1, AuCu₃ type [Jeitschko et al., 1964].

Lattice constant: [ibid.]

$$a = 5.011 \text{ \AA}$$

Density

(calculated) 8.245 g/cm³

Thermal parameters

Overall isotropic B = 1.0

Scattering factors

Ce⁰, Tl⁰ [International Tables, 1962].

Scale factors (integrated intensities)

$$\gamma = 2.09 \times 10^{-3}$$

I/I_C (calculated) = 37.2

References

International Tables for X-ray Crystallography III (1962), 211, 212.

Jeitschko, W., Nowotny, H., and Benesovsky, F. (1964). Monatsh. Chem. 95, 1040.

| d(Å) | I | Calculated Pattern (Peak heights) | | | 2θ (°) λ = 1.540598 Å |
|-------|-----|-----------------------------------|---|---|--------------------------|
| | | h | k | l | |
| 5.01 | 34 | 1 | 0 | 0 | 17.68 |
| 3.54 | 27 | 1 | 1 | 0 | 25.12 |
| 2.893 | 100 | 1 | 1 | 1 | 30.88 |
| 2.505 | 46 | 2 | 0 | 0 | 35.82 |
| 2.241 | 13 | 2 | 1 | 0 | 40.20 |
| 2.046 | 10 | 2 | 1 | 1 | 44.24 |
| 1.772 | 27 | 2 | 2 | 0 | 51.54 |
| 1.670 | 5 | 2 | 2 | 1 | 54.92 |
| 1.584 | 3 | 3 | 1 | 0 | 58.18 |
| 1.511 | 27 | 3 | 1 | 1 | 61.30 |
| 1.446 | 7 | 2 | 2 | 2 | 64.36 |
| 1.390 | 2 | 3 | 2 | 0 | 67.32 |
| 1.339 | 3 | 3 | 2 | 1 | 70.22 |
| 1.253 | 3 | 4 | 0 | 0 | 75.88 |
| 1.215 | 2 | 4 | 1 | 0 | 78.66 |
| 1.181 | 1 | 4 | 1 | 1 | 81.42 |
| 1.150 | 8 | 3 | 3 | 1 | 84.14 |
| 1.120 | 7 | 4 | 2 | 0 | 86.86 |
| 1.094 | 1 | 4 | 2 | 1 | 89.56 |
| 1.023 | 5 | 4 | 2 | 2 | 97.72 |
| .983 | 1 | 4 | 3 | 1 | 103.22 |
| .964 | 6 | 5 | 1 | 1 | 106.02 |
| .930 | 1 | 4 | 3 | 2 | 111.76 |
| .915 | 1 | 5 | 2 | 1 | 114.70 |
| .886 | 2 | 4 | 4 | 0 | 120.82 |
| .872 | 1 | 5 | 2 | 2 | 124.02 |
| .859 | 1 | 5 | 3 | 0 | 127.36 |
| .847 | 7 | 5 | 3 | 1 | 130.86 |
| .835 | 4 | 4 | 4 | 2 | 134.54 |
| .813 | 1 | 5 | 3 | 2 | 142.74 |
| .792 | 4 | 6 | 2 | 0 | 152.92 |
| .783 | 2 | 6 | 2 | 1 | 159.66 |

Cerium thallium, Ce₃Tl - continued

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-----|---|---|---------------|
| d(Å) | I | hkl | | | 2θ (°) |
| | | | | | λ = 1.540598Å |
| | | | | | |
| 5.01 | 30 | 1 | 0 | 0 | 17.69 |
| 3.54 | 26 | 1 | 1 | 0 | 25.11 |
| 2.593 | 100 | 1 | 1 | 1 | 30.88 |
| 2.505 | 50 | 2 | 0 | 0 | 35.81 |
| 2.241 | 14 | 2 | 1 | 0 | 40.21 |
| 2.076 | 11 | 2 | 1 | 1 | 44.24 |
| 1.772 | 33 | 2 | 2 | 0 | 51.54 |
| 1.670 | 1 | 3 | 0 | 0 | 54.92 |
| 1.670 | 5 | 2 | 2 | 1 | 54.92 |
| 1.585 | 5 | 3 | 1 | 0 | 58.17 |
| 1.511 | 37 | 3 | 1 | 1 | 61.31 |
| 1.447 | 10 | 2 | 2 | 2 | 64.35 |
| 1.390 | 3 | 3 | 2 | 0 | 67.32 |
| 1.379 | 5 | 3 | 2 | 1 | 70.22 |
| 1.253 | 4 | 4 | 0 | 0 | 75.89 |
| 1.215 | 2 | 4 | 1 | 0 | 78.66 |
| 1.215 | 2 | 3 | 2 | 2 | 78.66 |
| 1.191 | 1 | 3 | 3 | 0 | 81.41 |
| 1.181 | 2 | 4 | 1 | 1 | 81.41 |
| 1.150 | 13 | 3 | 3 | 1 | 84.14 |
| 1.120 | 12 | 4 | 2 | 0 | 86.86 |
| 1.093 | 2 | 4 | 2 | 1 | 89.57 |
| 1.068 | 1 | 3 | 3 | 2 | 92.28 |
| 1.023 | 9 | 4 | 2 | 2 | 97.72 |
| 1.002 | 1 | 4 | 3 | 0 | 100.46 |
| .993 | 2 | 4 | 3 | 1 | 103.23 |
| .983 | 1 | 5 | 1 | 0 | 103.23 |
| .964 | 9 | 5 | 1 | 1 | 106.02 |
| .964 | 3 | 3 | 3 | 3 | 106.02 |
| .931 | 1 | 5 | 2 | 0 | 111.75 |
| .931 | 2 | 4 | 3 | 2 | 111.75 |
| .915 | 2 | 5 | 2 | 1 | 114.70 |
| .886 | 4 | 4 | 4 | 0 | 120.82 |
| .872 | 1 | 4 | 4 | 1 | 124.03 |
| .872 | 1 | 5 | 2 | 2 | 124.03 |
| .859 | 1 | 5 | 3 | 0 | 127.36 |
| .859 | 1 | 4 | 3 | 3 | 127.36 |
| .847 | 18 | 5 | 3 | 1 | 130.85 |
| .835 | 2 | 6 | 0 | 0 | 134.54 |
| .835 | 10 | 4 | 4 | 2 | 134.54 |
| .824 | 1 | 6 | 1 | 0 | 138.47 |
| .813 | 2 | 5 | 3 | 2 | 142.74 |
| .813 | 1 | 6 | 1 | 1 | 142.74 |
| .792 | 15 | 6 | 2 | 0 | 152.93 |
| .793 | 2 | 5 | 4 | 0 | 159.67 |
| .783 | 4 | 6 | 2 | 1 | 159.67 |
| .783 | 2 | 4 | 4 | 3 | 159.67 |

Cobalt dysprosium, Co_2Dy

Structure

Cubic, Fd3m(227), $Z=8$, C15 type, isostructural with Cu_2Mg [Wernick and Geller, 1960].

Lattice constant: [ibid.]

$$a = 7.187(5)\text{\AA}$$

Density

(calculated) 10.033 g/cm^3

Thermal parameters

Overall isotropic $B = 1.0$

Scattering factors

Co^0 and Dy^0 [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)

$$\gamma = 0.510 \times 10^{-3}$$

$$I/I_C \text{ (calculated)} = 9.35$$

References

Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.

Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.

Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

| $d(\text{\AA})$ | I | Calculated Pattern (Integrated) | | | | $2\theta (\text{^\circ})$ |
|-----------------|-----|---------------------------------|---|---|--------------------------------|---------------------------|
| | | hkl | | | $\lambda = 1.540598\text{\AA}$ | |
| 4.15 | 13 | 1 | 1 | 1 | | 21.40 |
| 2.541 | 66 | 2 | 2 | 0 | | 35.29 |
| 2.167 | 100 | 3 | 1 | 1 | | 41.65 |
| 2.075 | 16 | 2 | 2 | 2 | | 43.59 |
| 1.649 | 3 | 3 | 3 | 1 | | 55.70 |
| 1.467 | 19 | 4 | 2 | 2 | | 63.35 |
| 1.383 | 19 | 5 | 1 | 1 | | 67.69 |
| 1.383 | 6 | 3 | 3 | 3 | | 67.69 |
| 1.270 | 17 | 4 | 4 | 0 | | 74.64 |
| 1.215 | 2 | 5 | 3 | 1 | | 78.70 |
| 1.136 | 7 | 6 | 2 | 0 | | 85.35 |
| 1.096 | 8 | 5 | 3 | 3 | | 89.31 |
| 1.083 | 4 | 6 | 2 | 2 | | 90.62 |
| .960 | 9 | 6 | 4 | 2 | | 106.65 |
| .936 | 11 | 7 | 3 | 1 | | 110.83 |
| .936 | 5 | 5 | 5 | 3 | | 110.83 |
| .898 | 3 | 8 | 0 | 0 | | 118.06 |
| .847 | 2 | 6 | 6 | 0 | | 130.86 |
| .847 | 5 | 8 | 2 | 2 | | 130.86 |
| .830 | 12 | 7 | 5 | 1 | | 136.31 |
| .830 | 2 | 5 | 5 | 5 | | 136.31 |
| .824 | 3 | 6 | 6 | 2 | | 138.25 |
| .789 | 2 | 7 | 5 | 3 | | 155.08 |
| .789 | 1 | 9 | 1 | 1 | | 155.08 |

Calculated Pattern (Peak heights)

| $d(\text{\AA})$ | I | Calculated Pattern (Peak heights) | | | | $2\theta (\text{^\circ})$ |
|-----------------|-----|-----------------------------------|---|---|--------------------------------|---------------------------|
| | | hkl | | | $\lambda = 1.540598\text{\AA}$ | |
| 4.15 | 16 | 1 | 1 | 1 | | 21.40 |
| 2.541 | 70 | 2 | 2 | 0 | | 35.30 |
| 2.167 | 100 | 3 | 1 | 1 | | 41.64 |
| 2.075 | 15 | 2 | 2 | 2 | | 43.58 |
| 1.649 | 2 | 3 | 3 | 1 | | 55.70 |
| 1.467 | 16 | 4 | 2 | 2 | | 63.34 |
| 1.383 | 19 | 5 | 1 | 1 | + | 67.68 |
| 1.271 | 13 | 4 | 4 | 0 | | 74.64 |
| 1.215 | 1 | 5 | 3 | 1 | | 78.70 |
| 1.136 | 5 | 6 | 2 | 0 | | 85.36 |
| 1.096 | 5 | 5 | 3 | 3 | | 89.30 |
| 1.084 | 2 | 6 | 2 | 2 | | 90.62 |
| .960 | 5 | 6 | 4 | 2 | | 106.66 |
| .936 | 8 | 7 | 3 | 1 | + | 110.82 |
| .898 | 2 | 8 | 0 | 0 | | 118.06 |
| .847 | 3 | 8 | 2 | 2 | + | 130.86 |
| .830 | 5 | 7 | 5 | 1 | + | 136.32 |
| .824 | 1 | 6 | 6 | 2 | | 138.26 |

Cobalt erbium, Co_2Er

Structure

Cubic, Fd3m(227), $Z=8$, C15 type, isostructural with Cu_2Mg [Wernick and Geller, 1960].

Lattice constant: [ibid.]

$$a = 7.144(5)\text{\AA}$$

Density

(calculated) 10.388 g/cm^3

Thermal parameters

Overall isotropic $B = 1.0$

Scattering factors

Co^0 and Er^0 [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)

$$\gamma = 0.762 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 9.76$$

References

- Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
 Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.
 Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-------|---|---|----------------------------|
| $d(\text{\AA})$ | I | hkl | | | $2\theta (\text{ }^\circ)$ |
| $\lambda = 1.540598\text{\AA}$ | | | | | |
| 4.12 | 15 | 1 | 1 | 1 | 21.53 |
| 2.526 | 68 | 2 | 2 | 0 | 35.51 |
| 2.154 | 100 | 3 | 1 | 1 | 41.91 |
| 2.062 | 15 | 2 | 2 | 2 | 43.87 |
| 1.639 | 3 | 3 | 3 | 1 | 56.07 |
| 1.458 | 20 | 4 | 2 | 2 | 63.77 |
| 1.375 | 19 | 5 | 1 | 1 | 68.15 |
| 1.375 | 6 | 3 | 3 | 3 | 68.15 |
| 1.263 | 17 | 4 | 4 | 0 | 75.17 |
| 1.208 | 2 | 5 | 3 | 1 | 79.27 |
| 1.130 | 7 | 6 | 2 | 0 | 85.99 |
| 1.089 | 8 | 5 | 3 | 3 | 89.99 |
| 1.077 | 4 | 6 | 2 | 2 | 91.32 |
| .955 | 9 | 6 | 4 | 2 | 107.59 |
| .930 | 11 | 7 | 3 | 1 | 111.83 |
| .930 | 5 | 5 | 5 | 3 | 111.83 |
| .893 | 4 | 8 | 0 | 0 | 119.22 |
| .842 | 2 | 6 | 6 | 0 | 132.39 |
| .842 | 5 | 8 | 2 | 2 | 132.39 |
| .825 | 13 | 7 | 5 | 1 | 138.07 |
| .825 | 2 | 5 | 5 | 5 | 138.07 |
| .819 | 3 | 6 | 6 | 2 | 140.10 |
| .784 | 2 | 7 | 5 | 3 | 158.43 |
| .784 | 1 | 9 | 1 | 1 | 158.43 |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|-------|---|---|----------------------------|
| $d(\text{\AA})$ | I | hkl | | | $2\theta (\text{ }^\circ)$ |
| $\lambda = 1.540598\text{\AA}$ | | | | | |
| 4.12 | 19 | 1 | 1 | 1 | 21.54 |
| 2.525 | 74 | 2 | 2 | 0 | 35.52 |
| 2.154 | 100 | 3 | 1 | 1 | 41.90 |
| 2.063 | 15 | 2 | 2 | 2 | 43.86 |
| 1.639 | 3 | 3 | 3 | 1 | 56.06 |
| 1.458 | 16 | 4 | 2 | 2 | 63.78 |
| 1.375 | 19 | 5 | 1 | 1 | 68.14 |
| 1.263 | 13 | 4 | 4 | 0 | 75.18 |
| 1.207 | 1 | 5 | 3 | 1 | 79.28 |
| 1.129 | 5 | 6 | 2 | 0 | 86.00 |
| 1.089 | 5 | 5 | 3 | 3 | 90.00 |
| 1.077 | 2 | 6 | 2 | 2 | 91.32 |
| .955 | 5 | 6 | 4 | 2 | 107.58 |
| .930 | 8 | 7 | 3 | 1 | 111.84 |
| .893 | 2 | 8 | 0 | 0 | 119.22 |
| .842 | 3 | 8 | 2 | 2 | 132.38 |
| .825 | 6 | 7 | 5 | 1 | 138.06 |
| .819 | 1 | 6 | 6 | 2 | 140.10 |

Cobalt erbium, Co_7Er_2

Structure

Hexagonal, $\bar{R}\bar{3}m$ (166), $Z = 6$. The structure was determined by Ostertag [1967].

Lattice constants: [ibid.]

$$a = 4.973 \text{ \AA}$$

$$c = 36.11$$

Density

(measured) 9.620 g/cm^3 [ibid.]
(calculated) 9.624 g/cm^3

Thermal parameters

Isotropic [Ostertag, op. cit.]

Scattering factors

Co^0 , Er^0 [International Tables, 1962].

Scale factors (integrated intensities)

$\gamma = 0.467 \times 10^{-3}$
 I/I_c (calculated) 6.70

References

International Tables for X-ray Crystallography III (1962), 204, 212.

Ostertag, W. (1967). J. Less-Common Metals, 13, 385.

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{^\circ})$ | | |
|-----------------|----|---------|---------------------------|---------------|---------------|
| | | | λ = 1.540598A | λ = 1.540598A | λ = 1.540598A |
| 1.987 | 8 | 0 2 7 | 45.62 | | |
| 1.944 | 12 | 2 0 8 | 46.70 | | |
| 1.917 | 8 | 1 1 12 | 47.40 | | |
| 1.905 | 7 | 0 1 17 | 47.70 | | |
| 1.801 | 3 | 2 0 11 | 50.66 | | |
| | | | | | |
| 1.730 | 3 | 1 1 15 | 52.90 | | |
| 1.720 | 4 | 0 0 21 | 53.22 | | |
| 1.665 | 6 | 0 1 20 | 55.12 | | |
| 1.653 | 1 | 2 0 14 | 55.54 | | |
| 1.626 | 2 | 2 1 1 | 56.56 | | |
| | | | | | |
| 1.561 | 2 | 1 1 18 | 59.12 | | |
| 1.558 | 2 | 0 2 16 | 59.28 | | |
| 1.534 | 3 | 1 0 22 | 60.30 | | |
| 1.512 | 1 | 2 0 17 | 61.24 | | |
| 1.505 | 1 | 0 0 24 | 61.58 | | |
| | | | | | |
| 1.484 | 13 | 2 1 10 | 62.54 | | |
| 1.458 | 11 | 1 2 11 | 63.76 | | |
| 1.436 | 9 | 3 0 0 | 64.90 | | |
| 1.425 | 6 | 0 2 19 | 65.44 | | |
| 1.414 | 12 | 1 1 21 | 66.00 | | |
| | | | | | |
| 1.384 | 8 | 2 0 20 | 67.66 | | |
| 1.377 | 4 | 1 2 14 | 68.06 | | |
| 1.369 | 2 | 1 0 25 | 68.46 | | |
| 1.352 | 20 | 3 0 9+ | 69.48 | | |
| 1.296 | 2 | 3 0 12+ | 72.96 | | |
| | | | | | |
| 1.292 | 4 | 1 2 17 | 73.20 | | |
| 1.287 | 3 | 1 1 24 | 73.50 | | |
| 1.269 | 1 | 2 0 23 | 74.78 | | |
| 1.243 | 19 | 2 2 0 | 76.58 | | |
| 1.233 | 1 | 3 0 15+ | 77.32 | | |
| | | | | | |
| 1.209 | 4 | 1 2 20 | 79.16 | | |
| 1.204 | 2 | 0 0 30 | 79.58 | | |
| 1.196 | 1 | 0 1 29 | 80.18 | | |
| 1.194 | 1 | 1 3 1 | 80.38 | | |
| 1.188 | 1 | 2 2 9 | 80.88 | | |
| | | | | | |
| 1.178 | 3 | 1 1 27 | 81.68 | | |
| 1.167 | 2 | 2 0 26+ | 82.60 | | |
| 1.156 | 2 | 2 1 22 | 83.60 | | |
| 1.149 | 1 | 2 2 12 | 84.20 | | |
| 1.134 | 5 | 1 3 10 | 85.58 | | |
| | | | | | |
| 1.124 | 3 | 1 0 31 | 86.48 | | |
| 1.122 | 5 | 3 1 11 | 86.68 | | |
| 1.106 | 2 | 0 2 28 | 88.26 | | |
| 1.102 | 6 | 0 3 21+ | 88.70 | | |
| 1.083 | 6 | 1 1 30+ | 90.62 | | |
| | | | | | |
| 1.080 | 4 | 2 1 25 | 90.92 | | |
| 1.076 | 4 | 4 0 1 | 91.42 | | |
| 1.057 | 8 | 2 2 18 | 93.60 | | |
| 1.047 | 1 | 0 4 8 | 94.70 | | |
| 1.041 | 2 | 3 1 17 | 95.44 | | |
| 1.041 | 2 | 3 1 17 | 95.44 | | |

Cobalt erbium, Co_7Er_2 - continued

| d (Å) | I | hkl | 2θ (°) | | Calculated Pattern (Integrated) | | |
|-------|----|---------|----------------|---|---------------------------------|-----|--------------|
| | | | λ = 1.540598 Å | ° | | | |
| 1.039 | 2 | 0 3 24+ | 95.74 | | 12.04 | 4 | 0 0 3 7.34 |
| 1.025 | 3 | 0 2 31 | 97.50 | | 6.02 | 1 | 0 0 6 14.71 |
| 1.007 | 4 | 2 2 21 | 99.74 | | 4.28 | 10 | 1 0 1 20.75 |
| 1.003 | 2 | 0 0 36 | 100.34 | | 4.19 | 1 | 0 1 2 21.19 |
| .9995 | 1 | 2 0 32 | 100.82 | | 4.01 | 4 | 0 0 0 22.14 |
| .9962 | 3 | 3 1 20 | 101.30 | | 3.89 | 3 | 1 0 4 22.86 |
| .9890 | 1 | 1 2 29 | 102.32 | | 3.116 | 2 | 0 1 8 28.63 |
| .9786 | 1 | 3 0 27+ | 103.84 | | 3.009 | 5 | 0 0 12 29.66 |
| .9658 | 1 | 1 3 22 | 105.80 | | 2.767 | 46 | 1 0 10 32.33 |
| .9584 | 1 | 2 2 24 | 106.98 | | 2.611 | 37 | 0 1 11 34.32 |
| .9530 | 5 | 3 2 10+ | 107.86 | | 2.487 | 55 | 1 1 0 36.00 |
| .9473 | 3 | 2 1 31 | 108.82 | | 2.407 | 2 | 0 0 15 37.32 |
| .9461 | 4 | 2 3 11 | 109.02 | | 2.334 | 1 | 1 0 13 38.54 |
| .9398 | 6 | 4 1 0 | 110.10 | | 2.213 | 9 | 0 1 14 40.74 |
| .9368 | 3 | 4 0 19 | 110.52 | | 2.150 | 38 | 0 2 1 42.00 |
| .9304 | 3 | 2 0 35+ | 111.78 | | 2.138 | 9 | 2 0 2 42.23 |
| .9247 | 3 | 0 4 20 | 112.82 | | 2.114 | 100 | 1 1 9 42.75 |
| .9224 | 6 | 3 0 30+ | 113.26 | | 2.095 | 6 | 0 2 4 43.15 |
| .9205 | 3 | 1 3 25 | 113.66 | | 2.064 | 4 | 2 0 5 43.84 |
| .9150 | 14 | 1 4 9+ | 114.66 | | 2.006 | 14 | 0 0 18 45.16 |
| .9106 | 1 | 2 2 27 | 115.54 | | 1.999 | 1 | 1 0 16 45.33 |
| .8971 | 2 | 1 4 12+ | 118.34 | | 1.987 | 7 | 0 2 7 45.61 |
| .8959 | 1 | 2 3 17 | 118.60 | | 1.944 | 12 | 2 0 8 46.70 |
| .8895 | 1 | 2 1 34+ | 120.00 | | 1.917 | 7 | 1 1 12 47.39 |
| .8835 | 1 | 1 0 40 | 121.34 | | 1.905 | 7 | 0 1 17 47.70 |
| .8755 | 1 | 1 4 15+ | 123.26 | | 1.801 | 3 | 2 0 11 50.66 |
| .8677 | 1 | 1 1 39 | 125.20 | | 1.730 | 3 | 1 1 15 52.89 |
| .8667 | 3 | 2 3 20 | 125.42 | | 1.720 | 4 | 0 0 21 53.23 |
| .8648 | 5 | 2 2 30 | 125.94 | | 1.665 | 7 | 0 1 20 55.11 |
| .8629 | 3 | 0 1 41 | 126.49 | | 1.653 | 1 | 2 0 14 55.55 |
| .8509 | 1 | 0 4 26+ | 129.70 | | 1.626 | 2 | 2 1 1 56.55 |
| .8465 | 1 | 3 2 22 | 131.00 | | 1.561 | 2 | 1 1 18 59.12 |
| .8378 | 2 | 0 5 10 | 133.68 | | 1.558 | 1 | 0 2 16 59.26 |
| .8370 | 1 | 2 1 37 | 133.92 | | 1.534 | 3 | 1 0 22 60.30 |
| .8339 | 3 | 1 3 31 | 134.94 | | 1.512 | 1 | 2 0 17 61.25 |
| .8331 | 2 | 5 0 11 | 135.20 | | 1.505 | 1 | 0 0 24 61.59 |
| .8288 | 3 | 3 3 0 | 136.68 | | 1.484 | 14 | 2 1 10 62.54 |
| .8265 | 2 | 4 0 28 | 137.44 | | 1.458 | 12 | 1 2 11 63.77 |
| .8247 | 8 | 4 1 21+ | 138.16 | | 1.436 | 10 | 3 0 0 64.90 |
| .8203 | 1 | 3 1 32 | 139.89 | | 1.425 | 6 | 0 2 19 65.45 |
| .8170 | 1 | 5 0 14 | 141.08 | | 1.414 | 13 | 1 1 21 66.00 |
| .8155 | 2 | 3 2 25+ | 141.70 | | 1.384 | 9 | 2 0 20 67.66 |
| .8137 | 6 | 2 4 1 | 142.42 | | 1.377 | 4 | 1 2 14 68.05 |
| .8126 | 3 | 1 1 42 | 142.90 | | 1.369 | 2 | 1 0 25 68.46 |
| .8117 | 10 | 3 3 9 | 143.24 | | 1.352 | 11 | 3 0 9 69.40 |
| .8106 | 2 | 2 4 4 | 143.70 | | 1.352 | 11 | 0 3 9 69.40 |
| .8088 | 1 | 4 2 5 | 144.52 | | 1.296 | 1 | 3 0 12 72.96 |
| .8062 | 1 | 0 1 44 | 145.68 | | 1.296 | 1 | 0 3 12 72.96 |
| .8040 | 1 | 2 4 7 | 146.72 | | 1.292 | 4 | 1 2 17 73.20 |
| .8010 | 2 | 4 2 8 | 148.19 | | 1.287 | 3 | 1 1 24 73.51 |

Cobalt erbium, Co_7Er_2 - continued

| d (Å) | I | hkl | 2θ (°) | |
|--------------------------------|----|--------|---------------|--|
| $\lambda = 1.540598\text{\AA}$ | | | | |
| 1.269 | 1 | 2 0 23 | 74.77 | |
| 1.243 | 21 | 2 2 0 | 76.57 | |
| 1.209 | 5 | 1 2 20 | 79.16 | |
| 1.204 | 1 | 0 0 30 | 79.58 | |
| 1.196 | 1 | 0 1 29 | 80.18 | |
| 1.194 | 1 | 1 3 1 | 80.37 | |
| 1.188 | 1 | 2 2 9 | 80.88 | |
| 1.178 | 3 | 1 1 27 | 81.69 | |
| 1.167 | 2 | 2 0 26 | 82.60 | |
| 1.156 | 2 | 2 1 22 | 83.59 | |
| 1.149 | 2 | 2 2 12 | 84.19 | |
| 1.134 | 6 | 1 3 10 | 85.57 | |
| 1.124 | 2 | 1 0 31 | 86.48 | |
| 1.122 | 5 | 3 1 11 | 86.67 | |
| 1.106 | 2 | 0 2 28 | 88.25 | |
| 1.105 | 1 | 2 2 15 | 88.43 | |
| 1.102 | 3 | 0 21 | 88.69 | |
| 1.102 | 3 | 0 3 21 | 88.69 | |
| 1.084 | 2 | 3 1 14 | 90.58 | |
| 1.083 | 5 | 1 1 30 | 90.63 | |
| 1.080 | 2 | 2 1 25 | 90.96 | |
| 1.076 | 4 | 0 1 | 91.41 | |
| 1.075 | 1 | 0 4 2 | 91.57 | |
| 1.057 | 9 | 2 2 18 | 93.59 | |
| 1.054 | 1 | 4 0 7 | 93.92 | |
| 1.047 | 1 | 0 4 8 | 94.70 | |
| 1.041 | 2 | 3 1 17 | 95.44 | |
| 1.039 | 1 | 3 0 24 | 95.74 | |
| 1.039 | 1 | 0 3 24 | 95.74 | |
| 1.025 | 4 | 0 2 31 | 97.50 | |
| 1.007 | 5 | 2 2 21 | 99.74 | |
| 1.003 | 2 | 0 0 36 | 100.34 | |
| .9995 | 1 | 2 0 32 | 100.83 | |
| .9962 | 3 | 3 1 20 | 101.20 | |
| .9890 | 1 | 1 2 29 | 102.31 | |
| .9786 | 1 | 0 3 27 | 103.85 | |
| .9786 | 1 | 3 0 27 | 103.85 | |
| .9658 | 2 | 1 3 22 | 105.80 | |
| .9584 | 1 | 2 2 24 | 106.98 | |
| .9530 | 5 | 3 2 10 | 107.86 | |
| .9525 | 2 | 0 2 34 | 107.94 | |
| .9473 | 4 | 2 1 31 | 108.81 | |
| .9461 | 4 | 2 3 11 | 109.01 | |
| .9398 | 7 | 4 1 0 | 110.10 | |
| .9368 | 2 | 4 0 19 | 110.62 | |
| .9304 | 3 | 2 0 35 | 111.77 | |
| .9302 | 1 | 1 1 36 | 111.80 | |
| .9274 | 1 | 1 2 32 | 112.32 | |
| .9247 | 4 | 0 4 20 | 112.81 | |
| .9227 | 2 | 2 3 14 | 113.20 | |

| d (Å) | I | hkl | 2θ (°) | |
|--------------------------------|----|--------|---------------|--|
| $\lambda = 1.540598\text{\AA}$ | | | | |
| .9224 | 2 | 3 0 30 | 113.26 | |
| .9224 | 2 | 0 3 30 | 113.26 | |
| .9205 | 2 | 1 3 25 | 113.61 | |
| .9150 | 10 | 4 1 9 | 114.67 | |
| .9150 | 10 | 1 4 9 | 114.67 | |
| .9106 | 1 | 2 2 27 | 115.55 | |
| .8971 | 1 | 4 1 12 | 118.34 | |
| .8971 | 1 | 1 4 12 | 118.34 | |
| .8959 | 2 | 2 3 17 | 118.60 | |
| .8895 | 1 | 2 1 34 | 120.00 | |
| .8835 | 2 | 1 0 40 | 121.34 | |
| .8677 | 1 | 1 1 39 | 125.19 | |
| .8667 | 4 | 2 3 20 | 125.43 | |
| .8648 | 6 | 2 2 30 | 125.94 | |
| .8629 | 2 | 0 1 41 | 126.43 | |
| .8620 | 1 | 3 1 29 | 126.67 | |
| .8509 | 1 | 0 4 26 | 129.71 | |
| .8465 | 2 | 3 2 22 | 131.01 | |
| .8378 | 3 | 0 5 10 | 133.67 | |
| .8370 | 1 | 2 1 37 | 133.93 | |
| .8339 | 5 | 1 3 31 | 134.94 | |
| .8331 | 3 | 5 0 11 | 135.21 | |
| .8325 | 1 | 0 2 40 | 135.41 | |
| .8288 | 5 | 3 3 0 | 136.68 | |
| .8265 | 2 | 4 0 28 | 137.50 | |
| .8247 | 8 | 4 1 21 | 138.16 | |
| .8247 | 8 | 1 4 21 | 138.16 | |
| .8222 | 1 | 0 3 36 | 139.05 | |
| .8222 | 1 | 3 0 36 | 139.05 | |
| .8203 | 1 | 3 1 32 | 139.79 | |
| .8170 | 1 | 5 0 14 | 141.07 | |
| .8155 | 2 | 3 2 25 | 141.67 | |
| .8152 | 2 | 2 0 41 | 141.80 | |
| .8137 | 11 | 2 4 1 | 142.41 | |
| .8131 | 2 | 4 2 2 | 142.67 | |
| .8126 | 2 | 1 1 42 | 142.88 | |
| .8117 | 15 | 3 3 9 | 143.25 | |
| .8106 | 2 | 2 4 4 | 143.71 | |
| .8088 | 1 | 4 2 5 | 144.51 | |
| .8062 | 2 | 0 1 44 | 145.69 | |
| .8040 | 3 | 2 4 7 | 146.73 | |
| .8010 | 4 | 4 2 8 | 148.18 | |
| .7991 | 2 | 3 3 12 | 149.15 | |
| .7982 | 2 | 5 0 17 | 149.60 | |
| .7971 | 3 | 4 1 24 | 150.21 | |
| .7971 | 3 | 1 4 24 | 150.21 | |
| .7937 | 2 | 1 3 34 | 152.11 | |
| .7907 | 8 | 4 0 31 | 153.94 | |
| .7900 | 3 | 4 2 11 | 154.37 | |
| .7895 | 9 | 2 1 40 | 154.69 | |

Cobalt gadolinium, CoGd₃

Structure

Orthorhombic, Pnma(62), Z=4, isostructural with CfFe₃, type D0₁₁. The structure was determined by Strydom and Alberts [1970].

Lattice constants: [ibid.]

$$\begin{aligned}a &= 7.05 \text{\AA} \\b &= 9.54 \\c &= 6.32\end{aligned}$$

Density
(calculated) 8.29 g/cm³

Thermal parameters

Isotropic [Strydom and Alberts, op. cit.].

Scattering factors

Co⁰, Gd⁰ [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\begin{aligned}\gamma &= 0.168 \times 10^{-3} \\I/I_c &\text{ (calculated) } 4.41\end{aligned}$$

References

- Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Strydom, O.A.W. and Alberts, L. (1970). J. Less-Common Metals, 22, 511.

| d (Å) | I | hkl | 2θ (°) | λ = 1.540598 Å |
|-------|----|--------|--------|----------------|
| 2.110 | 3 | 2 2 2 | 42.82 | |
| 1.975 | 7 | 2 4 0+ | 45.92 | |
| 1.891 | 2 | 2 3 2 | 48.08 | |
| 1.885 | 3 | 2 4 1 | 48.22 | |
| 1.859 | 16 | 1 2 3 | 48.96 | |
| 1.827 | 3 | 0 5 1 | 49.88 | |
| 1.811 | 3 | 3 3 1+ | 50.40 | |
| 1.777 | 1 | 2 1 3 | 51.40 | |
| 1.768 | 1 | 1 5 1 | 51.66 | |
| 1.754 | 3 | 3 2 2 | 52.12 | |
| 1.704 | 14 | 1 3 3 | 53.74 | |
| 1.698 | 16 | 4 0 1 | 53.96 | |
| 1.678 | 5 | 2 5 0 | 54.66 | |
| 1.671 | 4 | 4 1 1 | 54.80 | |
| 1.653 | 1 | 4 2 0 | 55.54 | |
| 1.622 | 24 | 3 3 2+ | 56.72 | |
| 1.599 | 2 | 4 2 1 | 57.60 | |
| 1.591 | 15 | 1 5 2+ | 57.92 | |
| 1.580 | 3 | 0 0 4 | 58.36 | |
| 1.569 | 10 | 3 0 3 | 58.82 | |
| 1.542 | 17 | 4 3 0+ | 59.96 | |
| 1.490 | 2 | 3 2 3 | 62.26 | |
| 1.482 | 3 | 2 5 2 | 62.64 | |
| 1.479 | 2 | 3 4 2 | 62.80 | |
| 1.467 | 2 | 1 2 4 | 63.36 | |
| 1.465 | 2 | 4 2 2 | 63.44 | |
| 1.442 | 2 | 3 5 1+ | 64.58 | |
| 1.426 | 1 | 2 1 4 | 65.42 | |
| 1.420 | 1 | 0 6 2 | 65.60 | |
| 1.413 | 1 | 2 6 1+ | 66.08 | |
| 1.392 | 3 | 1 6 2 | 67.18 | |
| 1.387 | 6 | 1 5 3+ | 67.50 | |
| 1.380 | 3 | 2 2 4 | 67.84 | |
| 1.362 | 1 | 5 1 1 | 68.88 | |
| 1.341 | 1 | 3 5 2 | 70.10 | |
| 1.332 | 1 | 0 7 1 | 70.64 | |
| 1.322 | 1 | 5 2 1 | 71.26 | |
| 1.317 | 1 | 0 4 4+ | 71.56 | |
| 1.301 | 1 | 4 2 3 | 72.64 | |
| 1.295 | 1 | 4 5 0+ | 73.02 | |
| 1.289 | 2 | 3 6 1 | 73.38 | |
| 1.268 | 1 | 4 5 1 | 74.80 | |
| 1.264 | 1 | 3 2 4 | 75.04 | |
| 1.243 | 4 | 5 2 2+ | 76.58 | |
| 1.234 | 1 | 2 4 4+ | 77.28 | |
| 1.232 | 1 | 1 7 2 | 77.38 | |
| 1.212 | 4 | 3 3 4 | 78.92 | |
| 1.199 | 1 | 1 5 4 | 79.94 | |
| 1.198 | 1 | 4 5 2 | 80.02 | |
| 1.194 | 1 | 5 3 2+ | 80.38 | |

Cobalt gadolinium, CoGd_3 - continued

| d (Å) | I | hkl | | | 20 (°) |
|---------|---|-----|----|----|--------------------------------|
| | | | | | $\lambda = 1.540598\text{\AA}$ |
| 1.190 | 1 | 2 | 0 | 5 | 80.64 |
| 1.181 | 1 | 2 | 1 | 5 | 81.46 |
| 1.175 | 3 | 0 | 3 | 5+ | 81.96 |
| 1.172 | 3 | 5 | 0 | 3 | 82.20 |
| 1.166 | 1 | 6 | 1 | 0 | 82.68 |
| 1.163 | 2 | 5 | 1 | 3 | 82.96 |
| 1.161 | 4 | 4 | 6 | 1 | 83.18 |
| 1.159 | 2 | 1 | 3 | 5 | 83.34 |
| 1.156 | 2 | 1 | 8 | 1 | 83.58 |
| 1.154 | 1 | 2 | 2 | 5 | 83.70 |
| 1.150 | 1 | 2 | 5 | 4 | 84.08 |
| 1.141 | 1 | 6 | 2 | 0+ | 84.94 |
| 1.138 | 1 | 5 | 2 | 3 | 85.20 |
| 1.133 | 1 | 5 | 4 | 2 | 85.66 |
| 1.130 | 2 | 2 | 8 | 0 | 85.98 |
| 1.123 | 1 | 6 | 2 | 1 | 86.64 |
| 1.121 | 1 | 0 | 6 | 4 | 86.84 |
| 1.117 | 3 | 3 | 6 | 3+ | 87.24 |
| 1.112 | 3 | 2 | 8 | 1 | 87.68 |
| 1.107 | 2 | 1 | 6 | 4 | 88.20 |
| 1.103 | 2 | 4 | 3 | 4+ | 88.54 |
| 1.102 | 2 | 1 | 8 | 2+ | 88.70 |
| 1.086 | 2 | 6 | 3 | 1 | 90.38 |
| 1.084 | 1 | 3 | 2 | 5 | 90.56 |
| 1.081 | 1 | 3 | 5 | 4 | 90.92 |
| 1.078 | 1 | 4 | 7 | 0 | 91.20 |
| 1.067 | 1 | 5 | 5 | 2 | 92.40 |
| 1.053 | 1 | 0 | 0 | 6 | 94.00 |
| 1.045 | 1 | 0 | 9 | 1+ | 94.92 |
| 1.042 | 1 | 1 | 5 | 5 | 95.30 |
| 1.027 | 3 | 1 | 8 | 3+ | 97.20 |
| 1.010 | 1 | 2 | 5 | 5 | 99.46 |
| 1.001 | 1 | 6 | 5 | 0 | 100.70 |
| .9985 | 2 | 5 | 5 | 3+ | 100.96 |
| .9882 | 1 | 6 | 5 | 1 | 102.44 |
| .9874 | 1 | 2 | 2 | 6 | 102.52 |
| .9596 | 2 | 7 | 0 | 2 | 106.78 |
| .9540 | 1 | 0 | 10 | 0 | 107.70 |
| .9493 | 1 | 3 | 8 | 3+ | 108.48 |
| .9433 | 1 | 1 | 8 | 4+ | 109.50 |
| .9240 | 1 | 3 | 9 | 2 | 112.94 |
| .9213 | 1 | 5 | 5 | 4 | 113.46 |
| .9189 | 1 | 2 | 8 | 4 | 113.92 |
| .8921 | 1 | 2 | 5 | 6 | 119.42 |
| .8906 | 1 | 4 | 7 | 4+ | 119.88 |
| .8781 | 1 | 0 | 6 | 6 | 122.64 |
| .8749 | 2 | 5 | 8 | 2+ | 123.38 |
| .8737 | 2 | 7 | 3 | 3 | 123.70 |
| .8697 | 1 | 4 | 3 | 6 | 124.68 |
| .8628 | 1 | 4 | 6 | 5 | 126.46 |
| .8586 | 1 | 8 | 2 | 1+ | 127.60 |

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-----|---|---|--------------------------------|
| d (Å) | I | hkl | | | 20 (°) |
| | | | | | $\lambda = 1.540598\text{\AA}$ |
| 4.22 | 1 | 1 | 1 | 1 | 21.03 |
| 3.525 | 1 | 2 | 0 | 0 | 25.24 |
| 3.350 | 23 | 1 | 2 | 1 | 26.5 ^a |
| 3.307 | 16 | 2 | 1 | 0 | 26.94 |
| 3.160 | 12 | 0 | 0 | 2 | 28.22 |
| 3.079 | 20 | 2 | 0 | 1 | 28.98 |
| 2.930 | 46 | 2 | 1 | 1 | 30.49 |
| 2.884 | 48 | 1 | 0 | 2 | 30.99 |
| 2.841 | 100 | 0 | 3 | 1 | 31.47 |
| 2.835 | 57 | 2 | 2 | 0 | 31.53 |
| 2.760 | 69 | 1 | 1 | 2 | 32.41 |
| 2.635 | 42 | 1 | 3 | 1 | 34.00 |
| 2.634 | 14 | 0 | 2 | 2 | 34.00 |
| 2.587 | 61 | 2 | 2 | 1 | 34.65 |
| 2.468 | 19 | 1 | 2 | 2 | 36.38 |
| 2.385 | 9 | 0 | 4 | 0 | 37.69 |
| 2.361 | 21 | 2 | 3 | 0 | 38.08 |
| 2.353 | 4 | 2 | 0 | 2 | 38.22 |
| 2.284 | 11 | 2 | 1 | 2 | 39.41 |
| 2.212 | 2 | 2 | 3 | 1 | 40.76 |
| 2.203 | 20 | 3 | 0 | 1 | 40.94 |
| 2.146 | 11 | 3 | 1 | 1 | 42.07 |
| 2.136 | 3 | 1 | 3 | 2 | 42.27 |
| 2.127 | 2 | 1 | 4 | 1 | 42.46 |
| 2.110 | 4 | 2 | 2 | 2 | 42.82 |
| 2.057 | 1 | 0 | 1 | 3 | 43.98 |
| 1.975 | 6 | 2 | 4 | 0 | 45.90 |
| 1.975 | 5 | 1 | 1 | 3 | 45.92 |
| 1.891 | 2 | 2 | 3 | 2 | 48.06 |
| 1.885 | 3 | 2 | 4 | 1 | 48.23 |
| 1.859 | 24 | 1 | 2 | 3 | 48.96 |
| 1.827 | 4 | 0 | 5 | 1 | 49.89 |
| 1.811 | 3 | 3 | 3 | 1 | 50.35 |
| 1.808 | 2 | 2 | 0 | 3 | 50.42 |
| 1.777 | 1 | 2 | 1 | 3 | 51.39 |
| 1.768 | 1 | 1 | 5 | 1 | 51.65 |
| 1.754 | 4 | 3 | 2 | 2 | 52.11 |
| 1.704 | 20 | 1 | 3 | 3 | 53.75 |
| 1.698 | 19 | 4 | 0 | 1 | 53.97 |
| 1.691 | 1 | 2 | 2 | 3 | 54.20 |
| 1.678 | 8 | 2 | 5 | 0 | 54.65 |
| 1.671 | 3 | 4 | 1 | 1 | 54.88 |
| 1.653 | 1 | 4 | 2 | 0 | 55.54 |
| 1.622 | 24 | 3 | 3 | 2 | 56.71 |
| 1.622 | 13 | 2 | 5 | 1 | 56.72 |
| 1.618 | 2 | 3 | 4 | 1 | 56.85 |
| 1.599 | 1 | 4 | 2 | 1 | 57.58 |
| 1.591 | 15 | 1 | 5 | 2 | 57.91 |
| 1.590 | 10 | 0 | 6 | 0 | 57.95 |
| 1.580 | 3 | 0 | 0 | 4 | 58.36 |

Cobalt gadolinium, CoGd₃ - continued

| d (Å) | I | hkl | | | 2θ (°) λ = 1.540598 Å |
|-------|----|-----|---|---|--------------------------|
| 1.572 | 1 | 2 | 3 | 3 | 58.68 |
| 1.569 | 14 | 3 | 0 | 3 | 58.82 |
| 1.548 | 1 | 3 | 1 | 3 | 59.69 |
| 1.542 | 8 | 1 | 0 | 4 | 59.95 |
| 1.542 | 14 | 4 | 3 | 0 | 59.96 |
| 1.541 | 5 | 1 | 4 | 3 | 59.99 |
| 1.490 | 3 | 3 | 2 | 3 | 62.25 |
| 1.482 | 5 | 2 | 5 | 2 | 62.63 |
| 1.479 | 1 | 3 | 4 | 2 | 62.77 |
| 1.467 | 3 | 1 | 2 | 4 | 63.35 |
| 1.465 | 1 | 4 | 2 | 2 | 63.45 |
| 1.442 | 2 | 3 | 5 | 1 | 64.57 |
| 1.441 | 1 | 2 | 4 | 3 | 64.63 |
| 1.426 | 2 | 2 | 1 | 4 | 65.41 |
| 1.420 | 1 | 0 | 6 | 2 | 65.60 |
| 1.413 | 1 | 2 | 6 | 1 | 66.09 |
| 1.392 | 4 | 1 | 6 | 2 | 67.19 |
| 1.387 | 2 | 1 | 3 | 4 | 67.46 |
| 1.387 | 6 | 1 | 5 | 3 | 67.50 |
| 1.385 | 4 | 4 | 3 | 2 | 67.56 |
| 1.383 | 1 | 4 | 4 | 1 | 67.69 |
| 1.380 | 3 | 2 | 2 | 4 | 67.85 |
| 1.362 | 1 | 5 | 1 | 1 | 68.88 |
| 1.341 | 2 | 3 | 5 | 2 | 70.11 |
| 1.332 | 2 | 0 | 7 | 1 | 70.65 |
| 1.322 | 2 | 5 | 2 | 1 | 71.26 |
| 1.309 | 1 | 1 | 7 | 1 | 72.09 |
| 1.301 | 1 | 4 | 2 | 3 | 72.64 |
| 1.295 | 1 | 4 | 5 | 0 | 73.02 |
| 1.289 | 3 | 3 | 6 | 1 | 73.38 |
| 1.268 | 2 | 4 | 5 | 1 | 74.79 |
| 1.264 | 1 | 3 | 2 | 4 | 75.07 |
| 1.244 | 1 | 1 | 0 | 5 | 76.51 |
| 1.243 | 5 | 5 | 2 | 2 | 76.58 |
| 1.234 | 1 | 2 | 4 | 4 | 77.26 |
| 1.232 | 1 | 1 | 7 | 2 | 77.39 |
| 1.212 | 7 | 3 | 3 | 4 | 78.91 |
| 1.212 | 1 | 3 | 5 | 3 | 78.95 |
| 1.199 | 1 | 1 | 5 | 4 | 79.93 |
| 1.198 | 1 | 4 | 5 | 2 | 80.03 |
| 1.194 | 1 | 5 | 3 | 2 | 80.39 |
| 1.190 | 1 | 2 | 0 | 5 | 80.69 |
| 1.181 | 2 | 2 | 1 | 5 | 81.45 |
| 1.175 | 1 | 6 | 0 | 0 | 81.93 |
| 1.175 | 4 | 0 | 3 | 5 | 81.96 |
| 1.172 | 1 | 5 | 0 | 3 | 82.20 |
| 1.166 | 1 | 6 | 1 | 0 | 82.68 |
| 1.163 | 3 | 5 | 1 | 3 | 82.95 |
| 1.161 | 5 | 4 | 6 | 1 | 83.17 |
| 1.159 | 1 | 1 | 3 | 5 | 83.34 |

| d (Å) | I | hkl | | | 2θ (°) λ = 1.540598 Å |
|-------|---|-----|----|---|--------------------------|
| 1.156 | 1 | 1 | 8 | 1 | 83.58 |
| 1.154 | 1 | 2 | 2 | 5 | 83.71 |
| 1.150 | 1 | 2 | 5 | 4 | 84.08 |
| 1.141 | 1 | 6 | 2 | 0 | 84.93 |
| 1.138 | 1 | 5 | 2 | 3 | 85.21 |
| 1.133 | 1 | 5 | 4 | 2 | 85.66 |
| 1.130 | 2 | 2 | 8 | 0 | 85.99 |
| 1.123 | 1 | 6 | 2 | 1 | 86.64 |
| 1.121 | 1 | 0 | 6 | 4 | 86.83 |
| 1.117 | 4 | 3 | 5 | 3 | 87.23 |
| 1.116 | 1 | 5 | 5 | 1 | 87.28 |
| 1.116 | 1 | 0 | 8 | 2 | 87.33 |
| 1.112 | 4 | 2 | 8 | 1 | 87.69 |
| 1.107 | 2 | 1 | 6 | 4 | 88.20 |
| 1.105 | 1 | 3 | 7 | 2 | 88.43 |
| 1.103 | 2 | 4 | 3 | 4 | 88.55 |
| 1.102 | 2 | 1 | 8 | 2 | 88.70 |
| 1.101 | 1 | 6 | 0 | 2 | 88.76 |
| 1.086 | 2 | 6 | 3 | 1 | 90.38 |
| 1.084 | 1 | 3 | 2 | 5 | 90.56 |
| 1.081 | 2 | 3 | 5 | 4 | 90.93 |
| 1.078 | 1 | 4 | 7 | 0 | 91.20 |
| 1.067 | 1 | 5 | 5 | 2 | 92.39 |
| 1.053 | 1 | 0 | 0 | 6 | 93.99 |
| 1.045 | 1 | 0 | 9 | 1 | 94.93 |
| 1.042 | 1 | 1 | 5 | 5 | 95.31 |
| 1.027 | 1 | 5 | 2 | 4 | 97.15 |
| 1.027 | 2 | 4 | 0 | 5 | 97.17 |
| 1.027 | 3 | 1 | 8 | 3 | 97.23 |
| 1.010 | 2 | 2 | 5 | 5 | 99.45 |
| 1.001 | 1 | 6 | 5 | 0 | 100.60 |
| .9985 | 3 | 5 | 5 | 3 | 100.97 |
| .9882 | 1 | 6 | 5 | 1 | 102.43 |
| .9874 | 1 | 2 | 2 | 6 | 102.55 |
| .9620 | 1 | 2 | 3 | 6 | 106.41 |
| .9596 | 2 | 7 | 0 | 2 | 106.79 |
| .9540 | 1 | 0 | 10 | 0 | 107.69 |
| .9493 | 1 | 3 | 8 | 3 | 108.47 |
| .9492 | 1 | 7 | 3 | 1 | 108.48 |
| .9433 | 1 | 1 | 8 | 4 | 109.50 |
| .9268 | 1 | 0 | 7 | 5 | 112.44 |
| .9240 | 1 | 3 | 9 | 2 | 112.95 |
| .9213 | 1 | 5 | 5 | 4 | 113.47 |
| .9189 | 1 | 2 | 8 | 4 | 113.92 |
| .9084 | 1 | 4 | 9 | 0 | 115.90 |
| .9025 | 1 | 5 | 3 | 5 | 117.20 |
| .8921 | 2 | 2 | 5 | 6 | 119.41 |
| .8802 | 1 | 1 | 2 | 7 | 122.13 |
| .8781 | 1 | 0 | 6 | 6 | 122.62 |
| .8749 | 3 | 5 | 8 | 2 | 123.39 |

Cobalt gadolinium, Co₂Gd

Structure

Cubic, Fd3m(227), Z=8, C15 type, isostructural with Cu₂Mg [Wernick and Geller, 1960].

Lattice constant: [ibid.]

$$a = 7.255(5)\text{\AA}$$

Density

(calculated) 9.571 g/cm³

Thermal parameters

Overall isotropic B = 1.0

Scattering factors

Co⁰ and Gd⁰ [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)

$$\gamma = 0.372 \times 10^{-3}$$

$$I/I_c \text{ (calculated} = 8.83$$

References

Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.

Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.

Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-----|---|---|----------------|
| d (Å) | I | hkl | | | 2θ (°) |
| | | | | | λ = 1.540598 Å |
| 4.19 | 10 | 1 | 1 | 1 | 21.19 |
| 2.565 | 63 | 2 | 2 | 0 | 34.95 |
| 2.187 | 100 | 3 | 1 | 1 | 41.24 |
| 2.094 | 17 | 2 | 2 | 2 | 43.16 |
| 1.664 | 2 | 3 | 3 | 1 | 55.14 |
| 1.481 | 18 | 4 | 2 | 2 | 62.68 |
| 1.396 | 19 | 5 | 1 | 1 | 66.97 |
| 1.396 | 6 | 3 | 3 | 3 | 66.97 |
| 1.283 | 18 | 4 | 4 | 0 | 73.83 |
| 1.226 | 1 | 5 | 3 | 1 | 77.83 |
| 1.147 | 7 | 6 | 2 | 0 | 84.37 |
| 1.106 | 8 | 5 | 3 | 3 | 88.25 |
| 1.094 | 4 | 6 | 2 | 2 | 89.54 |
| .969 | 9 | 6 | 4 | 2 | 105.22 |
| .945 | 10 | 7 | 3 | 1 | 109.28 |
| .945 | 5 | 5 | 5 | 3 | 109.28 |
| .907 | 3 | 8 | 0 | 0 | 116.29 |
| .855 | 2 | 6 | 6 | 0 | 128.56 |
| .855 | 4 | 8 | 2 | 2 | 128.56 |
| .838 | 11 | 7 | 5 | 1 | 133.71 |
| .838 | 2 | 5 | 5 | 5 | 133.71 |
| .832 | 3 | 6 | 6 | 2 | 135.52 |
| .796 | 1 | 7 | 5 | 3 | 150.61 |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|-----|---|---|----------------|
| d (Å) | I | hkl | | | 2θ (°) |
| | | | | | λ = 1.540598 Å |
| 4.19 | 12 | 1 | 1 | 1 | 21.20 |
| 2.564 | 64 | 2 | 2 | 0 | 34.96 |
| 2.187 | 100 | 3 | 1 | 1 | 41.24 |
| 2.094 | 17 | 2 | 2 | 2 | 43.16 |
| 1.664 | 2 | 3 | 3 | 1 | 55.14 |
| 1.481 | 15 | 4 | 2 | 2 | 62.68 |
| 1.396 | 19 | 5 | 1 | 1 | 66.96 |
| 1.283 | 13 | 4 | 4 | 0 | 73.82 |
| 1.226 | 1 | 5 | 3 | 1 | 77.82 |
| 1.147 | 4 | 6 | 2 | 0 | 84.36 |
| 1.106 | 5 | 5 | 3 | 3 | 88.26 |
| 1.094 | 3 | 6 | 2 | 2 | 89.54 |
| .970 | 5 | 6 | 4 | 2 | 105.22 |
| .945 | 8 | 7 | 3 | 1 | 109.28 |
| .907 | 2 | 8 | 0 | 0 | 116.30 |
| .855 | 3 | 8 | 2 | 2 | 128.56 |
| .838 | 5 | 7 | 5 | 1 | 133.70 |
| .832 | 1 | 6 | 6 | 2 | 135.52 |

Cobalt gadolinium, Co_7Gd_2

Structure

Hexagonal, $\bar{R}\bar{3}m(166)$, $Z = 6$. The structure was determined by Bertaut et al. [1965].

Lattice constants: [Ostertag, 1967]

$$\begin{aligned} a &= 5.023 \text{\AA} \\ c &= 36.29 \end{aligned}$$

Density
(calculated) 9.135 g/cm^3

Thermal parameters

Isotropic [Bertaut et al., op. cit.]

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

Scale factors (integrated intensities)

$$\begin{aligned} \gamma &= 0.302 \times 10^{-3} \\ I/I_c \text{ (calculated)} &= 6.84 \end{aligned}$$

References

Bertaut, E. F., Lemaire, F. G. R., and Schweizer, J. (1965). C. R. Acad. Sci. 260, 3595.

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

Ostertag, W. (1967). J. Less-Common Metals, 13, 385.

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|--------|---------------------------|---------------------------------|--|
| $d(\text{\AA})$ | I | hkl | $2\theta (\text{^\circ})$ | $\lambda = 1.540598 \text{\AA}$ | |
| 12.10 | 7 | 0 0 3 | 7.30 | | |
| 4.319 | 7 | 1 0 1 | 20.56 | | |
| 4.032 | 6 | 0 0 9 | 22.04 | | |
| 3.922 | 3 | 1 0 4 | 22.66 | | |
| 3.140 | 4 | 0 1 8 | 28.42 | | |
| 3.024 | 1 | 0 0 12 | 29.52 | | |
| 2.787 | 43 | 1 0 10 | 32.10 | | |
| 2.629 | 25 | 0 1 11 | 34.08 | | |
| 2.512 | 50 | 1 1 0 | 35.72 | | |
| 2.459 | 1 | 1 1 3 | 36.52 | | |
| 2.419 | 1 | 0 0 15 | 37.14 | | |
| 2.349 | 4 | 1 0 13 | 38.28 | | |
| 2.227 | 10 | 0 1 14 | 40.48 | | |
| 2.171 | 35 | 0 2 1 | 41.56 | | |
| 2.132 | 100 | 1 1 9 | 42.36 | | |
| 2.115 | 11 | 0 2 4 | 42.70 | | |
| 2.083 | 4 | 2 0 5 | 43.40 | | |
| 2.016 | 16 | 0 0 18 | 44.92 | | |
| 2.006 | 8 | 0 2 7 | 45.16 | | |
| 1.961 | 9 | 2 0 8 | 46.26 | | |

| $d(\text{\AA})$ | $^\circ$ | I | hkl | $2\theta (\text{^\circ})$ | $\lambda = 1.540598 \text{\AA}$ |
|-----------------|----------|----|---------|---------------------------|---------------------------------|
| 1.932 | | 2 | 1 1 12 | 47.00 | |
| 1.916 | | 5 | 0 1 17 | 47.40 | |
| 1.816 | | 1 | 2 0 11 | 50.20 | |
| 1.742 | | 3 | 1 1 15 | 52.48 | |
| 1.728 | | 2 | 0 0 21 | 52.94 | |
| 1.675 | | 4 | 0 1 20 | 54.78 | |
| 1.666 | | 1 | 2 0 14 | 55.06 | |
| 1.642 | | 1 | 2 1 1 | 55.94 | |
| 1.572 | | 4 | 1 1 18 | 58.68 | |
| 1.546 | | 1 | 1 2 8 | 59.78 | |
| 1.524 | | 1 | 2 0 17 | 60.74 | |
| 1.512 | | 1 | 0 0 24 | 61.26 | |
| 1.498 | | 10 | 2 1 10 | 61.90 | |
| 1.483 | | 2 | 0 1 23 | 62.58 | |
| 1.472 | | 7 | 1 2 11 | 63.14 | |
| 1.450 | | 7 | 3 0 0 | 64.18 | |
| 1.435 | | 7 | 0 2 19 | 64.92 | |
| 1.424 | | 5 | 1 1 21 | 65.52 | |
| 1.417 | | 2 | 2 1 13 | 65.86 | |
| 1.393 | | 7 | 2 0 20 | 67.12 | |
| 1.388 | | 5 | 1 2 14 | 67.38 | |
| 1.377 | | 1 | 1 0 25 | 68.04 | |
| 1.364 | | 18 | 0 3 9+ | 68.74 | |
| 1.303 | | 2 | 1 2 17 | 72.50 | |
| 1.205 | | 4 | 1 1 24 | 72.98 | |
| 1.277 | | 2 | 2 0 23 | 74.18 | |
| 1.256 | | 15 | 2 2 0 | 75.68 | |
| 1.244 | | 1 | 3 0 15+ | 76.54 | |
| 1.218 | | 3 | 1 2 20 | 78.44 | |
| 1.210 | | 1 | 0 0 30 | 79.10 | |
| 1.203 | | 1 | 1 1 29 | 79.66 | |
| 1.190 | | 1 | 2 2 9 | 79.94 | |
| 1.185 | | 2 | 1 1 27 | 81.08 | |
| 1.177 | | 1 | 3 0 18+ | 81.74 | |
| 1.175 | | 2 | 0 0 26 | 81.96 | |
| 1.145 | | 4 | 1 3 10 | 84.58 | |
| 1.138 | | 1 | 1 2 23 | 85.16 | |
| 1.133 | | 3 | 3 1 11 | 85.66 | |
| 1.113 | | 1 | 0 2 28+ | 87.56 | |
| 1.111 | | 3 | 0 3 21+ | 87.82 | |
| 1.094 | | 2 | 3 1 14 | 89.54 | |
| 1.090 | | 3 | 1 1 30 | 89.96 | |
| 1.087 | | 4 | 4 0 1+ | 90.24 | |
| 1.066 | | 8 | 2 2 18 | 92.56 | |
| 1.058 | | 1 | 0 4 8 | 93.50 | |
| 1.050 | | 1 | 3 1 17 | 94.34 | |
| 1.047 | | 2 | 0 3 24+ | 94.78 | |
| 1.037 | | 1 | 1 0 34 | 96.00 | |
| 1.021 | | 1 | 0 2 31 | 96.70 | |
| 1.016 | | 2 | 2 2 21 | 98.62 | |

Cobalt gadolinium, Co_7Gd_2 - continued

| $d(\text{\AA})$ | I | hkl | 20($^{\circ}$) | |
|-----------------|----|---------|--------------------------------|---|
| | | | $\lambda = 1.540598\text{\AA}$ | % |
| 1.007 | 2 | 1 1 33+ | 99.74 | |
| 1.005 | 2 | 3 1 20 | 100.12 | |
| .9958 | 1 | 1 2 29 | 101.36 | |
| .9857 | 1 | 0 3 27+ | 102.78 | |
| .9660 | 1 | 2 2 24 | 105.76 | |
| | | | | |
| .9622 | 3 | 3 2 10 | 106.36 | |
| .9582 | 2 | 0 2 34+ | 107.00 | |
| .9552 | 2 | 2 3 11 | 107.48 | |
| .9536 | 1 | 2 1 31 | 107.76 | |
| .9493 | 4 | 4 1 0 | 108.48 | |
| | | | | |
| .9451 | 2 | 4 0 19 | 109.12 | |
| .9359 | 1 | 2 0 35+ | 110.78 | |
| .9328 | 2 | 0 4 20 | 111.34 | |
| .9313 | 2 | 2 3 14 | 111.60 | |
| .9289 | 3 | 3 0 30+ | 112.04 | |
| | | | | |
| .9278 | 1 | 1 3 25 | 112.22 | |
| .9240 | 11 | 1 4 9+ | 112.96 | |
| .8953 | 2 | 2 1 34+ | 118.72 | |
| .8881 | 1 | 1 0 40 | 120.30 | |
| .8762 | 1 | 3 0 33+ | 123.08 | |
| | | | | |
| .8744 | 2 | 2 3 20 | 123.52 | |
| .8726 | 2 | 1 1 39 | 124.00 | |
| .8712 | 2 | 2 2 30 | 124.30 | |
| .8686 | 2 | 3 1 20 | 124.96 | |
| .8588 | 1 | 1 4 18+ | 127.52 | |
| | | | | |
| .8579 | 1 | 0 4 26 | 127.78 | |
| .8460 | 1 | 0 5 10 | 131.14 | |
| .8434 | 1 | 2 3 23 | 131.92 | |
| .8412 | 1 | 5 0 11 | 132.60 | |
| .8402 | 1 | 1 3 31 | 132.94 | |
| | | | | |
| .8372 | 2 | 3 3 0+ | 133.88 | |
| .8320 | 2 | 4 1 21+ | 135.60 | |
| .8285 | 1 | 1 0 43 | 136.80 | |
| .8273 | 1 | 2 2 33 | 137.20 | |
| .8219 | 3 | 2 4 1 | 139.18 | |
| | | | | |
| .8197 | 6 | 3 3 0 | 140.00 | |
| .8103 | 1 | 0 1 44 | 143.84 | |
| .8089 | 1 | 4 2 8 | 144.46 | |
| .8040 | 3 | 4 1 24+ | 146.72 | |
| .7994 | 1 | 1 3 34 | 148.98 | |
| | | | | |
| .7977 | 1 | 4 2 11 | 150.00 | |
| .7968 | 1 | 4 0 31 | 150.38 | |
| .7943 | 1 | 2 1 40 | 151.74 | |
| .7861 | 4 | 2 2 36 | 156.98 | |
| .7831 | 1 | 0 3 39+ | 159.22 | |

| Calculated Pattern (Integrated) | | | | |
|---------------------------------|-----|--------|--------------------------------|--|
| $d(\text{\AA})$ | I | hkl | 20($^{\circ}$) | |
| | | | $\lambda = 1.540598\text{\AA}$ | |
| 12.10 | 5 | 0 0 3 | 7.30 | |
| 4.319 | 6 | 1 0 1 | 20.55 | |
| 4.032 | 5 | 0 0 9 | 22.03 | |
| 3.922 | 3 | 1 0 4 | 22.65 | |
| 3.140 | 4 | 0 1 8 | 28.40 | |
| | | | | |
| 3.024 | 1 | 0 0 12 | 29.51 | |
| 2.787 | 40 | 1 0 10 | 32.09 | |
| 2.629 | 24 | 0 1 11 | 34.08 | |
| 2.512 | 48 | 1 1 0 | 35.72 | |
| 2.459 | 1 | 1 1 3 | 36.51 | |
| | | | | |
| 2.419 | 1 | 0 0 15 | 37.13 | |
| 2.349 | 4 | 1 0 13 | 38.29 | |
| 2.227 | 10 | 0 1 14 | 40.48 | |
| 2.171 | 33 | 0 2 1 | 41.56 | |
| 2.160 | 7 | 2 0 2 | 41.79 | |
| | | | | |
| 2.132 | 100 | 1 1 9 | 42.36 | |
| 2.115 | 5 | 0 2 4 | 42.72 | |
| 2.083 | 3 | 2 0 5 | 43.40 | |
| 2.016 | 16 | 0 0 18 | 44.92 | |
| 2.006 | 5 | 0 2 7 | 45.17 | |
| | | | | |
| 1.961 | 9 | 2 0 8 | 46.25 | |
| 1.932 | 2 | 1 1 12 | 46.99 | |
| 1.916 | 5 | 0 1 17 | 47.40 | |
| 1.816 | 1 | 2 0 11 | 50.20 | |
| 1.742 | 3 | 1 1 15 | 52.47 | |
| | | | | |
| 1.728 | 2 | 0 0 21 | 52.94 | |
| 1.675 | 5 | 0 1 20 | 54.77 | |
| 1.666 | 1 | 2 0 14 | 55.07 | |
| 1.642 | 1 | 2 1 1 | 55.94 | |
| 1.572 | 4 | 1 1 18 | 58.67 | |
| | | | | |
| 1.570 | 1 | 0 2 16 | 58.77 | |
| 1.546 | 1 | 1 2 8 | 59.78 | |
| 1.524 | 1 | 2 0 17 | 60.74 | |
| 1.512 | 1 | 0 0 24 | 61.25 | |
| 1.498 | 11 | 2 1 10 | 61.91 | |
| | | | | |
| 1.483 | 1 | 0 1 23 | 62.57 | |
| 1.472 | 7 | 1 2 11 | 63.12 | |
| 1.450 | 8 | 3 0 0 | 64.18 | |
| 1.435 | 7 | 0 2 19 | 64.92 | |
| 1.424 | 6 | 1 1 21 | 65.51 | |
| | | | | |
| 1.417 | 1 | 2 1 13 | 65.88 | |
| 1.393 | 7 | 2 0 20 | 67.12 | |
| 1.398 | 4 | 1 2 14 | 67.39 | |
| 1.377 | 1 | 1 0 25 | 68.03 | |
| 1.364 | 10 | 3 0 9 | 68.74 | |
| | | | | |
| 1.364 | 10 | 0 3 9 | 68.74 | |
| 1.303 | 2 | 1 2 17 | 72.51 | |
| 1.295 | 4 | 1 1 24 | 72.97 | |
| 1.277 | 2 | 2 0 23 | 74.19 | |
| 1.256 | 17 | 2 2 0 | 75.67 | |

Cobalt gadolinium, Co_7Gd_2 - continued

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ | $\lambda = 1.540598\text{\AA}$ |
|-----------------|---|--------|---------------------------|--------------------------------|
| 1.218 | 3 | 1 2 20 | 78.4 ² | |
| 1.210 | 1 | 0 0 30 | 79.11 | |
| 1.203 | 1 | 0 1 29 | 79.66 | |
| 1.199 | 1 | 2 2 9 | 79.95 | |
| 1.185 | 3 | 1 1 27 | 81.00 | |
| 1.175 | 2 | 2 0 26 | 81.95 | |
| 1.145 | 4 | 1 3 10 | 84.57 | |
| 1.138 | 1 | 1 2 23 | 85.16 | |
| 1.133 | 3 | 3 1 11 | 85.66 | |
| 1.113 | 1 | 0 2 28 | 87.55 | |
| 1.111 | 1 | 0 3 21 | 87.81 | |
| 1.111 | 1 | 3 0 21 | 87.81 | |
| 1.094 | 2 | 3 1 14 | 89.54 | |
| 1.090 | 4 | 1 1 30 | 89.95 | |
| 1.088 | 1 | 2 1 25 | 90.13 | |
| 1.097 | 3 | 4 0 1 | 90.25 | |
| 1.066 | 9 | 2 2 18 | 92.55 | |
| 1.058 | 1 | 0 4 8 | 93.50 | |
| 1.050 | 1 | 3 1 17 | 94.34 | |
| 1.047 | 1 | 3 0 24 | 94.79 | |
| 1.047 | 1 | 0 3 24 | 94.79 | |
| 1.037 | 1 | 1 0 34 | 95.99 | |
| 1.031 | 1 | 0 2 31 | 96.71 | |
| 1.016 | 2 | 2 2 21 | 98.62 | |
| 1.008 | 1 | 0 0 36 | 99.66 | |
| 1.007 | 2 | 1 1 33 | 99.76 | |
| 1.005 | 2 | 3 1 20 | 100.12 | |
| .9958 | 2 | 1 2 29 | 101.35 | |
| .9857 | 1 | 3 0 27 | 102.70 | |
| .9857 | 1 | 0 3 27 | 102.70 | |
| .9660 | 2 | 2 2 24 | 105.76 | |
| .9622 | 3 | 3 2 10 | 106.36 | |
| .9584 | 1 | 3 1 23 | 106.98 | |
| .9582 | 2 | 0 2 34 | 107.01 | |
| .9552 | 2 | 2 3 11 | 107.40 | |
| .9536 | 1 | 2 1 31 | 107.76 | |
| .9493 | 5 | 4 1 0 | 108.49 | |
| .9451 | 2 | 4 0 10 | 109.10 | |
| .9359 | 1 | 2 0 35 | 110.78 | |
| .9328 | 2 | 0 4 20 | 111.34 | |
| .9313 | 1 | 2 3 14 | 111.60 | |
| .9289 | 1 | 3 0 30 | 112.05 | |
| .9289 | 1 | 0 3 30 | 112.05 | |
| .9278 | 1 | 1 3 25 | 112.24 | |
| .9240 | 7 | 4 1 0 | 112.95 | |
| .9240 | 7 | 1 4 0 | 112.95 | |
| .9041 | 1 | 2 3 17 | 116.87 | |
| .9054 | 1 | 0 4 23 | 118.60 | |
| .9953 | 2 | 2 1 34 | 118.73 | |
| .8881 | 1 | 1 0 40 | 120.30 | |

| $d(\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ | $\lambda = 1.540598\text{\AA}$ |
|-----------------|----|--------|---------------------------|--------------------------------|
| .8762 | 1 | 0 3 33 | 123.07 | |
| .8762 | 1 | 3 0 33 | 123.07 | |
| .8744 | 2 | 2 3 20 | 123.50 | |
| .8726 | 1 | 1 1 30 | 123.97 | |
| .8712 | 3 | 2 2 30 | 124.30 | |
| .8686 | 2 | 3 1 20 | 124.97 | |
| .8588 | 1 | 4 1 18 | 127.51 | |
| .8588 | 1 | 1 4 18 | 127.51 | |
| .8579 | 1 | 0 4 26 | 127.78 | |
| .8460 | 2 | 0 5 10 | 131.14 | |
| .8434 | 1 | 2 3 23 | 131.93 | |
| .8423 | 1 | 2 1 37 | 132.27 | |
| .8412 | 1 | 5 0 11 | 132.60 | |
| .8402 | 1 | 1 3 31 | 132.94 | |
| .8372 | 3 | 3 3 0 | 133.89 | |
| .8331 | 1 | 4 0 28 | 135.23 | |
| .8320 | 2 | 4 1 21 | 135.59 | |
| .8320 | 2 | 1 4 21 | 135.59 | |
| .8285 | 2 | 1 0 43 | 136.70 | |
| .8273 | 2 | 2 2 33 | 137.21 | |
| .8248 | 1 | 5 0 14 | 138.11 | |
| .8224 | 1 | 3 2 25 | 139.00 | |
| .8219 | 6 | 2 4 1 | 139.10 | |
| .8212 | 1 | 4 2 2 | 139.43 | |
| .8197 | 9 | 3 3 9 | 140.02 | |
| .8187 | 1 | 2 4 4 | 140.30 | |
| .8110 | 1 | 2 4 7 | 143.14 | |
| .8103 | 2 | 0 1 44 | 143.83 | |
| .8089 | 1 | 4 2 8 | 144.45 | |
| .8040 | 3 | 1 4 24 | 146.72 | |
| .8040 | 3 | 4 1 24 | 146.72 | |
| .7904 | 3 | 1 3 34 | 148.98 | |
| .7977 | 1 | 4 2 11 | 149.88 | |
| .7968 | 2 | 4 0 31 | 150.30 | |
| .7943 | 4 | 2 1 40 | 151.73 | |
| .7911 | 1 | 3 3 15 | 153.64 | |
| .7968 | 1 | 0 2 43 | 156.40 | |
| .7861 | 12 | 2 2 36 | 156.98 | |
| .7845 | 2 | 5 0 20 | 158.17 | |
| .7836 | 1 | 4 2 14 | 158.84 | |
| .7831 | 2 | 0 3 30 | 159.23 | |
| .7831 | 2 | 3 0 39 | 159.23 | |

Cobalt gallium manganese, Co_2GaMn

Structure

Cubic, Fm3m(225), Z=4, Heusler alloy, type L₂1,
from powder data (x-ray and neutron) [Webster,
1971].

Lattice constant: [ibid.]

$$a = 5.770 \text{\AA}$$

Density

(calculated) 8.383 g/cm³

| d(\text{\AA}) | I | Calculated Pattern (Integrated) | | | $2\theta(^{\circ})$ $\lambda = 1.540598 \text{\AA}$ |
|---------------|-----|---------------------------------|---|---|--|
| | | h | k | l | |
| 3.331 | 1 | 1 | 1 | 1 | 26.74 |
| 2.040 | 100 | 2 | 2 | 0 | 44.37 |
| 1.4425 | 13 | 4 | 0 | 0 | 64.55 |
| 1.1778 | 23 | 4 | 2 | 2 | 81.69 |
| 1.0200 | 7 | 4 | 4 | 0 | 98.08 |
| .9123 | 11 | 6 | 2 | 0 | 115.20 |
| .8328 | 4 | 4 | 4 | 4 | 135.31 |

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co^0 , Ga^0 , Mn^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 0.851 \times 10^{-3}$$

$$I/I_C \text{ (calculated)} = 12.4$$

References

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

Webster, P.J. (1971). J. Phys. Chem. Solids, 32, 1221.

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|-------|---------------------|--|---------------------------------|
| d(\text{\AA}) | I | hkl | $2\theta(^{\circ})$ | | $\lambda = 1.540598 \text{\AA}$ |
| 3.331 | 1 | 1 1 1 | 26.74 | | |
| 2.040 | 100 | 2 2 0 | 44.37 | | |
| 1.4425 | 12 | 4 0 0 | 64.56 | | |
| 1.1778 | 20 | 4 2 2 | 81.70 | | |
| 1.0200 | 6 | 4 4 0 | 98.08 | | |
| .9123 | 8 | 6 2 0 | 115.20 | | |
| .8328 | 2 | 4 4 4 | 135.32 | | |

Cobalt gallium tantalum, Co_2GaTa

Structure

Cubic, $\text{Fm}3\text{m}(225)$, $Z=4$, Heusler alloy, type L₂1,
from powder data [Markiv et al., 1965].

Lattice constant: [ibid.]

$$a = 5.923 \text{\AA}$$

Density

(calculated) 11.780 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Ga^0 , Ta^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 1.56 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 18.7$$

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.

| $d(\text{\AA})$ | I | Calculated Pattern (Integrated) | | | $2\theta (\text{^\circ})$ |
|-----------------|-----|---------------------------------|---|---|---------------------------|
| | | h | k | l | |
| 3.420 | 21 | 1 | 1 | 1 | 26.04 |
| 2.961 | 16 | 2 | 0 | 0 | 30.15 |
| 2.094 | 100 | 2 | 2 | 0 | 43.17 |
| 1.786 | 10 | 3 | 1 | 1 | 51.10 |
| 1.710 | 4 | 2 | 2 | 2 | 53.55 |
| 1.481 | 14 | 4 | 0 | 0 | 62.69 |
| 1.359 | 4 | 3 | 3 | 1 | 69.07 |
| 1.324 | 5 | 4 | 2 | 0 | 71.12 |
| 1.209 | 26 | 4 | 2 | 2 | 79.16 |
| 1.140 | 2 | 5 | 1 | 1 | 85.03 |
| 1.140 | 1 | 3 | 3 | 3 | 85.03 |
| 1.047 | 8 | 4 | 4 | 0 | 94.73 |
| 1.001 | 3 | 5 | 3 | 1 | 100.60 |
| .9872 | 2 | 4 | 4 | 2 | 102.58 |
| .9365 | 13 | 6 | 2 | 0 | 110.68 |
| .9032 | 1 | 5 | 3 | 3 | 117.04 |
| .8929 | 2 | 6 | 2 | 2 | 119.24 |
| .8549 | 4 | 4 | 4 | 4 | 128.59 |
| .8294 | 2 | 5 | 5 | 1 | 136.49 |
| .8204 | 2 | 7 | 1 | 1 | 136.49 |
| .8214 | 3 | 6 | 4 | 0 | 139.38 |
| .7915 | 43 | 6 | 4 | 2 | 153.42 |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|---|---|----|---------------------------|
| $d(\text{\AA})$ | I | h | k | l | $2\theta (\text{^\circ})$ |
| 3.420 | 24 | 1 | 1 | 1 | 26.04 |
| 2.961 | 18 | 2 | 0 | 0 | 30.16 |
| 2.094 | 100 | 2 | 2 | 0 | 43.16 |
| 1.786 | 10 | 3 | 1 | 1 | 51.10 |
| 1.710 | 4 | 2 | 2 | 2 | 53.56 |
| 1.481 | 13 | 4 | 0 | 0 | 62.70 |
| 1.359 | 3 | 3 | 3 | 1 | 69.06 |
| 1.324 | 5 | 4 | 2 | 0 | 71.12 |
| 1.209 | 22 | 4 | 2 | 2 | 79.16 |
| 1.140 | 2 | 5 | 1 | 1+ | 85.03 |
| 1.047 | 6 | 4 | 4 | 0 | 94.74 |
| 1.001 | 3 | 5 | 3 | 1 | 100.60 |
| .9872 | 2 | 4 | 4 | 2+ | 102.58 |
| .9365 | 10 | 6 | 2 | 0 | 110.68 |
| .9032 | 1 | 5 | 3 | 3 | 117.04 |
| .8929 | 2 | 6 | 2 | 2 | 119.24 |
| .8549 | 3 | 4 | 4 | 4 | 128.59 |
| .8294 | 2 | 7 | 1 | 1+ | 136.49 |
| .8214 | 1 | 6 | 4 | 0 | 139.38 |
| .7915 | 16 | 6 | 4 | 2 | 153.42 |

Cobalt gallium titanium, Co_2GaTi

Structure

Cubic, Fm3m, Z=4, Heusler alloy, type L₂₁, from powder data (x-ray and neutron) [Webster and Ziebeck, 1973].

Lattice constant: [ibid.]

$$a = 5.848 \text{\AA}$$

Density

(calculated) 7.818 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co^0 , Ga^0 , Ti^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 0.885 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 11.9$$

References

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

Webster, P. J. and Ziebeck, K. R. A. (1973). J. Phys. Chem. Solids, 34, 1647.

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-----|---|--------|----------------|
| d (Å) | I | hkl | | 2θ (°) | λ = 1.540598 Å |
| 3.376 | 3 | 1 | 1 | 1 | 26.3° |
| 2.068 | 100 | 2 | 2 | 0 | 43.75 |
| 1.7632 | 2 | 3 | 1 | 1 | 51.81 |
| 1.4620 | 13 | 4 | 0 | 0 | 63.5° |
| 1.1937 | 23 | 4 | 2 | 2 | 80.3° |
| 1.0338 | 7 | 4 | 4 | 0 | 96.34 |
| .9246 | 11 | 6 | 2 | 0 | 112.83 |
| .8441 | 4 | 4 | 4 | 4 | 131.73 |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|-----|---|--------|----------------|
| d (Å) | I | hkl | | 2θ (°) | λ = 1.540598 Å |
| 3.376 | 3 | 1 | 1 | 1 | 26.3° |
| 2.068 | 100 | 2 | 2 | 0 | 43.76 |
| 1.7632 | 1 | 3 | 1 | 1 | 51.82 |
| 1.4620 | 12 | 4 | 0 | 0 | 63.6° |
| 1.1937 | 20 | 4 | 2 | 2 | 80.3° |
| 1.0338 | 6 | 4 | 4 | 0 | 96.34 |
| .9246 | 8 | 6 | 2 | 0 | 112.84 |
| .8441 | 2 | 4 | 4 | 4 | 131.72 |

Cobalt gallium vanadium, Co_2GaV

Structure

Cubic, $\text{Fm}3\bar{m}$ (225), $Z=4$, Heusler alloy, type L₂₁, from powder data (x-ray and neutron) [Ziebeck and Webster, 1974].

Lattice constant: [ibid.]

$$a = 5.786 \text{\AA}$$

Density

(measured) 8.15 g/cm^3 [ibid.]

(calculated) 8.177 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Ga^0 , V^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 0.893 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 12.0$$

References

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.

| $d(\text{\AA})$ | I | Calculated Pattern (Integrated) | | | $2\theta (\text{^\circ})$ | $\lambda = 1.540598 \text{\AA}$ |
|-----------------|-----|---------------------------------|---|---|---------------------------|---------------------------------|
| | | h | k | l | | |
| 3.341 | 2 | 1 | 1 | 1 | 26.66 | |
| 2.046 | 100 | 2 | 2 | 0 | 44.24 | |
| 1.7445 | 1 | 3 | 1 | 1 | 52.41 | |
| 1.4465 | 13 | 4 | 0 | 0 | 64.35 | |
| 1.1811 | 23 | 4 | 2 | 2 | 81.42 | |
| 1.0228 | 7 | 4 | 4 | 0 | 97.72 | |
| .9148 | 11 | 6 | 2 | 0 | 114.70 | |
| .8351 | 4 | 4 | 4 | 4 | 134.55 | |

| Calculated Pattern (Peak heights) | | | | | | |
|-----------------------------------|-----|-----|---------------------------|---|--------|---------------------------------|
| $d(\text{\AA})$ | I | hkl | $2\theta (\text{^\circ})$ | | | $\lambda = 1.540598 \text{\AA}$ |
| | | | 1 | 2 | 3 | |
| 3.341 | 3 | 1 | 1 | 1 | 26.62 | |
| 2.046 | 100 | 2 | 2 | 0 | 44.24 | |
| 1.7445 | 1 | 3 | 1 | 1 | 52.40 | |
| 1.4465 | 12 | 4 | 0 | 0 | 64.36 | |
| 1.1811 | 20 | 4 | 2 | 2 | 81.42 | |
| 1.0228 | 6 | 4 | 4 | 0 | 97.72 | |
| .9148 | 8 | 5 | 2 | 0 | 114.70 | |
| .8351 | 2 | 4 | 4 | 4 | 134.54 | |

Cobalt germanium manganese, Co_2GeMn

Structure

Cubic, Fm3m(225), Z=4, Heusler alloy, type L2₁, from powder data (x-ray and neutron) [Webster, 1971].

Lattice constant: [ibid.]

$$a = 5.743 \text{\AA}$$

Density

(calculated) 8.594 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co^0 , Ge^0 , Mn^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 0.851 \times 10^{-3}$$

$$I/I_C \text{ (calculated)} = 12.4$$

References

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

Webster, P.J. (1971). J. Phys. Chem. Solids, 32, 1221.

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-------|--------|--|--|
| d (Å) | I | hkl | 2θ (°) | | |
| $\lambda = 1.540598 \text{\AA}$ | | | | | |
| 3.316 | 2 | 1 1 1 | 26.87 | | |
| 2.0305 | 100 | 2 2 0 | 44.50 | | |
| 1.7316 | 1 | 3 1 1 | 52.83 | | |
| 1.4357 | 13 | 4 0 0 | 64.80 | | |
| 1.1723 | 23 | 4 2 2 | 82.16 | | |
| 1.0152 | 7 | 4 4 0 | 98.71 | | |
| .9080 | 12 | 6 2 0 | 116.05 | | |
| .8289 | 4 | 4 4 4 | 136.64 | | |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|-------|--------|--|--|
| d (Å) | I | hkl | 2θ (°) | | |
| $\lambda = 1.540598 \text{\AA}$ | | | | | |
| 3.316 | 2 | 1 1 1 | 26.88 | | |
| 2.0305 | 100 | 2 2 0 | 44.60 | | |
| 1.7316 | 1 | 3 1 1 | 52.82 | | |
| 1.4357 | 12 | 4 0 0 | 64.90 | | |
| 1.1723 | 20 | 4 2 2 | 82.16 | | |
| 1.0152 | 6 | 4 4 0 | 98.70 | | |
| .9080 | 9 | 6 2 0 | 116.06 | | |
| .8289 | 2 | 4 4 4 | 136.64 | | |

Cobalt germanium titanium, Co_2GeTi

Structure

Cubic, Fm3m(225), Z=4, Heusler alloy, type L₂1,
from powder data (Gladyshevskii et al., 1963).

Lattice constant: [ibid.]

$$a = 5.823 \text{\AA}$$

Density
(calculated) 8.018 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co^0 , Ge^0 , Ti^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 0.884 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 12.0$$

References

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

Gladyshevskii, E. I., Markiv, V. Ya., Kuz'ma, Yu. B. and Cherkashin, E. E. (1963). Titan Ego Splavy, No. 10, 71.

| d (Å) | I | Calculated Pattern (Integrated) | | | $2\theta (\circ)$ | $\lambda = 1.540598 \text{\AA}$ |
|-------|-----|---------------------------------|---|---|-------------------|---------------------------------|
| | | h | k | l | | |
| 3.362 | 3 | 1 | 1 | 1 | 26.49 | |
| 2.059 | 100 | 2 | 2 | 0 | 43.94 | |
| 1.756 | 2 | 3 | 1 | 1 | 52.04 | |
| 1.456 | 13 | 4 | 0 | 0 | 63.90 | |
| 1.189 | 23 | 4 | 2 | 2 | 80.80 | |
| 1.029 | 7 | 4 | 4 | 0 | 96.90 | |
| .921 | 11 | 6 | 2 | 0 | 113.58 | |
| .840 | 4 | 4 | 4 | 4 | 132.84 | |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|-------|-------------------|--|---------------------------------|
| d (Å) | I | hkl | $2\theta (\circ)$ | | $\lambda = 1.540598 \text{\AA}$ |
| 3.362 | 4 | 1 1 1 | 26.49 | | |
| 2.059 | 100 | 2 2 0 | 43.94 | | |
| 1.756 | 2 | 3 1 1 | 52.04 | | |
| 1.456 | 12 | 4 0 0 | 63.90 | | |
| 1.189 | 20 | 4 2 2 | 80.80 | | |
| 1.029 | 6 | 4 4 0 | 96.90 | | |
| .921 | 9 | 6 2 0 | 113.58 | | |
| .840 | 2 | 4 4 4 | 132.84 | | |

Cobalt indium, CoIn₃

Structure

Tetragonal, P4/mmb(127), Z=2. The structure was determined by Stadelmaier et al. [1973].

Lattice constants: [ibid.]

$$a = 6.830\text{ \AA}$$

$$c = 3.547$$

Density

(measured) 8.09 g/cm³ [ibid.]
(calculated) 8.097 g/cm³

Thermal parameters

Isotropic [Stadelmaier et al., op. cit.].

Scattering factors

Co⁰, In⁰ [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 0.451 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 7.04$$

References

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

Stadelmaier, H. H., Schöbel, J. D., Jones, R. A., and Shumaker, C. A. (1973). Acta Crystallogr. B29, 2926.

| d (Å) | I | hkl | | | 2θ (°) | λ = 1.540598 Å |
|-------|----|-----|---|----|--------|----------------|
| 1.403 | 1 | 4 | 2 | 1 | 66.62 | |
| 1.371 | 19 | 3 | 1 | 2 | 68.38 | |
| 1.339 | 1 | 5 | 1 | 0 | 70.22 | |
| 1.268 | 2 | 5 | 2 | 0 | 74.80 | |
| 1.253 | 3 | 5 | 1 | 1 | 75.86 | |
| 1.230 | 1 | 4 | 0 | 2 | 77.54 | |
| 1.211 | 2 | 4 | 1 | 2 | 79.04 | |
| 1.207 | 4 | 4 | 4 | 0 | 79.28 | |
| 1.194 | 11 | 5 | 2 | 1 | 80.34 | |
| 1.192 | 7 | 3 | 3 | 2 | 80.56 | |
| 1.171 | 1 | 5 | 3 | 0 | 82.24 | |
| 1.157 | 4 | 4 | 2 | 2 | 83.46 | |
| 1.148 | 2 | 1 | 1 | 3 | 84.24 | |
| 1.138 | 4 | 6 | 0 | 0 | 85.18 | |
| 1.117 | 2 | 2 | 0 | 3 | 87.18 | |
| 1.112 | 1 | 5 | 3 | 1 | 87.66 | |
| 1.103 | 5 | 2 | 1 | 3 | 88.64 | |
| 1.070 | 1 | 6 | 1 | 1 | 92.04 | |
| 1.069 | 1 | 5 | 1 | 2 | 92.22 | |
| 1.067 | 1 | 5 | 4 | 0 | 92.48 | |
| 1.033 | 3 | 6 | 2 | 1 | 96.42 | |
| 1.032 | 2 | 5 | 2 | 2 | 96.60 | |
| 1.021 | 3 | 5 | 4 | 1 | 97.90 | |
| .9981 | 3 | 4 | 4 | 2 | 101.04 | |
| .9774 | 1 | 5 | 3 | 2 | 104.02 | |
| .9720 | 2 | 4 | 0 | 3 | 104.84 | |
| .9623 | 2 | 4 | 1 | 3 | 106.34 | |
| .9580 | 5 | 6 | 0 | 2 | 107.04 | |
| .9529 | 2 | 3 | 3 | 3 | 107.86 | |
| .9320 | 3 | 7 | 1 | 1+ | 111.48 | |
| .9151 | 3 | 6 | 4 | 1 | 114.66 | |
| .9141 | 1 | 5 | 4 | 2 | 114.84 | |
| .9070 | 1 | 7 | 2 | 1 | 116.28 | |
| .8968 | 4 | 7 | 3 | 0 | 118.40 | |
| .8867 | 2 | 0 | 0 | 4+ | 120.64 | |
| .8648 | 4 | 5 | 2 | 3 | 125.92 | |
| .8516 | 1 | 2 | 1 | 4 | 129.52 | |
| .8491 | 1 | 5 | 5 | 1 | 130.24 | |
| .8472 | 1 | 8 | 1 | 0 | 130.84 | |
| .8324 | 1 | 2 | 2 | 4+ | 135.48 | |
| .8240 | 3 | 8 | 1 | 1 | 138.40 | |
| .8203 | 4 | 3 | 1 | 4 | 139.78 | |
| .8049 | 2 | 6 | 6 | 0 | 146.28 | |
| .8003 | 7 | 7 | 3 | 2 | 148.52 | |
| .7974 | 2 | 6 | 2 | 3 | 150.04 | |
| .7920 | 2 | 5 | 4 | 3 | 153.12 | |

Cobalt indium, CoIn₃ - continued

| Calculated Pattern (Integrated) | | | | |
|---------------------------------|-----|-------|--------|---------------|
| d(A) | I | hkl | 2θ(°) | λ = 1.540598A |
| 4.830 | 1 | 1 1 0 | 18.36 | |
| 3.547 | 2 | 0 0 1 | 25.09 | |
| 3.054 | 37 | 2 1 0 | 29.21 | |
| 2.859 | 52 | 1 1 1 | 31.26 | |
| 2.460 | 38 | 2 0 1 | 36.40 | |
| 2.415 | 13 | 2 2 0 | 37.20 | |
| 2.315 | 100 | 2 1 1 | 38.88 | |
| 2.160 | 60 | 3 1 0 | 41.70 | |
| 1.996 | 5 | 2 2 1 | 45.40 | |
| 1.773 | 16 | 0 0 2 | 51.40 | |
| 1.707 | 2 | 4 0 0 | 53.63 | |
| 1.671 | 3 | 3 2 1 | 54.90 | |
| 1.657 | 3 | 4 1 0 | 55.42 | |
| 1.610 | 4 | 3 3 0 | 57.17 | |
| 1.539 | 12 | 4 0 1 | 60.00 | |
| 1.534 | 7 | 2 1 2 | 60.30 | |
| 1.527 | 8 | 4 2 0 | 60.59 | |
| 1.501 | 10 | 4 1 1 | 61.76 | |
| 1.466 | 14 | 3 3 1 | 63.40 | |
| 1.429 | 4 | 2 2 2 | 65.22 | |
| 1.403 | 2 | 4 2 1 | 66.62 | |
| 1.371 | 22 | 3 1 2 | 68.39 | |
| 1.339 | 1 | 5 1 0 | 70.21 | |
| 1.268 | 2 | 5 2 0 | 74.80 | |
| 1.253 | 3 | 5 1 1 | 75.86 | |
| 1.230 | 1 | 4 0 2 | 77.55 | |
| 1.211 | 2 | 4 1 2 | 79.03 | |
| 1.207 | 3 | 4 4 0 | 79.28 | |
| 1.194 | 12 | 5 2 1 | 80.33 | |
| 1.192 | 2 | 3 3 2 | 80.51 | |
| 1.171 | 2 | 5 3 0 | 82.24 | |
| 1.157 | 5 | 4 2 2 | 83.46 | |
| 1.148 | 2 | 1 1 3 | 84.25 | |
| 1.138 | 5 | 6 0 0 | 85.17 | |
| 1.117 | 2 | 2 0 3 | 87.17 | |
| 1.112 | 1 | 5 3 1 | 87.67 | |
| 1.103 | 6 | 2 1 3 | 88.63 | |
| 1.070 | 2 | 6 1 1 | 92.04 | |
| 1.069 | 1 | 5 1 2 | 92.22 | |
| 1.067 | 1 | 5 4 0 | 92.47 | |
| 1.033 | 3 | 6 2 1 | 96.42 | |
| 1.032 | 2 | 5 2 2 | 96.61 | |
| 1.021 | 4 | 5 4 1 | 97.89 | |
| .9981 | 4 | 4 4 2 | 101.03 | |
| .9774 | 2 | 5 3 2 | 104.02 | |
| .9720 | 2 | 4 0 3 | 104.83 | |
| .9623 | 2 | 4 1 3 | 106.34 | |
| .9580 | 6 | 6 0 2 | 107.04 | |
| .9529 | 3 | 3 3 3 | 107.87 | |
| .9320 | 3 | 7 1 1 | 111.40 | |

| d(A) | I | hkl | 2θ(°) | λ = 1.540598A |
|-------|----|-------|--------|---------------|
| .9151 | 4 | 6 4 1 | 114.66 | |
| .9141 | 1 | 5 4 2 | 114.85 | |
| .9070 | 1 | 7 2 1 | 116.27 | |
| .8968 | 6 | 7 3 0 | 118.39 | |
| .8867 | 2 | 0 0 4 | 120.61 | |
| .8864 | 1 | 5 1 3 | 120.69 | |
| .8648 | 7 | 5 2 3 | 125.92 | |
| .8516 | 1 | 2 1 4 | 129.52 | |
| .8491 | 2 | 6 5 1 | 130.25 | |
| .8472 | 1 | 8 1 0 | 130.81 | |
| .8324 | 1 | 2 2 4 | 135.46 | |
| .8240 | 6 | 8 1 1 | 138.41 | |
| .8240 | 1 | 7 4 1 | 138.41 | |
| .8203 | 8 | 3 1 4 | 139.78 | |
| .8142 | 1 | 6 1 3 | 142.20 | |
| .8066 | 2 | 8 2 1 | 145.51 | |
| .8049 | 3 | 6 6 0 | 146.27 | |
| .8003 | 17 | 7 3 2 | 148.52 | |
| .7974 | 4 | 6 2 3 | 150.05 | |
| .7920 | 5 | 5 4 3 | 153.12 | |
| .7870 | 1 | 4 0 4 | 156.39 | |

Cobalt lanthanum, CoLa₃

Structure

Orthorhombic, Pnma(62), Z=4, isostructural with CeFe₃, type DO₁₁. The structure was determined by Cromer and Larson [1961].

Lattice constants: [ibid.]

$$a = 7.279 \text{ \AA}$$

$$b = 10.089$$

$$c = 6.578$$

(published value b = 10.088)

Density

(measured) 6.48 g/cm³ [ibid.]

(calculated) 6.539 g/cm³

Thermal parameters

Isotropic (Cromer and Larson, op. cit.).

Scattering factors

Co⁰, La⁰ [Forsyth and Wells, 1959].

Scale factors (integrated intensities)

$$\gamma = 0.200 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 4.15$$

References

Cromer, D. T. and Larson, A. C. (1961). Acta Crystallogr. 14, 1226.

Forsyth, J.B. and Wells, M. (1959). Acta Crystallogr. 12, 412.

| d(Å) | ° | I | hkl | | | 2θ(°) |
|--------|---|----|-----|---|----|----------------|
| | | | | | | λ = 1.540598 Å |
| 2.241 | | 3 | 1 | 4 | 1+ | 40.26 |
| 2.221 | | 6 | 3 | 1 | 1 | 40.60 |
| 2.197 | | 3 | 2 | 2 | 2 | 41.06 |
| 2.073 | | 4 | ? | 4 | 0 | 43.62 |
| 2.055 | | 3 | 1 | 1 | 3 | 44.02 |
| 1.977 | | 5 | 2 | 4 | 1+ | 45.88 |
| 1.953 | | 1 | 3 | 0 | 2 | 46.48 |
| 1.938 | | 15 | 1 | 2 | 3 | 46.84 |
| 1.885 | | 3 | 3 | 3 | 1 | 48.24 |
| 1.878 | | 3 | 2 | 0 | 3 | 48.38 |
| 1.821 | | 2 | 3 | 2 | 2+ | 50.06 |
| 1.781 | | 14 | 1 | 3 | 3 | 51.26 |
| 1.765 | | 6 | 2 | 5 | 0 | 51.76 |
| 1.760 | | 5 | 2 | 2 | 3 | 51.90 |
| 1.754 | | 11 | 4 | 0 | 1 | 52.10 |
| 1.728 | | 2 | 4 | 1 | 1 | 52.94 |
| 1.712 | | 1 | 4 | 2 | 0 | 53.50 |
| 1.704 | | 7 | 2 | 5 | 1 | 53.74 |
| 1.689 | | 15 | 3 | 3 | 2 | 54.28 |
| 1.681 | | 11 | 0 | 6 | 0 | 54.52 |
| 1.674 | | 12 | 1 | 5 | 2 | 54.80 |
| 1.645 | | 2 | 0 | 0 | 4 | 55.86 |
| 1.640 | | 2 | 2 | 3 | 3 | 56.02 |
| 1.627 | | 9 | 3 | 0 | 3 | 56.52 |
| 1.614 | | 4 | 1 | 4 | 3 | 57.02 |
| 1.604 | | 8 | 1 | 0 | 4 | 57.40 |
| 1.600 | | 12 | 4 | 3 | 0 | 57.54 |
| 1.584 | | 1 | 1 | 1 | 4 | 58.18 |
| 1.555 | | 4 | 2 | 5 | 2 | 59.38 |
| 1.548 | | 2 | 3 | 2 | 3 | 59.66 |
| 1.544 | | 2 | 3 | 4 | 2 | 59.84 |
| 1.529 | | 1 | 1 | 2 | 4 | 60.52 |
| 1.518 | | 1 | 4 | 2 | 2 | 60.96 |
| 1.510 | | 1 | 3 | 5 | 1 | 61.34 |
| 1.506 | | 1 | 2 | 4 | 3 | 61.50 |
| 1.4972 | | 1 | 0 | 6 | 2 | 61.92 |
| 1.4869 | | 1 | 2 | 6 | 1 | 62.40 |
| 1.4924 | | 2 | 2 | 1 | 4 | 62.60 |
| 1.4665 | | 3 | 1 | 6 | 2 | 63.38 |
| 1.4548 | | 3 | 1 | 5 | 3 | 63.94 |
| 1.4478 | | 1 | 1 | 3 | 4 | 64.28 |
| 1.4391 | | 3 | 4 | 3 | 2+ | 64.72 |
| 1.4366 | | 3 | 2 | 2 | 4 | 64.86 |
| 1.4075 | | 1 | 5 | 1 | 1+ | 66.36 |
| 1.4032 | | 2 | 3 | 5 | 2 | 66.58 |
| 2.873 | | 51 | 1 | 1 | 2 | 31.10 |
| 2.769 | | 32 | 1 | 3 | 1 | 32.30 |
| 2.693 | | 45 | 2 | 2 | 1 | 33.24 |
| 2.577 | | 12 | 1 | 2 | 2 | 34.80 |
| 2.522 | | 5 | 0 | 4 | 0 | 35.56 |
| 2.470 | | 16 | 2 | 3 | 0 | 36.34 |
| 2.440 | | 2 | 2 | 0 | 2 | 36.80 |
| 2.372 | | 8 | 2 | 1 | 2 | 37.90 |
| 2.312 | | 1 | 2 | 3 | 1 | 38.92 |
| 2.276 | | 13 | 3 | 0 | 1 | 39.56 |

Cobalt lanthanum, CoLa₃ - continued

| d (Å) | I | hkl | | | 2θ (°) λ = 1.540598 Å |
|--------|---|-----|---|----|--------------------------|
| 1.2989 | 1 | 1 | 7 | 2 | 72.74 |
| 1.2872 | 4 | 5 | 2 | 2 | 73.52 |
| 1.2618 | 5 | 3 | 3 | 4 | 75.24 |
| 1.2557 | 1 | 1 | 5 | 4 | 75.68 |
| 1.2528 | 1 | 2 | 6 | 3 | 75.90 |
| 1.2378 | 1 | 5 | 3 | 2+ | 76.98 |
| 1.2280 | 1 | 2 | 1 | 5 | 77.70 |
| 1.2252 | 4 | 0 | 3 | 5 | 77.92 |
| 1.2177 | 1 | 3 | 7 | 1 | 78.48 |
| 1.2138 | 4 | 4 | 6 | 1+ | 78.80 |
| 1.2082 | 1 | 1 | 3 | 5 | 79.22 |
| 1.2042 | 3 | 5 | 1 | 3+ | 79.54 |
| 1.2016 | 3 | 2 | 2 | 5 | 79.76 |
| 1.1916 | 1 | 2 | 8 | 0 | 80.54 |
| 1.1848 | 1 | 6 | 1 | 1+ | 81.10 |
| 1.1795 | 2 | 6 | 2 | 0+ | 81.56 |
| 1.1773 | 2 | 5 | 4 | 2+ | 81.74 |
| 1.1725 | 3 | 2 | 8 | 1 | 82.14 |
| 1.1692 | 4 | 3 | 6 | 3 | 82.42 |
| 1.1624 | 2 | 1 | 8 | 2+ | 83.04 |
| 1.1607 | 3 | 1 | 6 | 4+ | 83.16 |
| 1.1470 | 1 | 4 | 3 | 4 | 84.38 |
| 1.1412 | 1 | 6 | 3 | 0+ | 84.92 |
| 1.1382 | 1 | 6 | 0 | 2 | 85.18 |
| 1.1285 | 1 | 3 | 5 | 4 | 86.10 |
| 1.1273 | 1 | 3 | 2 | 5 | 86.20 |
| 1.1244 | 2 | 6 | 3 | 1 | 86.48 |
| 1.1051 | 1 | 0 | 9 | 1 | 88.38 |
| 1.0963 | 1 | 0 | 0 | 6 | 89.28 |
| 1.0896 | 1 | 1 | 5 | 5+ | 89.96 |
| 1.0811 | 2 | 1 | 8 | 3 | 90.88 |
| 1.0785 | 1 | 6 | 4 | 1+ | 91.16 |
| 1.0662 | 1 | 4 | 0 | 5+ | 92.54 |
| 1.0548 | 1 | 2 | 5 | 5 | 93.82 |
| 1.0441 | 1 | 2 | 1 | 6 | 95.08 |
| 1.0395 | 3 | 5 | 5 | 3+ | 95.64 |

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-----|---|---|--------------------------|
| d (Å) | I | hkl | | | 2θ (°) λ = 1.540598 Å |
| 5.51 | 1 | 0 | 1 | 1 | 16.07 |
| 5.04 | 1 | 0 | 2 | 0 | 17.57 |
| 4.88 | 2 | 1 | 0 | 1 | 18.16 |
| 4.39 | 1 | 1 | 1 | 1 | 20.20 |
| 3.508 | 20 | 1 | 2 | 1 | 25.37 |
| 3.424 | 18 | 2 | 1 | 0 | 26.01 |
| 3.289 | 13 | 0 | 0 | 2 | 27.09 |
| 3.185 | 19 | 2 | 0 | 1 | 28.00 |
| 3.037 | 41 | 2 | 1 | 1 | 29.39 |
| 2.997 | 43 | 1 | 0 | 2 | 29.78 |
| 2.994 | 100 | 0 | 3 | 1 | 29.81 |
| 2.952 | 43 | 2 | 2 | 0 | 30.26 |
| 2.873 | 72 | 1 | 1 | 2 | 31.10 |
| 2.769 | 44 | 1 | 3 | 1 | 32.30 |
| 2.755 | 10 | 0 | 2 | 2 | 32.47 |
| 2.693 | 66 | 2 | 2 | 1 | 33.24 |
| 2.577 | 17 | 1 | 2 | 2 | 34.79 |
| 2.522 | 7 | 0 | 4 | 0 | 35.56 |
| 2.470 | 23 | 2 | 3 | 0 | 36.34 |
| 2.440 | 2 | 2 | 0 | 2 | 36.80 |
| 2.372 | 12 | 2 | 1 | 2 | 37.90 |
| 2.312 | 1 | 2 | 3 | 1 | 38.92 |
| 2.276 | 19 | 3 | 0 | 1 | 39.56 |
| 2.241 | 2 | 1 | 4 | 1 | 40.21 |
| 2.238 | 2 | 1 | 3 | 2 | 40.27 |
| 2.221 | 9 | 3 | 1 | 1 | 40.50 |
| 2.197 | 4 | 2 | 2 | 2 | 41.06 |
| 2.073 | 6 | 2 | 4 | 0 | 43.63 |
| 2.055 | 4 | 1 | 1 | 3 | 44.02 |
| 1.977 | 6 | 2 | 4 | 1 | 45.86 |
| 1.878 | 2 | 2 | 0 | 3 | 48.43 |
| 1.821 | 2 | 3 | 2 | 2 | 50.05 |
| 1.820 | 1 | 4 | 0 | 0 | 50.09 |
| 1.781 | 21 | 1 | 3 | 3 | 51.26 |
| 1.765 | 8 | 2 | 5 | 0 | 51.76 |
| 1.760 | 1 | 2 | 2 | 3 | 51.91 |
| 1.754 | 16 | 4 | 0 | 1 | 52.11 |
| 1.728 | 4 | 4 | 1 | 1 | 52.95 |
| 1.712 | 1 | 4 | 2 | 0 | 53.49 |
| 1.704 | 11 | 2 | 5 | 1 | 53.74 |
| 1.690 | 1 | 3 | 4 | 1 | 54.24 |
| 1.689 | 22 | 3 | 3 | 2 | 54.28 |
| 1.681 | 12 | 0 | 6 | 0 | 54.53 |
| 1.674 | 17 | 1 | 5 | 2 | 54.80 |
| 1.645 | 3 | 0 | 0 | 4 | 55.36 |

Cobalt lanthanum, CoLa₃ - continued

| d(Å) | I | hkl | | | 2θ(°) λ = 1.540598 Å |
|--------|----|-----|---|---|-------------------------|
| 1.640 | 1 | 2 | 3 | 3 | 56.04 |
| 1.627 | 14 | 3 | 0 | 3 | 56.52 |
| 1.614 | 6 | 1 | 4 | 3 | 57.03 |
| 1.606 | 2 | 3 | 1 | 3 | 57.32 |
| 1.604 | 9 | 1 | 0 | 4 | 57.40 |
| 1.600 | 14 | 4 | 3 | 0 | 57.54 |
| 1.584 | 1 | 1 | 1 | 4 | 58.19 |
| 1.555 | 6 | 2 | 5 | 2 | 59.39 |
| 1.548 | 2 | 3 | 2 | 3 | 59.67 |
| 1.544 | 1 | 3 | 4 | 2 | 59.86 |
| 1.529 | 2 | 1 | 2 | 4 | 60.52 |
| 1.518 | 2 | 4 | 2 | 2 | 60.97 |
| 1.510 | 2 | 3 | 5 | 1 | 61.35 |
| 1.506 | 1 | 2 | 4 | 3 | 61.51 |
| 1.4972 | 1 | 0 | 6 | 2 | 61.93 |
| 1.4869 | 2 | 2 | 6 | 1 | 62.40 |
| 1.4824 | 2 | 2 | 1 | 4 | 62.62 |
| 1.4665 | 5 | 1 | 6 | 2 | 63.37 |
| 1.4548 | 5 | 1 | 5 | 3 | 63.94 |
| 1.4478 | 2 | 1 | 3 | 4 | 64.29 |
| 1.4391 | 4 | 4 | 3 | 2 | 64.72 |
| 1.4366 | 3 | 2 | 2 | 4 | 64.85 |
| 1.4079 | 1 | 0 | 7 | 1 | 66.34 |
| 1.4075 | 1 | 5 | 1 | 1 | 66.36 |
| 1.4032 | 2 | 3 | 5 | 2 | 66.59 |
| 1.3681 | 1 | 5 | 2 | 1 | 68.53 |
| 1.3525 | 4 | 3 | 6 | 1 | 69.43 |
| 1.3493 | 1 | 4 | 2 | 3 | 69.62 |
| 1.3237 | 2 | 4 | 5 | 1 | 71.17 |
| 1.3143 | 1 | 3 | 2 | 4 | 71.76 |
| 1.2989 | 2 | 1 | 7 | 2 | 72.75 |
| 1.2884 | 1 | 2 | 4 | 4 | 73.44 |
| 1.2872 | 7 | 5 | 2 | 2 | 73.52 |
| 1.2618 | 8 | 3 | 3 | 4 | 75.25 |
| 1.2557 | 1 | 1 | 5 | 4 | 75.68 |
| 1.2528 | 1 | 2 | 6 | 3 | 75.89 |
| 1.2378 | 1 | 5 | 3 | 2 | 76.97 |
| 1.2372 | 1 | 2 | 0 | 5 | 77.01 |
| 1.2280 | 2 | 2 | 1 | 5 | 77.70 |
| 1.2252 | 5 | 0 | 3 | 5 | 77.91 |
| 1.2210 | 1 | 1 | 8 | 1 | 78.23 |
| 1.2177 | 1 | 3 | 7 | 1 | 78.48 |
| 1.2138 | 6 | 4 | 6 | 1 | 78.78 |
| 1.2132 | 1 | 6 | 0 | 0 | 78.83 |
| 1.2128 | 1 | 5 | 0 | 3 | 78.86 |
| 1.2082 | 1 | 1 | 3 | 5 | 79.22 |
| 1.2045 | 1 | 6 | 1 | 0 | 79.51 |
| 1.2042 | 4 | 5 | 1 | 3 | 79.54 |
| 1.2031 | 1 | 2 | 5 | 4 | 79.62 |
| 1.2016 | 1 | 2 | 2 | 5 | 79.74 |

| d(Å) | I | hkl | | | 2θ(°) λ = 1.540598 Å | |
|--------|---|-----|---|---|-------------------------|-------|
| 1.1916 | 2 | | 2 | 8 | 0 | 80.55 |
| 1.1848 | 1 | | 6 | 1 | 1 | 81.11 |
| 1.1795 | 1 | | 6 | 2 | 0 | 81.54 |
| 1.1775 | 1 | | 0 | 8 | 2 | 81.71 |
| 1.1773 | 2 | | 5 | 4 | 2 | 81.73 |
| 1.1757 | 1 | | 0 | 6 | 4 | 81.87 |
| 1.1725 | 5 | | 2 | 8 | 1 | 82.14 |
| 1.1692 | 6 | | 3 | 6 | 3 | 82.42 |
| 1.1624 | 2 | | 1 | 8 | 2 | 83.01 |
| 1.1620 | 1 | | 5 | 5 | 1 | 83.04 |
| 1.1607 | 3 | | 1 | 6 | 4 | 83.16 |
| 1.1470 | 2 | | 4 | 3 | 4 | 84.38 |
| 1.1412 | 1 | | 6 | 3 | 0 | 84.91 |
| 1.1382 | 1 | | 6 | 0 | 2 | 85.18 |
| 1.1285 | 1 | | 3 | 5 | 4 | 86.09 |
| 1.1273 | 1 | | 3 | 2 | 5 | 86.21 |
| 1.1244 | 3 | | 6 | 3 | 1 | 86.48 |
| 1.1051 | 2 | | 0 | 9 | 1 | 88.38 |
| 1.0963 | 1 | | 0 | 0 | 6 | 89.27 |
| 1.0925 | 1 | | 1 | 9 | 1 | 89.67 |
| 1.0900 | 1 | | 5 | 0 | 4 | 89.93 |
| 1.0896 | 1 | | 1 | 5 | 5 | 89.97 |
| 1.0811 | 3 | | 1 | 8 | 3 | 90.88 |
| 1.0662 | 2 | | 4 | 0 | 5 | 92.52 |
| 1.0655 | 1 | | 5 | 2 | 4 | 92.60 |
| 1.0548 | 2 | | 2 | 5 | 5 | 93.82 |
| 1.0441 | 1 | | 2 | 1 | 6 | 95.08 |
| 1.0397 | 1 | | 6 | 5 | 0 | 95.61 |
| 1.0395 | 4 | | 5 | 5 | 3 | 95.64 |

Cobalt lutetium, Co_2Lu

Structure

Cubic, $\text{Fd}3m(227)$, $Z=8$, isostructural with Cu_2Mg , type C15, from powder data [Lemaire, 1971].

Lattice constant: [ibid.]

$$a = 7.102 \text{ \AA}$$

Density

(calculated) 10.860 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Lu^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 1.08 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 14.5$$

References

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

Lemaire, F. G. R. (1971). Solid State Commun. 9, 341.

| $d(\text{\AA})$ | I | Calculated Pattern (Integrated) | | | $2\theta (\text{^\circ})$ | $\lambda = 1.540598 \text{\AA}$ |
|-----------------|-----|---------------------------------|---|---|---------------------------|---------------------------------|
| | | h | k | l | | |
| 4.100 | 20 | 1 | 1 | 1 | 21.66 | |
| 2.511 | 73 | 2 | 2 | 0 | 35.73 | |
| 2.141 | 100 | 3 | 1 | 1 | 42.17 | |
| 2.050 | 12 | 2 | 2 | 2 | 44.14 | |
| 1.775 | 1 | 4 | 0 | 0 | 51.42 | |
| 1.629 | 5 | 3 | 3 | 1 | 56.43 | |
| 1.450 | 23 | 4 | 2 | 2 | 64.19 | |
| 1.367 | 20 | 5 | 1 | 1 | 68.61 | |
| 1.367 | 7 | 3 | 3 | 3 | 68.61 | |
| 1.255 | 18 | 4 | 4 | 0 | 75.69 | |
| 1.200 | 4 | 5 | 3 | 1 | 79.83 | |
| 1.123 | 9 | 6 | 2 | 0 | 86.62 | |
| 1.083 | 8 | 5 | 3 | 3 | 90.67 | |
| 1.071 | 3 | 6 | 2 | 2 | 92.02 | |
| .9945 | 1 | 5 | 5 | 1 | 101.53 | |
| .9945 | 1 | 7 | 1 | 1 | 101.53 | |
| .9490 | 12 | 6 | 4 | 2 | 108.52 | |
| .9246 | 6 | 5 | 5 | 3 | 112.84 | |
| .9246 | 12 | 7 | 3 | 1 | 112.84 | |
| .8877 | 4 | 8 | 0 | 0 | 120.39 | |
| .8676 | 1 | 7 | 3 | 3 | 125.20 | |
| .8370 | 7 | 8 | 2 | 2 | 133.95 | |
| .8370 | 3 | 6 | 6 | 0 | 133.95 | |
| .8201 | 15 | 7 | 5 | 1 | 139.87 | |
| .8201 | 2 | 5 | 5 | 5 | 139.87 | |
| .8147 | 2 | 6 | 6 | 2 | 142.02 | |
| .7940 | 2 | 8 | 4 | 0 | 151.92 | |

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|---|---|----|---------------------------------|
| $d(\text{\AA})$ | I | h | k | l | $2\theta (\text{^\circ})$ |
| | | | | | $\lambda = 1.540598 \text{\AA}$ |
| 4.100 | 24 | 1 | 1 | 1 | 21.66 |
| 2.511 | 77 | 2 | 2 | 0 | 35.74 |
| 2.141 | 100 | 3 | 1 | 1 | 42.18 |
| 2.050 | 13 | 2 | 2 | 2 | 44.14 |
| 1.775 | 1 | 4 | 0 | 0 | 51.42 |
| 1.629 | 5 | 3 | 3 | 1 | 56.44 |
| 1.450 | 21 | 4 | 2 | 2 | 64.20 |
| 1.367 | 23 | 5 | 1 | 1+ | 68.60 |
| 1.255 | 16 | 4 | 4 | 0 | 75.70 |
| 1.200 | 3 | 5 | 3 | 1 | 79.84 |
| 1.123 | 8 | 6 | 2 | 0 | 86.62 |
| 1.083 | 7 | 5 | 3 | 3 | 90.69 |
| 1.071 | 2 | 6 | 2 | 2 | 92.02 |
| .9945 | 2 | 7 | 1 | 1+ | 101.54 |
| .9490 | 10 | 6 | 4 | 2 | 108.52 |
| .9246 | 14 | 7 | 3 | 1+ | 112.84 |
| .8877 | 3 | 8 | 0 | 0 | 120.39 |
| .8676 | 1 | 7 | 3 | 3 | 125.20 |
| .8370 | 6 | 8 | 2 | 2+ | 133.94 |
| .8201 | 8 | 7 | 5 | 1+ | 139.89 |
| .8147 | 1 | 6 | 6 | 2 | 142.02 |
| .7940 | 1 | 8 | 4 | 0 | 151.92 |

Cobalt neodymium, Co_2Nd

Structure

Cubic, Fd3m (227), $Z = 8$, isostructural with Cu_2Mg , type C15, from powder data [Harris et al., 1965].

Lattice constant: [ibid.]

$$a = 7.2986 \text{\AA}$$

(published value 7.2834 kX)

Density

(calculated) 8.955 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Nd^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 0.571 \times 10^{-3}$$

I/I_c (calculated) = 12.2

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 (Integrated) | | | | | |
|---------------------------------|-----|-------|---|---------------------------|---------------------------------|
| $d(\text{\AA})$ | I | hkl | | $2\theta (\text{^\circ})$ | $\lambda = 1.540598 \text{\AA}$ |
| 4.214 | 11 | 1 | 1 | 1 | 21.07 |
| 2.5804 | 63 | 2 | 2 | 0 | 34.74 |
| 2.2006 | 100 | 3 | 1 | 1 | 40.98 |
| 2.1069 | 17 | 2 | 2 | 2 | 42.89 |
| 1.6744 | 2 | 3 | 3 | 1 | 54.78 |
| 1.4898 | 19 | 4 | 2 | 2 | 62.27 |
| 1.4046 | 19 | 5 | 1 | 1 | 66.52 |
| 1.4046 | 6 | 3 | 3 | 3 | 66.52 |
| 1.2902 | 18 | 4 | 4 | 0 | 73.31 |
| 1.2337 | 2 | 5 | 3 | 1 | 77.27 |
| 1.1540 | 7 | 6 | 2 | 0 | 83.75 |
| 1.1130 | 8 | 5 | 3 | 3 | 87.59 |
| 1.1003 | 4 | 6 | 2 | 2 | 88.87 |
| .9753 | 10 | 6 | 4 | 2 | 104.33 |
| .9502 | 11 | 7 | 3 | 1 | 108.32 |
| .9502 | 5 | 5 | 5 | 3 | 108.32 |
| .9123 | 3 | 8 | 0 | 0 | 115.20 |
| .8601 | 2 | 6 | 6 | 0 | 127.16 |
| .8601 | 5 | 8 | 2 | 2 | 127.16 |
| .8428 | 12 | 7 | 5 | 1 | 132.13 |
| .8428 | 2 | 5 | 5 | 5 | 132.13 |
| .8372 | 3 | 6 | 6 | 2 | 133.88 |
| .8011 | 2 | 7 | 5 | 3 | 148.11 |
| .8011 | 1 | 9 | 1 | 1 | 148.11 |
| .7780 | 13 | 6 | 6 | 4 | 163.83 |

Calculated Pattern (Peak heights)

| $d(\text{\AA})$ | I | hkl | | $2\theta (\text{^\circ})$ | $\lambda = 1.540598 \text{\AA}$ |
|-----------------|-----|-------|---|---------------------------|---------------------------------|
| 4.214 | 12 | 1 | 1 | 1 | 21.08 |
| 2.5804 | 65 | 2 | 2 | 0 | 34.74 |
| 2.2006 | 100 | 3 | 1 | 1 | 40.98 |
| 2.1069 | 16 | 2 | 2 | 2 | 42.91 |
| 1.6744 | 2 | 3 | 3 | 1 | 54.78 |
| 1.4898 | 17 | 4 | 2 | 2 | 62.26 |
| 1.4046 | 23 | 5 | 1 | 1+ | 66.52 |
| 1.2902 | 16 | 4 | 4 | 0 | 73.32 |
| 1.2337 | 2 | 5 | 3 | 1 | 77.28 |
| 1.1540 | 6 | 6 | 2 | 0 | 83.74 |
| 1.1130 | 6 | 5 | 3 | 3 | 87.58 |
| 1.1003 | 3 | 6 | 2 | 2 | 88.86 |
| 1.0220 | 1 | 7 | 1 | 1+ | 97.82 |
| .9753 | 7 | 6 | 4 | 2 | 104.34 |
| .9502 | 12 | 7 | 3 | 1+ | 108.32 |
| .9123 | 2 | 8 | 0 | 0 | 115.20 |
| .8601 | 4 | 8 | 2 | 2+ | 127.16 |
| .8428 | 7 | 7 | 5 | 1+ | 132.14 |
| .8372 | 1 | 5 | 6 | 2 | 133.88 |
| .8011 | 1 | 7 | 5 | 3+ | 148.10 |
| .7780 | 3 | 6 | 6 | 4 | 163.82 |

Cobalt nickel tin, $\text{Co}_{.75}\text{Ni}_{.75}\text{Sn}_{.75}$

Structure

Hexagonal, $P\bar{6}_3/mmc$ (194), $Z=2$, from powder data.
The atoms were assigned these positions: 1.5 Co plus 0.5 Ni in 2a; 1.5 Sn plus 0.5 Ni in 2c; and only 0.5 Ni in 2d. [Castelliz, 1953].

Lattice constants: [ibid.]

$$a = 4.095 \text{\AA}$$

$$c = 5.209$$

Density

(calculated) 7.781 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Ni^0 , Sn^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 0.453 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 6.08$$

References

Castelliz, L. (1953). Monatsh. Chem. 84, 49.

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

| Calculated Pattern (Peak heights) | | | | | |
|-----------------------------------|-----|-----|---|--------|----------------|
| d (Å) | I | hkl | | 2θ (°) | λ = 1.540598 Å |
| 2.931 | 100 | 1 | 0 | 1 | 30.48 |
| 2.604 | 7 | 0 | 0 | 2 | 34.42 |
| 2.099 | 87 | 1 | 0 | 2 | 43.06 |
| 2.048 | 88 | 1 | 1 | 0 | 44.20 |
| 1.679 | 14 | 2 | 0 | 1 | 54.64 |
| 1.610 | 7 | 1 | 1 | 2 | 57.18 |
| 1.559 | 11 | 1 | 0 | 3 | 59.20 |
| 1.466 | 20 | 2 | 0 | 2 | 63.40 |
| 1.302 | 5 | 0 | 0 | 4 | 72.54 |
| 1.298 | 11 | 2 | 1 | 1 | 72.80 |
| 1.241 | 4 | 2 | 0 | 3 | 76.76 |
| 1.192 | 16 | 2 | 1 | 2 | 80.52 |
| 1.182 | 9 | 3 | 0 | 0 | 81.32 |
| 1.099 | 14 | 1 | 1 | 4 | 89.02 |
| 1.076 | 2 | 3 | 0 | 2 | 91.39 |
| 1.061 | 5 | 2 | 1 | 3 | 93.10 |
| 1.024 | 5 | 2 | 2 | 0 | 97.60 |
| 1.000 | 2 | 1 | 0 | 5 | 100.82 |
| .967 | 3 | 3 | 1 | 1 | 105.68 |
| .953 | 1 | 2 | 2 | 2 | 107.90 |
| .920 | 7 | 3 | 1 | 2 | 113.68 |
| .898 | 2 | 2 | 0 | 5 | 118.08 |
| .875 | 7 | 3 | 0 | 4 | 123.30 |
| .874 | 2 | 4 | 0 | 1 | 123.60 |
| .856 | 3 | 3 | 1 | 3 | 128.34 |
| .843 | 3 | 1 | 0 | 6 | 131.98 |
| .839 | 3 | 4 | 0 | 2 | 133.22 |
| .823 | 3 | 2 | 1 | 5 | 138.94 |
| .805 | 7 | 2 | 2 | 4 | 146.32 |
| .804 | 3 | 3 | 2 | 1 | 146.78 |
| .799 | 1 | 1 | 1 | 6 | 149.04 |
| .790 | 1 | 4 | 0 | 3 | 154.60 |

Cobalt nickel tin, Co_{.75}Ni_{.75}Sn_{.75} - continued

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-----|---|---|--------------------|
| d(A) ^o | I | hkl | | | 2θ(°) ^o |
| λ = 1.540598A | | | | | |
| 2.931 | 100 | 1 | 0 | 1 | 30.47 |
| 2.604 | 7 | 0 | 0 | 2 | 34.41 |
| 2.099 | 93 | 1 | 0 | 2 | 43.06 |
| 2.048 | 95 | 1 | 1 | 0 | 44.20 |
| 1.679 | 17 | 2 | 0 | 1 | 54.63 |
| 1.610 | 9 | 1 | 1 | 2 | 57.18 |
| 1.559 | 13 | 1 | 0 | 3 | 59.20 |
| 1.466 | 24 | 2 | 0 | 2 | 63.41 |
| 1.302 | 6 | 0 | 0 | 4 | 72.53 |
| 1.298 | 12 | 2 | 1 | 1 | 72.80 |
| 1.241 | 5 | 2 | 0 | 3 | 76.77 |
| 1.192 | 21 | 2 | 1 | 2 | 80.53 |
| 1.182 | 11 | 3 | 0 | 0 | 81.32 |
| 1.099 | 17 | 1 | 1 | 4 | 89.02 |
| 1.076 | 2 | 3 | 0 | 2 | 91.38 |
| 1.061 | 6 | 2 | 1 | 3 | 93.10 |
| 1.024 | 7 | 2 | 2 | 0 | 97.60 |
| 1.000 | 3 | 1 | 0 | 5 | 100.82 |
| .967 | 5 | 3 | 1 | 1 | 105.60 |
| .953 | 2 | 2 | 2 | 2 | 107.80 |
| .920 | 10 | 3 | 1 | 2 | 113.60 |
| .898 | 2 | 2 | 0 | 5 | 118.09 |
| .875 | 12 | 3 | 0 | 4 | 123.30 |
| .874 | 2 | 4 | 0 | 1 | 123.61 |
| .856 | 5 | 3 | 1 | 3 | 128.34 |
| .843 | 6 | 1 | 0 | 6 | 131.98 |
| .839 | 6 | 4 | 0 | 2 | 133.21 |
| .823 | 6 | 2 | 1 | 5 | 138.93 |
| .805 | 17 | 2 | 2 | 4 | 146.31 |
| .804 | 7 | 3 | 2 | 1 | 146.78 |
| .799 | 2 | 1 | 1 | 6 | 149.05 |
| .790 | 4 | 4 | 0 | 3 | 154.60 |

Cobalt samarium, Co₅Sm

Structure

Hexagonal, P6/mmm(191), Z=1, isostructural with CaCu₅, type D_{2d}, from powder data [Khan and Feldmann, 1973].

Lattice constants: [ibid.]

$$a = 4.997 \text{ \AA}$$

$$c = 3.978$$

Density

(measured) 8.58 g/cm³ [ibid.]

(calculated) 8.590 g/cm³

Thermal parameters

Isotropic: overall B = 2.0

Scattering factors

Co⁰, Sm⁰ [Cromer and Mann, 1968].

Scale factors (integrated intensities)

$$\gamma = 0.320 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 6.73$$

References

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

Khan, Y. and Feldmann, D. (1973). J. Less-Common Metals, 31, 111.

| d(Å) | I | Calculated Pattern (Peak heights) | | | 2θ (°) λ = 1.540598 Å |
|-------|-----|-----------------------------------|---|---|--------------------------|
| | | h | k | l | |
| 4.328 | 2 | 1 | 0 | 0 | 20.52 |
| 3.978 | 8 | 0 | 0 | 1 | 22.34 |
| 2.929 | 60 | 1 | 0 | 1 | 30.50 |
| 2.498 | 36 | 1 | 1 | 0 | 35.92 |
| 2.164 | 36 | 2 | 0 | 0 | 41.72 |
| 2.116 | 100 | 1 | 1 | 1 | 42.70 |
| 1.999 | 24 | 0 | 0 | 2 | 45.58 |
| 1.901 | 5 | 2 | 0 | 1 | 47.82 |
| 1.556 | 11 | 1 | 1 | 2 | 59.34 |
| 1.513 | 10 | 2 | 1 | 1 | 61.22 |
| 1.464 | 14 | 2 | 0 | 2 | 63.48 |
| 1.443 | 4 | 3 | 0 | 0 | 64.56 |
| 1.356 | 14 | 3 | 0 | 1 | 69.22 |
| 1.268 | 2 | 1 | 0 | 3 | 74.84 |
| 1.249 | 9 | 2 | 2 | 0 | 76.14 |
| 1.171 | 7 | 1 | 1 | 3 | 82.24 |
| 1.168 | 6 | 3 | 0 | 2 | 82.52 |
| 1.149 | 3 | 3 | 1 | 1 | 84.20 |
| 1.082 | 2 | 4 | 0 | 0 | 90.80 |
| 1.058 | 8 | 2 | 2 | 2 | 93.46 |
| 1.030 | 2 | 2 | 1 | 3 | 96.80 |
| .994 | 1 | 0 | 0 | 4 | 101.54 |
| .976 | 3 | 3 | 0 | 3 | 104.20 |
| .963 | 1 | 3 | 2 | 1 | 106.20 |
| .950 | 2 | 4 | 0 | 2 | 108.30 |
| .944 | 1 | 4 | 1 | 0 | 109.32 |
| .924 | 1 | 1 | 1 | 4 | 112.96 |
| .919 | 5 | 4 | 1 | 1 | 113.94 |
| .904 | 2 | 2 | 0 | 4 | 116.96 |
| .890 | 1 | 3 | 1 | 3 | 119.92 |
| .853 | 2 | 4 | 1 | 2 | 129.10 |
| .819 | 1 | 3 | 0 | 4 | 140.38 |
| .818 | 1 | 4 | 2 | 0 | 140.74 |
| .815 | 2 | 3 | 3 | 1 | 141.80 |
| .795 | 1 | 3 | 2 | 3 | 151.52 |

Cobalt samarium, Co₅Sm - continued

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-----|---|---|----------------|
| d (Å) | I | hkl | | | 2θ (°) |
| | | | | | λ = 1.540598 Å |
| 4.328 | 2 | 1 | 0 | 0 | 20.51 |
| 3.978 | 7 | 0 | 0 | 1 | 22.33 |
| 2.929 | 56 | 1 | 0 | 1 | 30.50 |
| 2.498 | 35 | 1 | 1 | 0 | 35.91 |
| 2.164 | 36 | 2 | 0 | 0 | 41.71 |
| 2.116 | 100 | 1 | 1 | 1 | 42.70 |
| 1.989 | 25 | 0 | 0 | 2 | 45.57 |
| 1.901 | 5 | 2 | 0 | 1 | 47.81 |
| 1.556 | 12 | 1 | 1 | 2 | 59.34 |
| 1.513 | 11 | 2 | 1 | 1 | 61.22 |
| 1.464 | 15 | 2 | 0 | 2 | 63.48 |
| 1.443 | 4 | 3 | 0 | 0 | 64.55 |
| 1.356 | 16 | 3 | 0 | 1 | 69.23 |
| 1.268 | 3 | 1 | 0 | 3 | 74.83 |
| 1.249 | 10 | 2 | 2 | 0 | 76.14 |
| 1.192 | 1 | 2 | 2 | 1 | 80.53 |
| 1.171 | 8 | 1 | 1 | 3 | 82.24 |
| 1.168 | 3 | 3 | 0 | 2 | 82.55 |
| 1.149 | 3 | 3 | 1 | 1 | 84.10 |
| 1.082 | 2 | 4 | 0 | 0 | 90.80 |
| 1.058 | 10 | 2 | 2 | 2 | 93.46 |
| 1.030 | 2 | 2 | 1 | 3 | 96.81 |
| .994 | 1 | 0 | 0 | 4 | 101.53 |
| .976 | 4 | 3 | 0 | 3 | 104.20 |
| .963 | 2 | 3 | 2 | 1 | 106.20 |
| .950 | 3 | 4 | 0 | 2 | 108.29 |
| .944 | 2 | 4 | 1 | 0 | 109.31 |
| .924 | 2 | 1 | 1 | 4 | 112.95 |
| .919 | 7 | 4 | 1 | 1 | 113.94 |
| .904 | 2 | 2 | 0 | 4 | 116.96 |
| .890 | 2 | 3 | 1 | 3 | 119.92 |
| .853 | 3 | 4 | 1 | 2 | 129.10 |
| .846 | 1 | 5 | 0 | 1 | 131.24 |
| .833 | 1 | 3 | 3 | 0 | 135.31 |
| .819 | 2 | 3 | 0 | 4 | 140.37 |
| .818 | 3 | 4 | 2 | 0 | 140.74 |
| .815 | 4 | 3 | 3 | 1 | 141.81 |
| .795 | 2 | 3 | 2 | 3 | 151.51 |
| .782 | 2 | 1 | 0 | 5 | 159.75 |

Cobalt tin, Co_3Sn_2

Structure

Hexagonal, $P6_3/mmc$ (194), $Z = 1$, isostructural with Ni_3Sn_2 , type $B8_2$, from powder data [Rajeswari and Manohar, 1970].

Lattice constants: [ibid.]

$$a = 4.109 \text{ \AA}$$

$$c = 5.180$$

Density

(calculated) 9.080 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Polymorphism

This phase was annealed above 550°C , and quenched to room temperature. A low-temperature, more ordered modification also exists [Rajeswari and Manohar, op. cit.].

Scattering factors

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

Scale factors (integrated intensities)

$$\gamma = 0.383 \times 10^{-3}$$

$$I/I_c \text{ (calculated)} = 6.62$$

References

- Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
 Rajeswari, H. and Manohar, H. (1970). Indian J. Pure Appl. Phys. 8, 363.

| $d(\text{\AA})$ | I | Calculated Pattern (Peak heights) | | | | $2\theta (\text{^\circ})$ |
|-----------------|-----|-----------------------------------|---|---|---------------------------------|---------------------------|
| | | h | k | l | $\lambda = 1.540598 \text{\AA}$ | |
| 3.558 | 2 | 1 | 0 | 0 | | 25.02 |
| 2.933 | 82 | 1 | 0 | 1 | | 30.46 |
| 2.590 | 12 | 0 | 0 | 2 | | 34.60 |
| 2.094 | 88 | 1 | 0 | 2 | | 43.16 |
| 2.055 | 100 | 1 | 1 | 0 | | 44.04 |
| 1.683 | 12 | 2 | 0 | 1 | | 54.48 |
| 1.610 | 14 | 1 | 1 | 2 | | 57.19 |
| 1.553 | 9 | 1 | 0 | 3 | | 59.46 |
| 1.467 | 21 | 2 | 0 | 2 | | 63.38 |
| 1.302 | 9 | 2 | 1 | 1 | | 72.56 |
| 1.295 | 6 | 0 | 0 | 4 | | 73.00 |
| 1.230 | 4 | 2 | 0 | 3 | | 76.80 |
| 1.194 | 18 | 2 | 1 | 2 | | 80.38 |
| 1.186 | 11 | 3 | 0 | 0 | | 81.00 |
| 1.096 | 15 | 1 | 1 | 4 | | 89.36 |
| 1.078 | 3 | 3 | 0 | 2 | | 91.16 |
| 1.061 | 4 | 2 | 1 | 3 | | 93.10 |
| 1.027 | 6 | 2 | 2 | 0 | | 97.16 |
| .995 | 2 | 1 | 0 | 5 | | 101.50 |
| .970 | 3 | 3 | 1 | 1 | | 105.22 |
| .955 | 2 | 2 | 2 | 2 | | 107.54 |
| .922 | 7 | 3 | 1 | 2 | | 113.28 |
| .895 | 1 | 2 | 0 | 5 | | 118.72 |
| .877 | 2 | 4 | 0 | 1 | | 122.94 |
| .875 | 9 | 3 | 0 | 4 | | 123.44 |
| .857 | 3 | 3 | 1 | 3 | | 128.06 |
| .841 | 3 | 4 | 0 | 2 | | 132.56 |
| .839 | 4 | 1 | 0 | 6 | | 133.28 |
| .821 | 2 | 2 | 1 | 5 | | 139.62 |
| .806 | 3 | 3 | 2 | 1 | | 145.58 |
| .805 | 8 | 2 | 2 | 4 | | 146.34 |
| .796 | 2 | 1 | 1 | 6 | | 150.84 |
| .791 | 1 | 4 | 0 | 3 | | 153.84 |

Cobalt tin, Co_3Sn_2 - continued

| Calculated Pattern (Integrated) | | | | | |
|---------------------------------|-----|-----|---|--------------------------------|--------|
| d (Å) | I | hkl | | 2θ (°) | % |
| | | | | $\lambda = 1.540598\text{\AA}$ | |
| 3.558 | 2 | 1 | 0 | 0 | 25.00 |
| 2.933 | 76 | 1 | 0 | 1 | 30.45 |
| 2.590 | 12 | 0 | 0 | 2 | 34.60 |
| 2.094 | 89 | 1 | 0 | 2 | 43.17 |
| 2.055 | 100 | 1 | 1 | 0 | 44.04 |
| 1.683 | 13 | 2 | 0 | 1 | 54.49 |
| 1.610 | 15 | 1 | 1 | 2 | 57.18 |
| 1.553 | 10 | 1 | 0 | 3 | 59.45 |
| 1.467 | 24 | 2 | 0 | 2 | 63.37 |
| 1.302 | 10 | 2 | 1 | 1 | 72.56 |
| 1.295 | 6 | 0 | 0 | 4 | 73.09 |
| 1.239 | 4 | 2 | 0 | 3 | 76.87 |
| 1.194 | 20 | 2 | 1 | 2 | 80.38 |
| 1.186 | 12 | 3 | 0 | 0 | 80.99 |
| 1.096 | 18 | 1 | 1 | 4 | 89.36 |
| 1.078 | 3 | 3 | 0 | 2 | 91.17 |
| 1.061 | 5 | 2 | 1 | 3 | 93.10 |
| 1.027 | 7 | 2 | 2 | 0 | 97.16 |
| .995 | 2 | 1 | 0 | 5 | 101.50 |
| .970 | 4 | 3 | 1 | 1 | 105.22 |
| .955 | 3 | 2 | 2 | 2 | 107.55 |
| .922 | 10 | 3 | 1 | 2 | 113.29 |
| .895 | 2 | 2 | 0 | 5 | 118.72 |
| .877 | 2 | 4 | 0 | 1 | 122.94 |
| .875 | 13 | 3 | 0 | 4 | 123.44 |
| .857 | 4 | 3 | 1 | 3 | 128.05 |
| .841 | 5 | 4 | 0 | 2 | 132.56 |
| .839 | 6 | 1 | 0 | 6 | 133.31 |
| .821 | 5 | 2 | 1 | 5 | 139.61 |
| .806 | 6 | 3 | 2 | 1 | 145.57 |
| .805 | 18 | 2 | 2 | 4 | 146.33 |
| .796 | 4 | 1 | 1 | 6 | 150.85 |
| .791 | 4 | 4 | 0 | 3 | 153.82 |

CUMULATIVE INORGANIC INDEX

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|---|-----------------|------|---|-----------------|------|
| Aluminum, Al | 1 | 11 | Ammonium copper bromide hydrate, $(\text{NH}_4)_2\text{CuBr}_4 \cdot 2\text{H}_2\text{O}$ | 10m | 6 |
| Aluminum antimony, AlSb | 4 | 72 | Ammonium copper chloride, NH_4CuCl_3 | 7m | 7 |
| Aluminum bismuth oxide, $\text{Al}_4\text{Bi}_2\text{O}_9$.. | 11m | 5 | Ammonium copper chloride hydrate, $(\text{NH}_4)_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$ | 12m | 6 |
| Aluminum chloride, AlCl_3 | 9m | 61 | Ammonium copper fluoride, NH_4CuF_3 .. | 11m | 8 |
| Aluminum chloride hydrate (chloraluminite), $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ | 7 | 3 | Ammonium gallium sulfate hydrate, $\text{NH}_4\text{Ga}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 9 |
| Aluminum fluoride hydroxide silicate, topaz, $\text{Al}_2(\text{F},\text{OH})_2\text{SiO}_4$ | 1m | 4 | Ammonium germanium fluoride, $(\text{NH}_4)_2\text{GeF}_6$ | 6 | 8 |
| Aluminum nitride, AlN | 12m | 5 | Ammonium hydrogen carbonate (teschemacherite), $(\text{NH}_4)\text{HCO}_3$ | 9 | 5 |
| Aluminum nitrate hydrate, $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ | 11m | 6 | Ammonium hydrogen phosphate, $\text{NH}_4\text{H}_2\text{PO}_4$ | 4 | 64 |
| Aluminum oxide (corundum), $\alpha\text{-Al}_2\text{O}_3$ | 9 | 3 | Ammonium iodate, NH_4IO_3 | 10m | 7 |
| Aluminum oxide hydrate (boehmite), $\alpha\text{-Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$ | 3 | 38 | Ammonium iodide, NH_4I | 4 | 56 |
| Aluminum oxide hydrate, diaspore, $\beta\text{-Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$ | 3 | 41 | Ammonium iridium chloride, $(\text{NH}_4)_2\text{IrCl}_6$ | 8 | 6 |
| Aluminum phosphate, $\text{Al}(\text{PO}_3)_3$ | 2m | 3 | Ammonium iron fluoride, $(\text{NH}_4)_3\text{FeF}_6$ | 9m | 9 |
| Aluminum phosphate (berlinite), AlPO_4 (trigonal) | 10 | 3 | Ammonium iron sulfate, $\text{NH}_4\text{Fe}(\text{SO}_4)_2$.. | 10m | 8 |
| Aluminum phosphate, AlPO_4 (orthorhombic) | 10 | 4 | Ammonium iron sulfate hydrate, $\text{NH}_4\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 10 |
| Aluminum silicate (mullite), $\text{Al}_6\text{Si}_2\text{O}_{13}$ | 3m | 3 | Ammonium lead chloride, $(\text{NH}_4)_2\text{PbCl}_6$.. | 11m | 10 |
| Aluminum tungsten oxide, $\text{Al}_2(\text{WO}_4)_3$ | 11m | 7 | Ammonium magnesium aluminum fluoride, $\text{NH}_4\text{MgAlF}_6$ | 10m | 9 |
| Ammonium aluminum fluoride, $(\text{NH}_4)_3\text{AlF}_6$ | 9m | 5 | Ammonium magnesium chromium oxide hydrate, $(\text{NH}_4)_2\text{Mg}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 10 |
| Ammonium aluminum selenate hydrate, $\text{NH}_4\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 9m | 6 | Ammonium manganese chloride hydrate, $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$ | 11m | 11 |
| Ammonium aluminum sulfate, $\text{NH}_4\text{Al}(\text{SO}_4)_2$ | 10m | 5 | Ammonium manganese(II) fluoride, NH_4MnF_3 | 5m | 8 |
| Ammonium aluminum sulfate hydrate (tschermigite), $\text{NH}_4\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 3 | Ammonium manganese sulfate, $(\text{NH}_4)_2\text{Mn}_2(\text{SO}_4)_3$ | 7m | 8 |
| Ammonium azide, NH_4N_3 | 9 | 4 | Ammonium manganese sulfate hydrate, $(\text{NH}_4)_2\text{Mn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 12 |
| Ammonium beryllium fluoride, $(\text{NH}_4)_2\text{BeF}_4$ | 3m | 5 | Ammonium mercury chloride, NH_4HgCl_3 | 8m | 14 |
| Ammonium boron fluoride, NH_4BF_4 ... | 3m | 6 | Ammonium molybdenum oxide phosphate hydrate, $(\text{NH}_4)_3(\text{MoO}_3)_2 \text{PO}_4 \cdot 4\text{H}_2\text{O}$... | 8 | 10 |
| Ammonium bromide, NH_4Br | 2 | 49 | Ammonium nickel(II) chloride, NH_4NiCl_3 | 6m | 6 |
| Ammonium cadmium chloride, NH_4CdCl_3 | 5m | 6 | Ammonium nickel chromium oxide hydrate, $(\text{NH}_4)_2\text{Ni}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 16 |
| Ammonium cadmium sulfate, $(\text{NH}_4)_2\text{Cd}_2(\text{SO}_4)_3$ | 7m | 5 | Ammonium nitrate (nitrammite), NH_4NO_3 | 7 | 4 |
| Ammonium cadmium sulfate hydrate, $(\text{NH}_4)_2\text{Cd}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 5 | Ammonium osmium bromide, $(\text{NH}_4)_2\text{OsBr}_6$.. | 3 | 71 |
| Ammonium calcium sulfate, $(\text{NH}_4)_2\text{Ca}_2(\text{SO}_4)_3$ | 8m | 7 | Ammonium osmium chloride, $(\text{NH}_4)_2\text{OsCl}_6$ | 1m | 6 |
| Ammonium chlorate, NH_4ClO_4 (orthorhombic) | 7 | 6 | Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_4$ | 6 | 6 |
| Ammonium chloride (sal-ammoniac), NH_4Cl | 1 | 59 | Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_6$ | 8 | 7 |
| Ammonium chromium sulfate hydrate, $\text{NH}_4\text{Cr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 7 | Ammonium platinum bromide, $(\text{NH}_4)_2\text{PtBr}_6$ | 9 | 6 |
| Ammonium cobalt (II) chloride, NH_4CoCl_3 | 6m | 5 | Ammonium platinum chloride, $(\text{NH}_4)_2\text{PtCl}_6$ | 5 | 3 |
| Ammonium cobalt fluoride, NH_4CoF_3 | 8m | 9 | Ammonium rhenium oxide, NH_4ReO_4 | 9 | 7 |
| | | | Ammonium selenium bromide, $(\text{NH}_4)_2\text{SeBr}_6$ | 8 | 4 |
| | | | Ammonium silicon fluoride (cryptothalite), $(\text{NH}_4)_2\text{SiF}_6$ | 5 | 5 |
| | | | Ammonium sulfate (mascagnite), $(\text{NH}_4)_2\text{SO}_4$ | 9 | 8 |
| | | | Ammonium tellurium bromide, $(\text{NH}_4)_2\text{TeBr}_6$ | 8 | 5 |

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

m - Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE INORGANIC INDEX - Continued

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|--|-----------------|------|--|-----------------|------|
| Ammonium tellurium chloride, | | | Barium lead nitrate, | | |
| $(\text{NH}_4)_2\text{TeCl}_6$ | 8 | 8 | $\text{Ba}_{.33}\text{Pb}_{.67}(\text{NO}_3)_2$ | 12m | 40 |
| Ammonium tin chloride, $(\text{NH}_4)_2\text{SnCl}_6$ | 5 | 4 | Barium lead nitrate, | | |
| Ammonium vanadium oxide, NH_4VO_3 | 8 | 9 | $\text{Ba}_{.67}\text{Pb}_{.33}(\text{NO}_3)_2$ | 12m | 40 |
| Ammonium zinc fluoride, NH_4ZnF_3 | 8m | 18 | Barium molybdenum oxide, BaMoO_4 | 7 | 7 |
| Ammonium zirconium fluoride, | | | Barium molybdenum oxide, Ba_2MoO_5 | 12m | 10 |
| $(\text{NH}_4)_3\text{ZrF}_7$ | 6 | 14 | Barium nitrate (nitrobarite), | | |
| Antimony, Sb | 3 | 14 | $\text{Ba}(\text{NO}_3)_2$ | 11m | 14 |
| Antimony(III) fluoride, SbF_3 | 2m | 4 | Barium oxide, BaO | 9m | 63 |
| Antimony(III) iodide, SbI_3 | 6 | 16 | Barium oxide, BaO_2 | 6 | 18 |
| Antimony(III) oxide (senarmontite), | | | Barium phosphate, $\text{Ba}_3(\text{PO}_4)_2$ | 12m | 12 |
| Sb_2O_3 (cubic) | 3 | 31 | Barium selenide, BaSe | 5m | 61 |
| Antimony(III) oxide, valentinite, | | | Barium silicate, $\beta\text{-BaSiO}_3$ | 13m | 8 |
| Sb_2O_3 (orthorhombic) | 10 | 6 | Barium silicate (sanbornite), | | |
| Antimony(IV) oxide (cervantite), | | | $\beta\text{-BaSi}_2\text{O}_5$ | 13m | 10 |
| Sb_2O_4 | 10 | 8 | Barium silicate, Ba_2SiO_4 | 13m | 12 |
| Antimony(V) oxide, Sb_2O_5 | 10 | 10 | Barium silicate, $\text{Ba}_2\text{Si}_3\text{O}_8$ | 13m | 13 |
| Antimony selenide, Sb_2Se_3 | 3m | 7 | Barium silicate, Ba_3SiO_5 | 13m | 15 |
| Antimony(III) sulfide (stibnite), | | | Barium silicate, $\text{Ba}_3\text{Si}_5\text{O}_{13}$ | 13m | 17 |
| Sb_2S_3 | 5 | 6 | Barium silicon fluoride, BaSiF_6 | 4m | 7 |
| Antimony telluride, Sb_2Te_3 | 3m | 8 | Barium strontium nitrate, | | |
| Arsenic, As | 3 | 6 | $\text{Ba}_{.25}\text{Sr}_{.75}(\text{NO}_3)_2$ | 12m | 42 |
| Arsenic(III) iodide, AsI_3 | 13m | 7 | Barium strontium nitrate, | | |
| Arsenic oxide (arsenolite), | | | $\text{Ba}_{.50}\text{Sr}_{.50}(\text{NO}_3)_2$ | 12m | 42 |
| As_2O_3 (cubic) | 1 | 51 | Barium strontium nitrate, | | |
| Arsenic oxide, claudetite, As_2O_3 | | | $\text{Ba}_{.75}\text{Sr}_{.25}(\text{NO}_3)_2$ | 12m | 42 |
| (monoclinic) | 3m | 9 | Barium sulfate (baryte), BaSO_4 | 10m | 12 |
| Barium, Ba | | | Barium sulfide, BaS | 7 | 8 |
| Barium aluminum oxide, BaAl_2O_4 | 5m | 11 | Barium tin oxide, BaSnO_3 | 3m | 11 |
| Barium aluminum oxide, $\text{Ba}_3\text{Al}_2\text{O}_6$ | 12m | 7 | Barium titanium oxide, BaTiO_3 | 3 | 45 |
| Barium arsenate, $\text{Ba}_3(\text{AsO}_4)_2$ | 2m | 6 | Barium titanium silicate (fresnoite), | | |
| Barium borate, BaB_4O_7 | 4m | 6 | $\text{Ba}_2\text{TiSi}_2\text{O}_8$ | 9m | 14 |
| Barium borate, high form, BaB_2O_4 .. | 4m | 4 | Barium tungsten oxide, BaWO_4 | 7 | 9 |
| Barium borate, $\text{BaB}_8\text{O}_{13}$ | 7m | 10 | Barium tungsten oxide, Ba_2WO_5 | 12m | 14 |
| Barium bromate hydrate, | | | Barium zirconium oxide, BaZrO_3 | 5 | 8 |
| $\text{Ba}(\text{BrO}_3)_2 \cdot \text{H}_2\text{O}$ | 8m | 19 | Beryllium, alpha, Be | | |
| Barium bromide, BaBr_2 | 10m | 63 | Beryllium aluminum oxide | | |
| Barium bromide fluoride, BaBrF | 10m | 10 | (chrysoberyl), BeAl_2O_4 | 9 | 10 |
| Barium bromide hydrate, $\text{BaBr}_2 \cdot \text{H}_2\text{O}$ | 3m | 10 | Beryllium aluminum silicate, beryl, | | |
| Barium calcium nitrate, | | | $\text{Be}_3\text{Al}_2(\text{SiO}_3)_6$ | 9 | 13 |
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| Norbergite, $Mg_2SiO_4 \cdot MgF_2$ | 10 | 39 | Strontianite, $SrCO_3$ | 3 | 56 |
| Oldhamite, CaS | 7 | 15 | Struvite, $MgNH_4PO_4 \cdot 6H_2O$ | 3m | 41 |
| Otavite, $CdCO_3$ | 7 | 11 | Sulfur, S (orthorhombic) | 9 | 54 |
| Oxammite, $(NH_4)_2C_2O_4 \cdot H_2O$ | 7 | 5 | Sylvite, KCl | 1 | 65 |
| Palladium, Pd | 1 | 21 | *Tellurite, TeO_2 | 9 | 57 |
| *Paratellurite, TeO_2 | 10 | 55 | Tellurium, Te | 1 | 26 |
| Paratellurite, TeO_2 | 7 | 56 | Tellurobismuthite, Bi_2Te_3 | 3m | 16 |
| Periclase, MgO | 1 | 37 | Tenorite, CuO | 1 | 49 |
| Perovskite, $CaTiO_3$ | 9m | 17 | Teschemacherite, NH_4HCO_3 | 9 | 5 |
| *Phenakite, Be_2SiO_4 | 8 | 11 | Thenardite, Na_2SO_4 | 2 | 59 |
| Picromerite, $K_2Mg(SO_4)_2 \cdot 6H_2O$ | 8m | 54 | Thermonatrite, $Na_2CO_3 \cdot H_2O$ | 8 | 54 |
| *Pirssonite, $Na_2Ca(CO_3)_2 \cdot 2H_2O$ | 9m | 106 | *Thomsenolite, $NaCaAlF_6 \cdot H_2O$ | 8m | 132 |
| Platinum, Pt | 1 | 31 | Thorianite, ThO_2 | 1 | 57 |
| Portlandite, $Ca(OH)_2$ | 1 | 58 | Thortveitite, $Sc_2Si_2O_7$ | 7m | 58 |
| Powellite, $CaMoO_4$ | 6 | 22 | Tiemannite, $HgSe$ | 7 | 35 |
| Pyrargyrite, Ag_3SbS_3 | 5m | 51 | Tin, α -Sn (cubic) | 2 | 12 |
| Pyrite, FeS_2 | 5 | 29 | Tin, β -Sn (tetragonal) | 1 | 24 |
| *Pyroaurite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$, phase II | 10m | 104 | *Topaz, $Al_2SiO_4(F,OH)_2$ | 1m | 4 |
| Pyrolusite, β - MnO_2 | 10m | 39 | Trevorite, $NiFe_2O_4$ | 10 | 44 |
| Pyrope, $Mg_3Al_2(SiO_4)_3$ | 4m | 24 | Tschermigite, $NH_4Al(SO_4)_2 \cdot 12H_2O$ | 6 | 3 |
| *Quartz, SiO_2 (α or low) | 3 | 24 | Tungstenite, WS_2 | 8 | 65 |
| Rammelsbergite, $NiAs_2$ | 10 | 42 | Uraninite, UO_2 | 2 | 33 |
| Retgersite, $NiSO_4 \cdot 6H_2O$ | 7 | 36 | Uvarovite, $Ca_3Cr_2(SiO_4)_3$ | 10 | 17 |
| Rhodochrosite, $MnCO_3$ | 7 | 32 | *Valentinite, Sb_2O_3 | 10 | 6 |
| Romarchite, SnO | 4 | 28 | Valentinite, Sb_2O_3 | 10 | 6 |
| Rutile, TiO_2 | 7m | 83 | Villiaumite, NaF | 1 | 63 |
| Safflorite, $CoFeAs_4$ | 10 | 28 | Willemite, Zn_2SiO_4 | 7 | 62 |
| Sal-ammoniac, NH_4Cl | 1 | 59 | Witherite, $BaCO_3$ | 2 | 54 |
| Sanbornite, β - $BaSi_2O_5$ | 13m | 10 | Wulfenite, $PbMoO_4$ | 7 | 23 |
| Sanmartinite, $ZnWO_4$ | 2m | 40 | Wurtzite, ZnS | 2 | 14 |
| Scachlite, $MnCl_2$ | 8m | 43 | *Xanthoconite, Ag_3AsS_3 | 8m | 126 |
| *Scheelite, $CaWO_4$ | 6 | 23 | Xenotime, YPO_4 | 8 | 67 |
| Selenium, Se | 5 | 54 | Zinc, Zn | 1 | 16 |
| Selenolite, SeO_2 | 7m | 60 | Zincite, ZnO | 2 | 25 |
| Sellaite, MgF_2 | 4 | 33 | Zinkosite, $ZnSO_4$ | 7 | 64 |
| Senarmontite, Sb_2O_3 | 3 | 31 | *Zircon, $ZrSiO_4$ | 4 | 68 |
| Shcherbinaite, V_2O_5 | 8 | 66 | Zircosulfate, $Zr(SO_4)_2 \cdot 4H_2O$ | 7 | 66 |
| Silver, Ag | 1 | 23 | | | |

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| U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET | | | | 1. PUBLICATION OR REPORT NO. NBS-MN25, Section 13 | 2. Gov't Accession No. | 3. Recipient's Accession No. |
| 4. TITLE AND SUBTITLE Standard X-ray Diffraction Powder Patterns Section 13 - Data for 58 Substances | | | | 5. Publication Date June 1976 | 6. Performing Organization Code | |
| 7. AUTHOR(S) Marlene C. Morris, Howard F. McMurdie, Eloise H. Evans Boris Paretzkin, Johan H. de Groot, Camden R. Hubbard and Simon | | | | 8. Performing Organ. Report No. J. Carmel | 10. Project/Task/Work Unit No. 3130163 | |
| 9. PERFORMING ORGANIZATION NAME AND ADDRESS NATIONAL BUREAU OF STANDARDS DEPARTMENT OF COMMERCE WASHINGTON, D.C. 20234 | | | | 11. Contract/Grant No. | 13. Type of Report & Period Covered Interim | |
| 12. Sponsoring Organization Name and Complete Address (Street, City, State, ZIP) Same as Item 9. | | | | 14. Sponsoring Agency Code | | |
| 15. SUPPLEMENTARY NOTES Library of Congress Catalog Card Number: 53-61386 | | | | | | |
| 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 58 substances. Thirty-one of these patterns represent experimental data and 27 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns. | | | | | | |
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